LOW-RANK DRIVING IN QUANTUM SYSTEMS

DISSERTATION

Presented to the Faculty of

The University of Texas at Dallas

in Partial Fulfillment

of the Requirements

for the Degree of

DOCTOR OF PHILOSOPHY IN PHYSICS

May, 1989

Ronald Steven Burkey, B.S., M.S.

May, 1989. First printing.

March, 2003. Translated into LaTeX. No intentional content changes were made, except for the correction of a small number of obvious misprints, though many formatting changes were made. Endnotes have been converted to footnotes, and their numbering has changed slightly because of added editorial notes. Figures are now embedded in the text rather than collected at the ends of chapters. Many figures have been redrawn.

[1] (The copyright notice above is believed to be correct; information to the contrary should be sent to info@sandroid.org.)

LOW-RANK DRIVING IN QUANTUM SYSTEMS

APPROVED BY SUPERVISORY COMMITTEE:

Cyrus D. Cantrell, III, Chairman

Carl B. Collins

Wolfgang Rindler

Roy C. Chaney

John Hoffman

DEDICATION

This work is dedicated to the memory of my mother and to my father, who probably thought that it would never be finished.

Contents

ACKNOWLEDGEMENTS **ix**

ABSTRACT **xi**

I. INTRODUCTION **1**
1.1. Introduction 1
1.2. The Concept of Low Driver-Rank 4
1.3. The Continuum-Continuum System and Coherent Population-Trapping . . 6
1.4. Future Directions 8
1.5. How to Find it 8

II. Survey of the Literature **11**
2.1. Introduction 11
2.2. Studies of the Undamped 2-Level System 11
2.3. Studies of the $(1, \mathrm{N})$ System 15
2.4. Studies of the Ladder System 20
2.5. Studies of Continua 21
2.6. Coherent Population Trapping 23

III. BASIC DEFINITIONS AND NOTATION **27**
3.1. Schrödinger's Equation 27
3.2 Low Driver-Rank 29
3.3. $(1, \mathrm{N})$ and $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ Systems 30
3.4. "Continuous Matrix" Notation 34
3.5. Some Commonly Employed $(1, \mathsf{BAND})$ Systems 37
3.6. Some Simple Factorizations 40
3.7. The Rotating-Wave Approximation (RWA) 43

IV. SYSTEMS WITH CONSTANT DRIVING **45**
4.1. Introduction 45
4.2. Eigenvalues and Eigenvectors 47
4.3. Laplace Transforms 50
4.4. Laplace Transform of the Ground State 51
4.5. A Simple Algebraic Example 52
4.6. Population Trapping in the Continuum 55
4.6.1. Odd-Rank Population Trapping 56

4.6.2. Continuum-Continuum Population Trapping 58
4.7. Laplace Inversion for Rational Bands 70
4.8. Conclusion 73
4.9. Appendix A: Reality of Characteristic Polynomial 73

V. THE INTEGRAL EQUATIONS **75**
5.1. Integral Form of Schrödinger's Equation 75
5.2. Several Driving Fields 78
5.3. Generalizing the Weisskopf-Wigner and Golden-Rule Approximations 79
5.4. Reconstructing the Differential Equations, I: Effective Hamiltonian 83
5.5. Reconstructing the Differential Equations, II: Rational Functions 85
5.6. Reconstructing the Differential Equations, III: Gaussian Integration 87
5.7. A Quirky Case: The Discrete-Lorentzian Band 92
5.8. Numerical Examples 94
5.9. $(\mathrm{CONTINUUM}, \mathrm{CONTINUUM})$ Population Trapping 108

VI. BAND-DIAGONALIZATION OF THE HAMILTONIAN **113**
6.1. Definition of Band-Diagonalization 113
6.2. Constructing the Band-diagonal Hamiltonian 115
6.3. The $(1, \mathrm{CONTINUUM})$ System 119
6.4. Continuum-Continuum Population Trapping and Time-Varying Interactions 125

VII. APPROXIMATE BAND-DIAGONALIZATION **129**
7.1. Introduction 129
7.2. Polynomial Approximations and the $(1, \mathrm{CONTINUUM})$ System 130
7.3. Generalization: $(\mathrm{N}, \mathrm{CONTINUUM})$ Transitions 138
7.4. Generalization: $(\mathrm{CONTINUUM}, \mathrm{CONTINUUM})$ Transitions 139
7.5. Generalization: $(\underline{\mathrm{CONTINUUM}})$ Transitions 141
7.6. Unlimited Continua 142
7.7. Multi-Dimensional Continua 143
7.8. Summary of the Theoretical Discussion 145

VIII. DYNAMICS OF THE CHEBYCHEV LADDER **149**
8.1. Introduction 149
8.2. The Dispersion Relation for the Chebychev Ladder 150
8.3. Non-Hermitian δ-Truncation of the Chebychev Ladder 153
8.4. Rational λ-Termination 163
8.5. The Rest of the Story 167
8.6. $(\mathrm{CONTINUUM}, \mathrm{CONTINUUM})$ Population Trapping in Strictly Limited Continua 173
8.7. Appendix A: Tables 176

IX. SUMMARY **179**
9.1. Why a Summary? 179
9.2. Low Driver-Rank 179
9.3. Exact Methods 179
9.3.1. Constant $H'(t)$—Eigenvalues and Eigenvectors 179

9.3.2. Constant $H'(t)$—Laplace Transform 179
9.3.3. Time-Varying $H'(t)$—Integral Equations 180
9.3.4. Time-Varying $H'(t)$—Band-Diagonalization 180
9.4. Consequences of the Exact Methods 180
9.4.1. Rational Continua 180
9.4.2. The $(1, \mathsf{DISCRETE\,LORENTZIAN})$ System 180
9.4.3. Weisskopf-Wigner Approximations (Langevin Equations) 180
9.4.4. Gaussian Discretization of the Continuum 181
9.4.5. Tridiagonalization of the $(1, \mathsf{CONTINUUM})$ System 181
9.4.6. The $(1, \mathsf{CHEBYCHEV\,2ND\,KIND})$ System 181
9.5. Approximate Low Driver-Rank 181
9.5.1. Approximate Tridiagonalization of the Hamiltonian 181
9.5.2. Wave Packets in the Chebychev Ladder 181
9.5.3. Non-Hermitian Ladder Termination 181
9.6. $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ Population Trapping 182
9.6.1. The Broad-Continuum Case 182
9.6.2. The Narrow-Continuum Case 182
9.6.3. The Limited-Continuum Case 182
9.6.5. The $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ System 182
9.7. Population Non-Decay 182
9.8. What Remains to be Done 182

VITA **185**

ACKNOWLEDGEMENTS

Of course, the primary credit for guiding me in my research belongs to my advisor, C. D. Cantrell, III. In addition to introducing me to the existing work and instructing me in the necessary modes of thought for producing research in my field, his comments and suggestions (not to mention collaboration) have proved invaluable. Many of the ideas presented herein are presaged in papers of his (see Chap. II) published prior to my involvement. My only regret is that, in developing fully some of the ideas presented here, I was forced to neglect pursuing a (still promising) reduced-density-matrix technique which he devised (in 1981) and which provided much of the original stimulation for my thought.

There are other people and organizations without whom this dissertation would not exist in its present form.

First, I would like to thank B. DePaola, G. Peterson, and D. R. Adams for various conversations which stimulated to some extent the development of some of the ideas to be presented. Also, I would like to acknowledge that the germ of much of this work (though not its actual substance) is present in certain publications of R. Haydock, A. Makarov, V. Platonenko, and V. Tyakht.

I am very grateful to the Robert A. Welch Foundation for supporting me financially as a Predoctoral Fellow during much of this work. A. Glosson and particularly W. M. Lee were helpful in dealing with certain practical details involved in producing this dissertation. Also, Heads Up Technologies, Inc., generously provided some of the computer facilities used.

Finally, I would like to thank M. Renfrow for acting as my “second mom” and helping me past some of the difficulties that often attend being a graduate student.

ABSTRACT

A new property of quantum systems called *low-rank driving* is introduced. Numerous simplifications in the solution of the time-dependent Schrödinger equation are pointed out for systems having this property. These simplifications are in the areas of finding eigenvalues, taking the Laplace transform, converting Schrödinger's equation to an integral form, discretizing the continuum, generalizing the Weisskopf-Wigner approximation, band-diagonalizing the Hamiltonian, finding new exact solutions to Schrödinger's equation, and so forth. The principal physical application considered is the phenomenon of coherent population-trapping in continuum-continuum interactions.

CHAPTER I
INTRODUCTION

1.1. Introduction

Many authors have published studies concerning the properties of quantum systems having continuous bands of energy levels.[1] The simplest example of such a system is an extension of the familiar $(1, \mathrm{N})$ system having a discrete ground state coupled to a "band" of N energy levels.[2] This system is depicted in Fig. (1.1a). In Fig. (1.1b), the band of energy levels becomes continuous in the limit $\mathrm{N} \to \infty$, as the spacing between the energy levels becomes infinitesimal. The structure of this model, known as the $(1, \mathsf{CONTINUUM})$ system, is simple: we have merely a discrete ground state coupled to a continuum. Of course, one can imagine many more complicated examples of continuous quantum systems, such as: a continuum coupled to several discrete (perhaps embedded) energy levels; a continuum coupled to a second continuum;[3] or perhaps a continuum allowing internal transitions among two of its own energy levels.

Continuous quantum systems are of interest for several reasons. While continuous systems have found few uses to date in realistic problems, they are often employed in theoretical investigations of very idealized model systems. This happens because continuous bands of energy levels can model several interesting effects. Primarily, multi-atomic molecules can have dense bands of closely spaced *discrete* energy levels due to rotational splitting,[4] and continuous bands can sometimes be used to model the general (but not detailed) effects of such bands. For example, in Intramolecular Relaxation (IMR) one studies the redistribution (relaxation) of molecular population among the densely packed energy levels in such bands.[5] As another example, in the study of the so-called quasi-continuum, the dense energy levels of the quasi-continuum are often modeled instead by continuous

[1] Many examples are provided below. Of course, the best-known example to most physicists is the ionization continuum.

[2] G. Stey and R. Gibberd, *Physica* (Utr.) **60**, 1 (1972).

[3] For example, Z. Deng and J. H. Eberly, *Phys. Rev. A* **34**, 2492 (1986).

[4] G. Herzberg, *Molecular Spectra and Molecular Structure, I. Spectra of Diatomic Molecules*, second edition (Van Nostrand, Princeton, New Jersey, 1977), ch. 2.

[5] E. Borsella, R. Fantoni, A. Giardini-Guidoni, D. R. Adams, and C. D. Cantrell, *Chem. Phys. Lett.* **101**, 86 (1983); U. del Bello, E. Borsella, R. Fantoni, A. Giardini-Guidoni, and C. D. Cantrell, *Chem. Phys. Lett.* **114**, 467 (1985); C. D. Cantrell in *Proceedings of the International Conference on Lasers '81*, ed. by C. B. Collins (STS Press, 1982), p. 936.

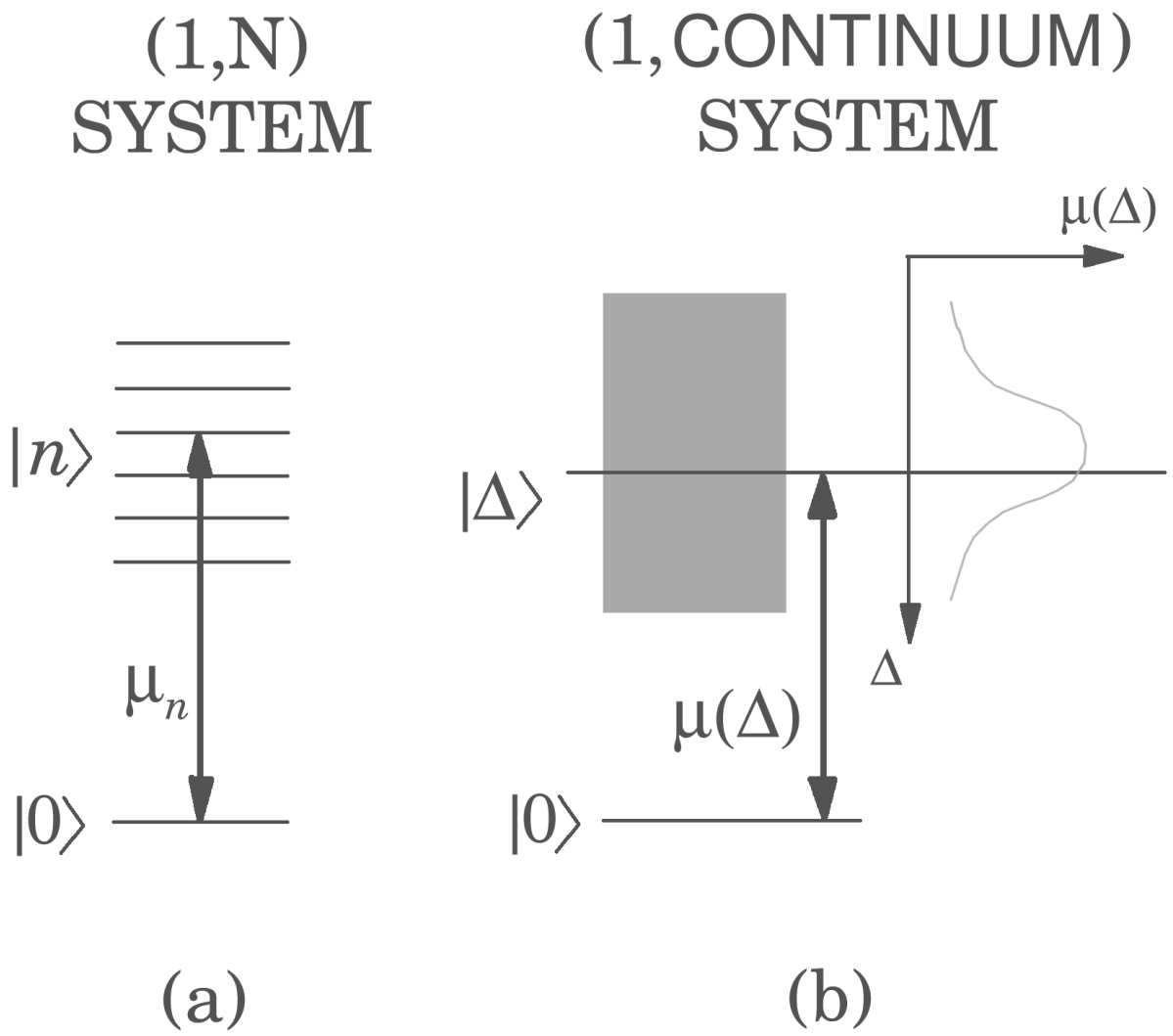

FIGURE 1.1.

Side-by-side comparison of: a) the discrete $(1, \mathrm{N})$ system, and b) the (1,CONTINUUM) system. The discrete energy levels are indexed by an integer n, while the continuous energy levels are indexed by a continuous quantity Δ (representing, perhaps, the detuning of the level from a laser field). In this example, we have a dipole interaction. The dipole operator's matrix elements are μ_n in the discrete case and $\mu(\Delta)$ in the continuous case. These matrix elements result in transitions between the "ground state" $|0\rangle$ and the energy levels of the band but, conventionally, transitions between two levels of the band are forbidden.

bands.[6] Of course, true continua such as ionization continua, as opposed to continuous approximations, also appear in quantum systems.

There are no generally adequate methods, either analytical or computational, for dealing with systems of this kind. Several approaches have been tried, each having a certain regime in which they are of use:

- The use of eigenvalue/eigenvector methods in continuous systems was pioneered by U. Fano.[7]
- Laplace-transform methods have been employed by many authors.[8]
- The methods of perturbation theory lead alternately to the approximations of Wigner and Weisskopf[9] or to the Golden-Rule approximation.[10]
- Integral-equation techniques lead to "memory-function"[11] and other novel approaches.
- Coarse-graining techniques[12] attempt to lump together the many levels of the continuum into a kind of unified (and simplified) whole.
- In some cases, the continuum can be treated as a kind of thermal reservoir.[13]
- Various miscellaneous methods apply to restricted cases.[14]

While all of these approaches have a certain validity, they also have certain flaws, when considered as a group:

First, they are generally very specific to the $(1, \mathsf{CONTINUUM})$ system. Indeed, these methods are often specific to a particular class of $(1, \mathsf{CONTINUUM})$ system, and not to $(1, \mathsf{CONTINUUM})$ systems in general. Of course, there are exceptions. One common variation[15] is the study of autoionizing model systems having *two* discrete levels interacting with an ionization continuum.

Second, of those methods which could be applied to a wider group of problems (such as continuum-continuum interactions), there is usually no *systematic* way of doing so. Thus, we might be able to solve a quantum system containing two interacting continua

[6] N. Bloembergen, C. D. Cantrell, and D. M. Larsen in *Tunable Lasers and Applications*, ed. by A. Mooradian, T. Jaeger, and P. Stokseth (Springer, Heidelberg, 1976); N. Isenor, V. Merchant, R. Hallsworth, and M. Richardson, *Can. J. Phys.* **51**, 1281 (1973); C. D. Cantrell, V. Letokhov, and A. Makarov, in *Coherent Nonlinear Optics, Recent Advances*, ed. by M. Feld and V. Letokhov (Springer, Heidelberg, 1980), ch. 5.

[7] U. Fano, *Phys. Rev.* **124**, 1866 (1961).

[8] For example, A. Makarov, V. Platonenko, and V. Tyakht, *Sov. Phys. JETP* **48**, 1044 (1978).

[9] Generally attributed to V. Weisskopf and E. Wigner, *Z. Phys.* **63**, 54 (1930), but actually due to L. Landau, *Z. Phys.* **45**, 430 (1927), according to P. Milonni, J. Ackerhalt, and H. Galbraith, *Phys. Rev. A* **28**, 32 (1983).

[10] E. Merzbacher, *Quantum Mechanics*, second edition (Wiley, New York, 1970), ch. 18.

[11] R. Lefebvre and J. Savolainen, *J. Chem. Phys.* **60**, 2509 (1974).

[12] For example, J. J. Yeh, C. M. Bowden, and J. H. Eberly, *J. Chem. Phys.* **76**, 5936 (1982).

[13] W. Louisell, *Quantum Statistical Properties of Radiation* (John Wiley, New York, 1973), ch. 6.

[14] For example, R. S. Burkey and C. D. Cantrell, *Opt. Commun.* **43**, 64 (1982).

[15] For example, A. Lami and N. Rahman, *Phys. Rev. A* **33**, 782 (1986).

using the Laplace transform but, if so, it would generally require a significant amount of algebra even to determine the feasibility of such an approach.

Third, among the popular approximations, there is no good way of determining the level of accuracy obtained from the calculation. Indeed, in most cases these exists *no* accurate calculation method. That is, approximations are adopted not because they are the best available approximation, but simply because there is no other alternative.

Fourth, there is generally no way to incorporate time-varying stimuli into the system. If, for example, we consider a molecule stimulated by a quasi-monochromatic laser field (with a time-varying envelope), or perhaps several differing quasi-monochromatic laser fields, we are left with very few alternative approaches in analyzing the system.

In short, while various attempts have been made to deal with specific cases of immediate interest, there is no truly adequate way to analyze the continuous quantum system.

1.2. The Concept of Low Driver-Rank

A set of widely useful tools for dealing with continuous systems can be constructed by means of a new concept—that of *low driver-rank*. This concept is vaguely analogous (but unrelated in any practical sense) to the idea behind perturbation theory.

In perturbation theory, one divides the Hamiltonian of the system under investigation into two parts. The undriven (or unperturbed) part of the Hamiltonian is supposed to be *large* relative to the driving part of the Hamiltonian (the perturbation). This allows one to conclude that the system behaves mainly according to the undriven part of the Hamiltonian, but with small corrections.[16] Whether one part of the Hamiltonian operator is larger than the other part is determined simply by an arithmetic comparison of the corresponding matrix elements of the operators.

In a low-driver-rank quantum system, on the other hand, the sizes of the matrix elements are of no concern whatever. Indeed, the driving operator can be much larger than the undriven Hamiltonian operator. What is of interest instead is the *ranks* of these operators, considered as matrices. [17] If the matrix rank of the driving part of the Hamiltonian is very small compared to the matrix rank of the undriven Hamiltonian, then the system is said to be of *low driver-rank*. In practical terms, the rank of the undriven Hamiltonian is generally infinite in a continuous system, and we require the matrix rank of the driving term to be a small (integer) number. This concept, while admittedly novel, has the advantage that it describes most continuous model quantum systems analytically solved in the literature.[18] For example, in the $(1, \mathsf{CONTINUUM})$ system of Fig. (1.1b), the undriven Hamiltonian is of infinite matrix rank, while the driving term is merely of rank 2.

In fact, the concept of low driver-rank is very powerful and will be developed in detail below. A set of tools based on the low-driver-rank concept, intended to aid in solving continuous quantum systems, will be developed there. A summary description of these

[16] L. Landau and E. Lifshitz, *Quantum Mechanics*, third edition (Pergamon, Elmsford, New York, 1977), ch. 6.

[17] F. E. Hohn, *Elementary Matrix Algebra*, third edition (Macmillan, New York, 1973), ch. 6.

[18] Actually, I do not know of a continuous system whose time variation has been presented in closed form in the literature, except for Refs. 3 and 19, and various minor modifications of the $(1, \mathsf{CONTINUUM})$ system.

tools appears below.

In order to understand the power of these methods, we require a numerical measure of the complexity of the quantum systems involved. This measure involves the matrix ranks of the undriven Hamiltonian and the driving part of the Hamiltonian. For the sake of discussion, we'll give these values special names:

$$\begin{aligned} \mathrm{N} &= \text{matrix rank of undriven Hamiltonian} \\ &= \text{number of energy levels in the system.} \\ \mathrm{M} &= \text{matrix rank of driving part of Hamiltonian.} \end{aligned}$$

For continuous systems, which are our main concern, $\mathrm{N} \to \infty$. However, to simplify our discussion let's just suppose for the moment that N is some "very large" integer such that $\mathrm{N} \gg \mathrm{M}$.

The low-driver-rank idea is used principally to systematize or to extend methods previously applicable only to $(1, \mathsf{CONTINUUM})$ systems. However, it also allows several wholly new methods of attack. Here is a brief summary of the new mathematical methods to be developed, as contrasted to the similar methods used in systems with smaller numbers of energy levels:

- Eigenvalues and eigenvectors: In a low-driver-rank system, eigenvalues and eigenvectors can be computed by diagonalizing an $\mathrm{M} \times \mathrm{M}$ matrix rather than an $\mathrm{N} \times \mathrm{N}$ (Hamiltonian) matrix. (Chapter IV.)

- Laplace transform: The Laplace transform of a low-driver-rank system is computed by inverting an $\mathrm{M} \times \mathrm{M}$ matrix rather than an $\mathrm{N} \times \mathrm{N}$ matrix. If knowledge of the ground state alone is desired, only an $(\mathrm{M}-2) \times (\mathrm{M}-2)$ matrix must be inverted. (Chapter IV.)

- Integral equations: An integral representation of Schrödinger's equation consisting of $\leq \mathrm{M}$ coupled integral equations exists for low-driver-rank systems. This holds even for time-varying stimuli such as electric fields applied externally to the system. (Chapter V.) For non-low-driver-rank systems, N coupled equations would be required. These integral equations have many uses, of which the following will be elaborated:

  - The extension of the Weisskopf-Wigner and Golden Rule approximations to systems other than the $(1, \mathsf{CONTINUUM})$,
  - The discretization of continuous bands of energy levels, and
  - Detailed modeling of continua by reservoirs.

- Band diagonalization. The Hamiltonian of a low-driver-rank system may be band-diagonalized (even in the case of time-varying stimuli) by means of a similarity transformation that is independent of time. The number of distinct co-diagonals of the Hamiltonian is $\leq \mathrm{M}$. For example, the Hamiltonian of the $(1, \mathsf{CONTINUUM})$ system can be tridiagonalized. (Chapters VI and VII.)

- New analytic solutions of various systems. (Especially Chapter VIII.)

- Plus, as the saying goes, much much more.

1.3. The Continuum-Continuum System and Coherent Population-Trapping

The physical system to which these mathematical methods will be principally applied is the (CONTINUUM, CONTINUUM) which, obviously, consists of two coupled continuous bands. [See Fig. (1.2).] Although this is not a "realistic" system in the sense of modeling closely any molecular or atomic system it is nevertheless of some interest,[19] particularly in relation to the problem of coherent population trapping.[20] Problems similar to this have been investigated previously, but since adequate tools for solving continuous systems were lacking, only very simple cases could be considered.

In coherent population trapping, the population of a quantum system remains closely confined to a small set of states not obviously decoupled from the remainder of the system. This can happen in the (CONTINUUM, CONTINUUM) system in rather odd ways. The parameters at our disposal in investigating the (CONTINUUM, CONTINUUM) system, not including the detailed interaction, are these:

1. The widths of the continuous bands in frequency space.
2. The strength of the interaction coupling the bands.
3. The initial population distribution .
4. Whether the coupling interaction is time-varying and (if so) how fast?

This suggests investigation of the following issues:

- Effects when one continuous band is much narrower in frequency space than the other.
- Effects when the interaction strength is much larger than the bandwidths.
- Effects of a very large interaction strength, with still larger bandwidths.
- Effects of time-varying interactions or differing initial population distributions on anything interesting discovered above.

While a number of interesting points will arise from these investigations, two results will command the most attention:

The first result concerns bands which are very broad in frequency space. We find that increasing the interaction strength (between the two continua) to very high levels

[19] R. S. Burkey, A. Glosson, and C. D. Cantrell, to be published in *Phys. Rev. A*, March 1, 1989.

[20] R. M. Whitley and C. R. Stroud, Jr., *Phys. Rev. A* **14**, 1498 (1976); J. D. Stettler, C. M. Bowden, N. M. Witriol, and J. H. Eberly, *Phys. Lett.* **73A**, 171 (1979); F. T. Hioe and J. H. Eberly, *Phys. Rev. Lett.* **47**, 838 (1981); P. M. Radmore and P. L. Knight, *J. Phys. B* **15**, 561 (1982); S. Swain, *J. Phys. B* **15**, 3405 (1982); Z. Deng, *Opt. Commun.* **48**, 284 (1983); D. A. Cardimona, M. G. Raymer, and C. R. Stroud, Jr., *J. Phys. B* **15**, 55 (1982); P. Lambropoulos and P. Zoller, *Phys. Rev. A* **24**, 379 (1981); P. E. Coleman and P. L. Knight, *J. Phys. B* **15**, L235 (1982); Z. Deng, *J. Opt. Soc. Am. B* **1**, 874 (1984); Z. Deng, *Phys. Lett.* **105A**, 43 (1984).

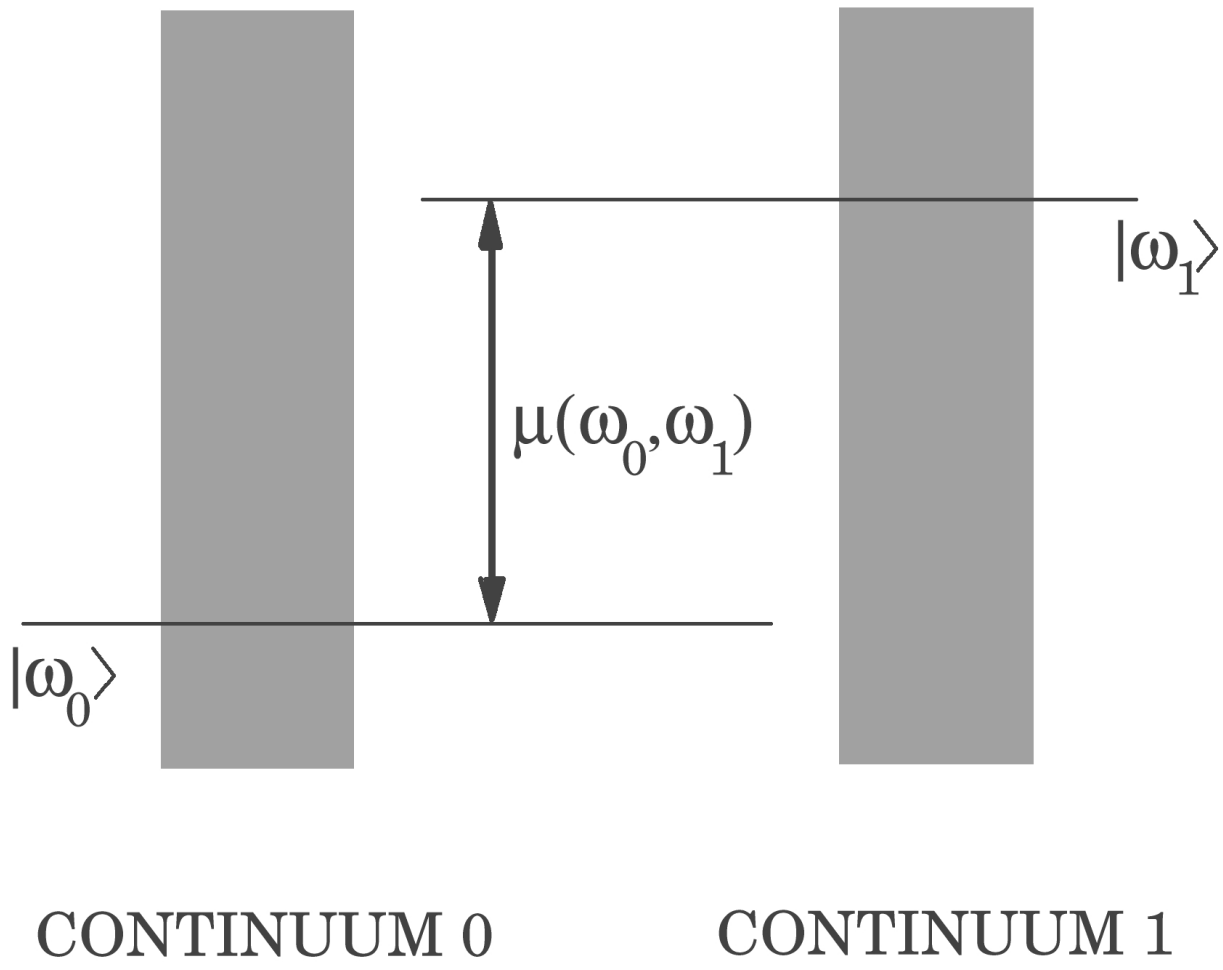

FIGURE 1.2.

A (CONTINUUM, CONTINUUM) system. In this example, there are two coupled continuous bands of energy levels. Each energy level in continuum 0 has an allowed dipole transition to each level in continuum 1, and vice versa. There are no transitions between two levels of the same continuum. In the general case the (CONTINUUM, CONTINUUM) system is not actually of low driver-rank, but it can be approximated to any desired accuracy as a low-driver-rank system.

does not result in very strong coupling between the two continua. As the interaction strength increases, we would expect the population to be completely mixed between the two continua: in the steady state, each continuum would host 50% of the population. In fact, past a certain point the level of coupling decreases until (for an infinite interaction strength) the bands are totally decoupled. Thus, at very high interaction strengths, the population is entirely trapped in the continuum initially containing it. This is closely related to (and prompted by) the results reported in Ref. 2.

The second result concerns bands of energy levels confined to a finite frequency range. In this case, increasing the interaction strength does increase the coupling between the continua in an expected way. When the interaction strength is much larger than the widths of the continua (in energy space), each continuum acts something like a single discrete energy level, so the system as a whole acts something like a two-level system. Thus, as the interaction strength is turned up, the population oscillates between the two continua more and more rapidly. The surprise has to do with damping. Even though the population mainly oscillates, the finite width of the continua (which is very small, but still non-zero) should cause a non-recoverable absorption of population by the continua. Thus the oscillations should eventually decay into a steady-state population distribution of 50% in each continuum. This does happen at moderate interaction strengths, but not at high interaction strengths. At high interaction strengths the population continues oscillating (without damping) forever.

1.4. Future Directions

The reader may find that there is more of mathematical method than of physics in this dissertation. This was not my original intent, but turned out to be a practical necessity as the full scope of the low-driver-rank assumption became apparent. Limitations of time and space made it literally impossible to develop the mathematical techniques *and* to pursue any significant concrete physical problem (as opposed to the rather abstract problem of population trapping) at the same time. I wish this could have been otherwise, but I do not apologize for it.

I hope that the methods presented herein are developed in sufficient detail to allow their application in some of the problems being solved in our Quantum Optics research group. The particular application which springs to mind (and which motivated this work) is the modeling and inclusion of vibrational bands of polyatomic molecules in propagation problems, for which these techniques would be ideal. In propagation problems involving the coupled Maxwell-Schrödinger equations, the Schrödinger equation must be solved simultaneously at many points in space, necessitating highly efficient solution methods.

Additional directions in which this work can be advanced are outlined briefly in §9.8.

1.5. How to Find it

In Chapter II, a review of the literature will be presented. In Chapter III, various terms and notation are defined. New results are presented in Chapters IV-VIII. Thus, some

readers may want to proceed directly to Chapter IV and treat Chapters II and III as reference material. (This warning is provided for the benefit of those readers who find reading sixty or seventy pages of introductory material too tiring.)

CHAPTER II
Survey of the Literature

2.1. Introduction

The treatment of continuous bands of energy levels in (model) quantum systems has been dealt with only infrequently in the air we will adopt. Our study is firmly rooted in the tradition of many investigations of model 2-level systems, $(1, \mathrm{N})$ systems, and ladder systems.

We will study continua using methods which are similar in character (though not in detail) to the methods used earlier on these "predecessor" model systems. Therefore, it is appropriate to consider the history of investigations of the 2-level system and its generalization as the $(1, \mathrm{N})$ system, of which the simpler continuous systems are direct generalizations. Studies of the ladder system would not seem to be as closely related to studies of the continuum; however, we will find in Chapter VIII that they are indeed related in an odd and unexpected way. Thus, we will also consider the history of ladder-system investigations.

Though a few investigations of continua have adopted the attitudes and methods characteric of the study of $(1, \mathrm{N})$ systems, most continuum investigations have adopted the methods of perturbation theory, and of various approximating theories. It is thus appropriate to consider the history of these investigations.

Finally, since we will be applying our results to the problem of coherent population trapping, we will consider these investigations as well.

2.2. Studies of the Undamped 2-Level System

Of course, the two-level system has been studied from the earliest days of quantum theory, and its study has reached the point where it is mainly a textbook subject (though it is also still an active area of research). In particular, there is an authoritative book by Allen and Eberly[1] on the theory and practice of 2-level systems. Other extensive sources are Agarwal[2] and Sargent *et al*.[3] Because of this, we will only review some of the highlights of 2-level-system study, beginning with a basic historical background, and proceeding to

[1] L. Allen and J. H. Eberly, *Optical Resonance and Two-Level Atoms* (Wiley, New York, 1975).
[2] G. S. Agarwal in *Springer Tracts in Modern Physics* (Springer, Berlin, 1974), vol. 70.
[3] M. Sargent III, M. O. Scully, and W. E. Lamb, Jr., *Laser Physics* (Addison-Wesley, Reading, Mass., 1974).

some of the methods (primarily mathematical) for solving such systems. The interested reader should refer to these sources for more details. Systems with damping are covered in §2.5.

The 2-level system was apparently first introduced by Weisskopf and Wigner in 1930.[4] It is a natural approximation to many quantum systems in which a given transition is driven resonantly. If a system is prepared with all its population in a given state and an interaction is then supplied which is resonant with the transition between this state and a second state, the population will sometimes simply cycle between these two states at the Rabi frequency.[5] All other states of the system receive very little population, and are therefore essentially irrelevant to the time-evolution of the system. As another example, Bebb and Gold[6] have shown that in a ladder of resonant transitions, only the two extreme states hold much population (*via* multiphoton transitions), and the intermediate states can be discarded to leave just an approximate 2-level system.

Of course, there are also many situations in which this doesn't hold. Perhaps the given states are degenerate. Perhaps the applied interaction isn't exactly resonant. Perhaps there is a large number of nearly resonant transitions. Perhaps the applied interaction itself is changing in time, so that different transitions are resonant at different times. These conditions necessitate more complex models, such as those discussed in §2.3 and §2.4. In comparison to the systems we will be dealing with in the remainder of this paper, the 2-level system is fairly trivial in a theoretical and computational sense. It is true that there is no closed-form analytical solution to the time-evolution of the 2-level system in the case of a general time-dependent Hamiltonian. (We are referring to the Schrödinger picture, in which the Hamiltonian is time-independent except in the case of an externally applied interaction.[7]) On the other hand, there are numerous techniques for solving the system in various special cases.

In the case of a time-independent Hamiltonian operator, there are several ways of producing a closed-form solution for the time-evolution. The eigenvalues and eigenvectors of the Hamiltonian are well-known, and can be used to construct the full solution. Alternately, one can compute the time-evolution operator $U(t) = e^{-iHt}$. Pauli[8] showed that if the Hamiltonian H is decomposed into a linear combination of spin-matrices, then e^{-iHt} can be written in a simple way in terms of the coefficients of this decomposition. This is related closely to the theory of infinitesimal rotations and quaternions.[9] The time-development operator is still useful in the case of a *periodic* time-varying Hamiltonian. It is a consequence of Floquet's theorem (see the work of Shirley,[10] Barone *et al.*,[11] Milfeld and Wyatt,[12] and Salzman[13]) that $U(t)$ can be written as the product of a *periodic unitary operator* (whose period is the same as that of the Hamiltonian) times an exponential e^{-iMt}

[4] V. Weisskopf and E. Wigner, *Z. Phys.* **63**, 54 (1930).
[5] I. I. Rabi, *Phys. Rev.* **51**, 652 (1937).
[6] H. B. Bebb and A. Gold, *Phys. Rev.* **143**, 1 (1966).
[7] P. Roman, *Advanced Quantum Theory* (Addison-Wesley, Reading, Mass., 1965), §1-5a.
[8] W. Pauli, *Zeits. f. Physik* **43**, 601 (1927).
[9] W. R. Hamilton, *Elements of Quaternions*, vol. I, third ed. (Chelsea, New York, 1969).
[10] J. H. Shirley, *Phys. Rev. B* **138**, 979 (1965).
[11] S. R. Barone, M. A. Narcowich, and F. J. Narcowich, *Phys. Rev. A* **15**, 1109 (1977).
[12] K. F. Milfeld and R. E. Wyatt, *Phys. Rev. A* **27**, 72 (1983).
[13] W. R. Salzman, *Phys. Rev. A* **10**, 461 (1974).

(where M is time-independent).

For a more general time-dependent Hamiltonian (for example, for a system stimulated by an externally applied laser field whose amplitude is changing in time), one can no longer find a closed-form solution except for special types of interactions. In the degenerate case (or the case of equal detunings under the RWA—see below), a relatively simple closed-form solution can be written (see Gibbs,[14] for example). When this is not the case, only special types of time-variation can produce closed-form solutions. Thus, Zon and Katsnel'son[15] have solved the case of a symmetrical cusp pulse. Bambini and Berman[16] have found a class of pulse-shapes for which a closed-form solution exists and, in so doing, have generalized the solution of Rosen and Zener[17] for the hyperbolic secant pulse. Radmore,[18] Wilson and Friedmann,[19] and Burkey and Cantrell[20] have produced closed-form solutions in the case of an exponentially increasing interaction. Additionally, Ref. 19 considered the case of a pulse which increases from zero exponentially, remains at a constant strength for an interval, and then declines exponentially to zero again. Ref. 20 solved the two-level system for what the authors called the "semi-exponential" pulse, which superficially resembles the so-called Fermi pulse.

In some cases, it is possible to employ approximations which, while not exact, are tremendously accurate and produce closed-form solutions. The "adiabatic" approximation in quantum mechanics stems from work of Einstein[21] and Ehrenfest.[22] (See also Grischkowsky,[23] Crisp,[24] or Lehmberg and Reintjes.[25]) According to the adiabatic theorem, if the externally applied interaction varies in time slowly enough, the system always remains in an instantaneous eigenstate of the Hamiltonian. Of course, this principle applies more widely than just to 2-level systems. Recent authors who have used this principle in more general applications include Kuz'min and Sazonov,[26] Peterson and Cantrell,[27] and Peterson.[28] The latter works are very useful general references on the adiabatic approximation.

Actually, the time-independent case is *also* often considered to be an approximation: that of an interaction turned on very rapidly at time zero. Since time zero is also the beginning of the observation (or computation) period, the Hamiltonian is time-independent during the observation period, but not for all time. This view is taken in various pub-

[14] H. M. Gibbs, *Phys. Rev. A* **8**, 446 (1973).
[15] B. A. Zon and B. G. Katsnel'son, *Sov. Phys. JETP* **40**, 462 (1975).
[16] A. Bambini and P. R. Berman, *Phys. Rev. A* **23**, 2496 (1981).
[17] N. Rosen and C. Zener, *Phys. Rev.* **40**, 502 (1932).
[18] P. M. Radmore, *Phys. Lett.* **87A**, 285 (1982).
[19] A. D. Wilson and H. Friedman, *Chem. Phys.* **23**, 105 (1977).
[20] R. S. Burkey and C. D. Cantrell, *Opt. Commun.* **43**, 64 (1982).
[21] A. Einstein, *Verh. d. D. Phys. Ges.* **16**, 826 (1914).
[22] P. Ehrenfest, *Phil. Mag.* **33**, 500 (1917).
[23] M. D. Grischkowsky, *Phys. Rev. Lett.* **24**, 866 (1970).
[24] M. D. Crisp, *Phys. Rev. A* **8**, 2128 (1973).
[25] R. H. Lehmberg and J. Reintjes, *Phys. Rev. A* **12**, 2574 (1975).
[26] M. V. Kuz'min and V. N. Sazonov, *Sov. Phys. JETP* **52**, 889 (1980); M. V. Kuz'min, *Sov. J. Quantum Electron.* **11**, 9 (1981); M. V. Kuz'min and V. N. Sazonov, *Sov. Phys. JETP* **56**, 27 (1982).
[27] G. L. Peterson and C. D. Cantrell, *Phys. Rev. A* **31**, 807 (1985).
[28] G. L. Peterson, doctoral dissertation, University of Texas at Dallas, 1986.

lications of Stone and Goodman, and their collaborators.[29] See also S. Mukamel and J. Jortner[30] and C. D. Cantrell and H. W. Galbraith.[31]

Of course, there is no reason to limit our discussion to analytic solutions. There have probably been few recent investigators of multilevel systems who have not had to resort to computer or qualitative solutions at one time or another. Schrödinger's equations for a 2-level system consist simply of two coupled ordinary differential equations. Such systems are quite easy to solve using standard black-box computer programs (such as those found in IMSL[32]) as long as one is not obliged to deal with large collections of such systems, as in propagation problems. (See M. Crenshaw *et al*.[33] and D. D. Chu and C. D. Cantrell.[34]) The primary difficulty encountered is that there are several different time-scales in the problem, and they can differ wildly from each other. For example, transition frequencies may be optical (in the case of an externally applied laser field), while the time scale of change of the laser amplitude (which is the time scale on which interesting changes to the system occur) can be many orders of magnitude larger. This could mean that a tremendously large number of computational time-steps would be needed to observe any interesting features of the time-evolution. This problem is partially overcome by use of the the so-called Rotating-Wave Approximation (RWA).[35] In the RWA, the optical frequency components are removed in a safe way, and are replaced with detuning frequencies (which are much smaller near resonance) instead. The RWA is generally considered quite safe. It is widely used (as, for example, in the famous study of the two-level atom interacting with a quantized electromagnetic field by Jaynes and Cummings[36]). However, Tavis and Cummings[37] have pointed out that the RWA fails at high field-strengths. Milonni *et al*.[38] have shown that collections of two-level systems which exhibit quantum chaos (in the sense of being very sensitive to the exact initial conditions) when solved exactly, sometimes have only quasi-periodic behavior in the RWA.

A visual and intuitive approach which is familiar and appealing to many physicists is the Bloch-vector approach introduced by Feynman *et al*.[39] In this approach, the *two* probability amplitudes in the 2-level system are manipulated to produce a *three*-vector called the *Bloch vector*. The Bloch vector obeys an equation of motion very different from

[29] For example: M. Goodman and E. Thiele, *Phys. Rev. A* **5**, 135 (1972); J. Stone, E. Thiele, and M. F. Goodman, *J. Chem. Phys.* **59**, 2909 (1973); J. Stone, E. Thiele, and M. F. Goodman, *J. Chem. Phys.* **63**, 2936 (1975); M. F. Goodman, J. Stone, and E. Thiele, *J. Chem. Phys.* **59**, 2919 (1973); M. F. Goodman, J. Stone, and E. Thiele, *J. Chem. Phys.* **63**, 2929 (1973); J. Stone and M. F. Goodman, *Phys. Rev. A* **14**, 380 (1976); M. F. Goodman, J. Stone, and D. A. Dows, *J. Chem. Phys.* **65**, 5052 (1976); J. Stone, M. F. Goodman, and D. A. Dows, *J. Chem. Phys.* **65**, 5062 (1976).

[30] S. Mukamel and J. Jortner, J. Chem. Phys. 65, 5204 (1976); *Chem. Phys. Lett.* **40**, 150 (1976).

[31] C. D. Cantrell and H. W. Galbraith, *Optics. Comm.* **21**, 374 (1977).

[32] International Mathematical and Statistical Library, by IMSL, Inc.

[33] M. E. Crenshaw, C. D. Cantrell, D. D. Chu, and C. A. Glosson, in *Science and Engineering on Cray Supercomputers*, ed. by John E. Aldag (Cray Research, Inc., Minneapolis, 1987), pp. 477-490.

[34] D. D. Chu and C. D. Cantrell, to be published.

[35] The multilevel RWA is discussed by T. Einwohner, J. Wong, and J. C. Garrison, *Phys. Rev. A* **14**, 1452 (1976); the case of bound-free transitions is discussed by J. Javanainen, *J. Phys. B* **16**, 1343 (1983).

[36] E. Jaynes and F. Cummings, *Proc. IEEE* **51**, 89 (1963).

[37] M. Tavis and F. Cummings, *Phys. Rev.* **170**, 379 (1968).

[38] P. Milonni, J. Ackerhalt, and H. Galbraith, *Phys. Rev. Lett.* **50**, 966 (1983).

[39] R. P. Feynman, F. L. Vernon, Jr., and R. W. Hellwarth, *J. Appl. Phys.* **28**, 49 (1957).

the coupled Schrödinger equations. In fact, it resembles the equation of motion for a magnetic dipole in a time-varying (if the Hamiltonian is time-varying) magnetic field. This is, of course, closely related to the spin-matrix approach mentioned earlier. The solution to the optical Bloch equations was originally given by Torrey.[40] R.G. Brewer and E. L. Hahn[41] have constructed a similar vector model for a three-level system.

Also closely related is the *density-matrix* approach introduced by Neumann[42] and Landau[43]). (See also the review articles by Fano[44] and ter Haar.[45]) Here, instead of solving the two coupled differential equations for the components of the 2-vector $\psi(t)$, one attempts to solve the four coupled differential equations for the components of the 2×2 matrix $\rho = \psi\psi^\dagger$, which is known as the density matrix. As it happens, only three of these equations are independent, and they are linear combinations of the Bloch-vector components. However, there are several other advantages to using the density matrix. The primary advantage is that we can factor in our *ignorance* of the initial conditions, over and above the uncertainties dictated already by the quantum approach. For example, an ensemble of atoms obeying a thermal distribution can be described by a density matrix; a superposition, on the other hand, can only describe a *single* atom. Second, it provides a natural arena for figuring in phenomenological damping (due to collisions,[46] random motion of atoms in the ensemble, and other items falling under the loose heading of "line broadening"). Thus, for example, the well-known work of Icsevgi and Lamb[47] uses a density matrix approach in dealing with a gas of two-level atoms.

Incidentally, though the mathematical methods developed in Chapters VI-VIII below can be applied to simplify the density-matrix equation of motion, we have nevertheless used them herein exclusively in the solution of Schrödinger's equation. Perhaps this would be a direction of useful future extension to the method.

2.3. Studies of the $(1, \mathrm{N})$ System

The $(1, \mathrm{N})$ system was introduced by Rice[48] in 1933 as a natural extension to the 2-level system. In this system, there is a "background" of N states with nearly resonant transitions to a given state (see §3.3). The $(1, \mathrm{N})$ system is characterized by a "row-column bordered" Hamiltonian. In Rice's system, the background states were all equally spaced in frequency. Though this is a commonly studied special case, the equal-spacing requirement is generally relaxed, and the background states may be distributed in any desired way. Probably the generally best-known study of $(1, N)$ systems is that by Stey and Gib-

[40] H. C. Torrey, *Phys. Rev.* **76**, 1059 (1949).
[41] R. G. Brewer and E. L. Hahn, *Phys. Rev.* A **11**, 1641 (1975).
[42] J. von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Berlin, Julius Springer, 1931).
[43] L. Landau, *Z. Phys.* **45**, 430 (1927).
[44] U. Fano, *Rev. Mod. Phys.* **29**, 74 (1957).
[45] D. ter Haar, Rep. *Prog. Phys.* **24**, 304 (1961).
[46] A good exposition appears in J. B. Halsted, *Physics of Atomic Collisions*, 2nd ed. (Elsevier, New York, 1972), Ch. 13. Reviews can be found in S. Ch'en and M. Takeo, *Rev. Mod. Phys.* **29**, 20 (1957); R. Breene, *Rev. Mod. Phys.* **29**, 94 (1957); H. van Regemorteur, *Ann. Rev. Astrophys.* **3**, 71 (1965).
[47] A. Icsevgi and W. E. Lamb, Jr., *Phys. Rev.* **185**, 517 (1969).
[48] O. K. Rice, *J. Chem. Phys.* **1**, 375 (1933).

berd,[49] in which (among other things) the effects of departures from even spacing are derived. By the way, a satisfactory brief review of the field may be found in Shore.[50]

The $(1, \mathrm{N})$ system can be used to model the closely spaced rotational levels in vibrational bands of polyatomic molecules.[51] Bixon and Jortner[52] have used it as a model for studying Intra-Molecular Relaxation (IMR) for this very reason. In IMR, one wants to study the natural (*i.e.*, unstimulated) redistribution of population among the various states of the molecule. Additional discussions appear in Freed and Jortner,[53] Freed,[54] Borsella *et al.*,[55] del Bello *et al.*,[56] Cantrell,[57] and Robinson and Langhoff.[58]

The $(1, \mathrm{N})$ system is also typically used to study the behavior of the so-called quasi-continuum introduced by Bloembergen *et al*.[59] and Isenor *et al.*,[60] though its properties (in particular, its selection rules) differ markedly from the quasi-continuum.

The $(1, \mathrm{N})$ system and $(1, \mathsf{CONTINUUM})$ system (in which $\mathrm{N} \to \infty$) have been used to model many other physical situations as well. Indeed, there are too many such studies to mention. However, one recent example is the study of Fu and Haken,[61] in which the $(1, \mathsf{CONTINUUM})$ system is adopted as a semi-classical model for the dye laser.

Analytic solutions to the $(1, \mathrm{N})$ system are rarer than solutions to the 2-level system, though the theoretical approaches used are rather numerous. In the first place, there is no closed-form solution for the eigenvalues and/or eigenvectors of the Hamiltonian matrix. However, the problem has been thoroughly studied (see Wilkinson[62]). A simple (but implicit) equation for the eigenvalues exists, and the properties of the eigenvalues are well-understood. (For example: if the energies of the background states are arranged in ascending order, then there is precisely one eigenvalue between each of them, as well as one which is less than the smallest energy and one which is greater than the largest energy.)

---

[49] G. Stey and R. Gibberd, *Physica (Utr)* **60**, 1 (1972).

[50] B. W. Shore, *Chem. Phys. Lett.* **99**, 240 (1983).

[51] One might mention: O. K. Rice, *Phys. Rev.* **33**, 748 (1929); O. K. Rice, *Phys. Rev.* **34**, 1451 (1929); O. K. Rice, *Proc. Nat. Acad. Sci. U.S.* **15**, 459 (1929); G. W. Robinson and R. P. Frosch, *J. Chem. Phys.* **37**, 1962 (1962); G. W. Robinson and R. P. Frosch, *J. Chem. Phys.* **38**, 1187 (1963); G. W. Robinson in *Excited States*, Vol. 1, ed. by E. C. Lim (Academic Press, New York, 1974); S. Nordholm and S. Rice, *J. Chem. Phys.* **61**, 203 and 768 (1974); J. Jortner, *Pure and Appl. Chem.* **24**, 165 (1970); J. Jortner and S. Mukamel in *The World of Quantum Chemistry*, ed. by R. Daudel and B. Pullman (Reidel, Dordrecht, 1974); K. Freed, *J. Chem. Phys.* **52**, 1354 (1970).

[52] M. Bixon and J. Jortner, *J. Chem. Phys.* **48**, 715 (1968).

[53] K. F. Freed and J. Jortner, *J. Chem. Phys.* **50**, 2916 (1969).

[54] K. F. Freed, *Curr. Topics Chem.* **31**, 105 (1972); K. F. Freed, *Chem. Phys. Lett.* **42**, 600 (1976).

[55] E. Borsella, R. Fantoni, A. Giardini-Guidoni, D. R. Adams, and C. D. Cantrell, *Chem. Phys. Lett.* **101**, 86 (1983).

[56] U. del Bello, E. Borsella, R. Fantoni, A. Giardini-Guidoni, and C. D. Cantrell, *Chem. Phys. Lett.* **114**, 467 (1985).

[57] C. D. Cantrell in *Proceedings of the International Conference on Lasers '81*, ed. by C. B. Collins (STS Press, 1982), p. 936.

[58] G. W. Robinson and C. A. Langhoff, *Chem. Phys.* **5**, 1 (1974).

[59] N. Bloembergen, C. D. Cantrell, and D. M. Larsen, in *Tunable Lasers and Applications*, ed. by A. Mooradian, T. Jaeger, and P. Stokseth (Springer, Heidelberg, 1976).

[60] N. Isenor, V. Merchant, R. Hallsworth, and M. Richardson, *Can. J. Phys.* **51**, 1281 (1973).

[61] H. Fu and H. Haken, *Phys. Rev. A* **36**, 4802 (1987).

[62] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford Press, Cambridge, 1965).

Laplace transforms can sometimes produce closed-form solutions for the time-evolution of a $(1, \mathrm{N})$ or $(1, \mathsf{CONTINUUM})$ system. By this means Makarov *et al.*[63] have calculated an analytical solution for a $(1, \infty)$ system, in which the background states follow the form of a "discrete Lorentzian" (see Chapter III). The same authors also found the solution in the case of background states following a continuous Lorentzian distribution. However, the Laplace transform is more often used for the approximations it allows than for its exact solutions (see §2.5). The case of a broad, featureless background has also been solved using the Laplace transform technique, by several authors, including Kyrölä[64] and Deng.[65]

Again, there are several approaches to solving the time-dependent Schrödinger equation in the case of a time-dependent Hamiltonian. In spite of all these methods, I know of no published closed-form solutions to any such $(1, \mathrm{N})$ systems, except those presented in the remainder of the paper (and my related publications), and these relate only to the $(1, \mathsf{CONTINUUM})$ system. Burkey and Cantrell in Ref. 20 found the solution to the $(1, \mathsf{CONTINUUM})$ system stimulated by an exponentially increasing interaction, if the background states follow a continuous Lorentzian distribution. Later, the same authors introduced rules for extending all closed-form solutions of the 2-level system to closed-form solutions of the Lorentzian-background system.[66] Generalized forms of these rules are consequences of the developments in Chapter V.

The time-evolution of the $(1, \mathrm{N})$ and $(1, \mathsf{CONTINUUM})$ systems can be treated using a single integro-differential equation rather than the $\mathrm{N} + 1$ coupled Schrödinger equations for the probability amplitudes. This technique is used so frequently that we cannot possibly provide a historical review here, but it dates at least to Weisskopf and Wigner (Ref. 4). Examples of recent use include the discussion of deviations from the Weisskopf-Wigner exponential decay (see below) by Seke and Herfort,[67] and the study of a $(2, \mathsf{CONTINUUM})$ autoionizing system by Deng and Eberly.[68]

The kernel of the integro-differential equation represents a "memory function". When approximated, the integro-differential equation becomes a delay-differential equation (according to Milonni *et al.*[69]), in which the present time-derivative of the probability amplitude is related to the probability amplitude at a (discrete set of) previous time(s). Such equations have been shown to contribute to quantum chaos by Ikeda *et al.*[70] The simpler Markov approximation (which destroys the memory of the system) results in the Weisskopf-Wigner approximation.

The comments in §2.2 concerning the adiabatic approximation, the density-matrix approach, and computer-generated solutions apply equally well here. For example,

[63] A. A. Makarov, V. T. Platonenko, and V. V. Tyakht, *Sov. Phys. JETP* **48(6)**, 1044 (1978).
[64] E. Kyrölä, *J. Opt. Soc. Am. B* **1**, 737 (1984).
[65] See below.
[66] R. S. Burkey and C. D. Cantrell, *J. Opt. Soc. Am. B* **1**, 169 (1984).
[67] J. Seke and W. N. Herfort, *Phys. Rev. A* **38**, 833 (1988).
[68] Z. Deng and J. H. Eberly, *Phys. Rev. A* **36**, 2750 (1987).
[69] P. W. Milonni, J. R. Ackerhalt, H. W. Galbraith, and M.-L. Shih, *Phys. Rev. A* **28**, 32 (1983). This reference also contains an interesting discussion of entropy of such a system.
[70] K. Ikeda, K. Kondo, and O. Akimoto, *Phys. Rev. Lett.* **49**, 1467 (1982).

Yeh *et al.*[71] and Eberly *et al.*[72] have used the adiabatic approximation in solving the $(1, \mathrm{CONTINUUM})$ system, while others (such as Peterson *et al.*[73]) have used the adiabatic approximation in non-trivial generalizations of the $(1, \mathrm{N})$ system. Quack[74] has solved the $(1, \mathrm{N})$ system numerically. Interestingly, Bloch vectors also have some application, though it is not generally known. Elgin[75] and Hioe and Eberly[76] have shown that the Bloch vector idea can be extended to higher-order systems [not just the $(1, \mathrm{N})$ system], though not necessarily in a way having the appeal of the 3-dimensional Bloch vectors of the 2-level system. They have related these ideas to some "conservation laws" for the density matrix. They have found that in the absence of damping, that $\mathrm{trace}(\rho^n) = constant$ (in time) for any n. (The constants are all equal to unity for an unmixed state.) Contrast this with the better-known relationship $\mathrm{trace}(\rho) \equiv 1$. See also P. Milonni and J. Eberly.[77] Of course, this is not the only approach to solving the density-matrix equations of motion. Most of the techniques that can be applied to the state-vector Schrödinger equation can also be applied to the density-matrix form as well. For example, Goodman and Thiele[78] showed how to expand the density matrix in terms of its eigen-matrices.

As far as simple numerical integration of Schrödinger's equation is concerned, Haydock[79] has presented a computational algorithm, based on the method of Lanczos,[80] for tridiagonalizing any time-independent Hamiltonian [not just those of the $(1, N)$ system]. Burkey and Cantrell (Ref. 66) have improved on this result in the case of $(1, \mathrm{CONTINUUM})$ systems by giving analytically a similarity transformation that tridiagonalizes the time-*dependent* Hamiltonian. Burkey and Cantrell[81] have also given approximations which allow a similar treatment for the $(\mathrm{N}, \mathrm{CONTINUUM})$ system. Schek and Wyatt[82] have found a way of computing the tridiagonalized matrix elements in a way that is useful at high field-strengths.

Closely related is the work of Nauts and Wyatt,[83] Adams *et al.*,[84] and Schek and Wy-

[71] J. J. Yeh, C. M. Bowden, and J. H. Eberly, *J. Chem. Phys.* **76**, 5936 (1982).
[72] J. H. Eberly, J. J. Yeh, and C. M. Bowden, *Chem. Phys. Lett.* **86**, 76 (1982).
[73] for example, G. L. Peterson, C. D. Cantrell, and R. S. Burkey, *Opt. Commun.* **43**, 123 (1982); G. L. Peterson and C. D. Cantrell, *Phys. Rev. A* **31**, 807 (1985); G. L. Peterson and C. D. Cantrell in *Multiple-Photon Excitation and Dissociation of Polyatomic Molecules*, ed. by C. D. Cantrell (Springer-Verlag, Berlin, 1986), pp. 215-221.
[74] M. Quack, *J. Chem. Phys.* **69**, 1282 (1978).
[75] J. N. Elgin, *Physical Letters* **80A**, 140 (1980).
[76] F. T. Hioe and J. H. Eberly, *Phys. Rev. Lett.* **47**, 838 (1981); F. T. Hioe and J. H. Eberly, *Phys. Rev. A* **25**, 2168 (1982).
[77] P. W. Milonni and J. H. Eberly, *J. Chem. Phys.* **68**, 1602 (1978).
[78] M. F. Goodman and E. Thiele, *Phys. Rev. A* **5**, 1355 (1972).
[79] R. Haydock in *Solid State Physics*, ed. by E. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1980), Vol. 35, p. 215; R. Haydock, *Computer Physics Communications* **20**, 11 (1980); R. Haydock, V. Heine, and M. J. Kelly, *J. Phys.* **C8**, 2591 (1975).
[80] C. Lanczos, *J. Res. Natl. Bur. Std.* **45**, 255 (1950).
[81] R. S. Burkey and C. D. Cantrell, *J. Opt. Soc. Am. B* **2**, 451 (1985).
[82] I. Schek and R. Wyatt, *J. Chem. Phys.* **89**, 4924 (1988).
[83] A. Nauts and R. E. Wyatt, *Phys. Rev. Lett.* **51**, 2238 (1983); A. Nauts and R. E. Wyatt, *Phys. Rev. A* **30**, 872 (1984).
[84] D. R. Adams, C. D. Cantrell, R. S. Burkey, and G. L. Peterson, *Proc. Lasers '85* (1985).

att,[85] in which the time-development operator e^{-iHt} of a general discrete quantum system is written in terms of a finite computation involving only the eigenvalues (and not the eigenvectors) of the Hamiltonian. This technique has been applied by Schek *et al.*[86] to the study of quantum chaos in a $(2, \mathrm{N})$ system (actually, a 2-level system in which the upper level is coupled to a set of background states).

Other general [not just $(1, \mathrm{N})$ system] techniques for computing the time-development operator $U(t)$ include the Dyson expansion,[87] the Magnus expansion,[88] and (more recently) the method of Jolicard and Billing.[89] Salzman[90] has elucidated the relationship between the Dyson and Magnus expansions.

Lefebvre and Savolainen[91] have introduced a slightly extended version of the $(1, \mathrm{N})$ model, in which the background states and the ground state experience damping through coupling with additional reservoirs of states. Their formalism is identical to that of usual $(1, \mathrm{N})$ systems, except that the Hamiltonian is no longer Hermitian. Other, less-known efforts in this direction include the studies of Witriol *et al.*[92] and Witriol.[93] Incidentally, all of these efforts use the integro-differential equation approach in attempting to solve their model systems.

These are not the only attempts at producing simple, solvable extensions to the $(1, \mathrm{N})$ system. For example, Galbraith *et al.*[94] have extended the concept by splitting each energy level into two. Walter *et al.*[95] have studied the eigenvalue problem for the general (N, M) non-Hermitian system.

The behavior of the $(1, \mathrm{N})$ and $(1, \mathsf{CONTINUUM})$ systems educed from these investigations is actually rather simple. The probability amplitude of the ground state decays "exponentially", as implied by the Weisskopf-Wigner approximation, in the case of the continuum. Though the "decay" is always present, the exact exponential form depends on a Lorentzian continuum lineshape (as implied, for example, in Refs. 63 and 66, and in the work of Robiscoe and Hermanson[96]). Deviations from strict exponential decay during spontaneous emission are mentioned, for example, in Knight and Milonni.[97] However, even in the case of a non-Lorentzian lineshape, exponential decay can be a good approximation if coupling of the ground-state to the continuum is weak, as indicated by the work

[85] I. Schek and R. E. Wyatt in *Methods of Laser Spectroscopy*, ed. by Y. Prior, A. Ben-Reuven, and M. Rosenbluh (Plenum, New York, 1986); I. Schek and R. E. Wyatt, *J. Chem. Phys.* **84(8)**, 4497 (1986); I. Schek and R. E. Wyatt, *Chem. Phys. Lett.* **129**, 99 (1986).
[86] I. Schek, N. Moiseyev, and R. E. Wyatt, *Phys. Rev. A* **36**, 3743 (1987).
[87] F. J. Dyson, *Phys. Rev.* **75**, 486 (1949).
[88] W. Magnus, *Commun. Pure Appl. Math.* **7**, 649 (1954); D. W. Robinson, *Helv. Phys. Acta* **36**, 140 (1968); P. Pechukas and J. C. Light, *J. Chem. Phys.* **44**, 3897 (1966).
[89] G. Jolicard and G. D. Billing, *Chem. Phys.* **104**, 357 (1986).
[90] W. R. Salzman, *J. Chem. Phys.* **32**, 822 (1985).
[91] R. Lefebvre and J. Savolainen, *J. Chem. Phys.* **60**, 2509 (1974).
[92] N. M. Witriol, A. J. Galli, W. H. Brumage, and C. M. Bowden, *Opt. Lett.* **5**, 24 (1980).
[93] N. M. Witriol, *Chem. Phys. Lett.* **98**, 77 (1983).
[94] H. W. Galbraith, J. R. Ackerhalt, and P. W. Milonni, *J. Chem. Phys.* **78**, 790 (1984).
[95] O. Walter, L. S. Cedarbaum, and J. Schirmer, *J. Math. Phys.* **25**, 729 (1984).
[96] R. T. Robiscoe and J. C. Hermanson, *Am. J. Phys.* **40**, 1443 (1972); R. T. Robiscoe and J. C. Hermanson, *Am. J. Phys.* **41**, 414 (1973).
[97] P. L. Knight and P. W. Milonni, *Phys. Lett.* **56A**, 275 (1976).

of Pietenpol.[98] On the other hand, Khalfin[99] has shown that if the energy spectrum is bounded from below, then there must be a long-term deviation on the order of $\frac{1}{t}$ from pure exponential decay.

In the case of the (discrete) $(1, \mathrm{N})$ system, this initial somewhat-exponential decay of the ground-state probability amplitude is still in evidence. However, the system experiences periodic *recurrences* or *collapse and revival*. (See, for example, Refs. 63 and 78, or the work of Fonda and Ghirardi.[100]) Here, the ground-state population decays smoothly, but then suddenly builds to a peak at a later time. The cycle of rapid buildup followed by slow decay is then repeated, with the buildup becoming less perfect as time goes on (so that after a number of repetitions, the pattern is no longer evident).

2.4. Studies of the Ladder System

The ladder system is a generalization of the 2-level system which is very different from the $(1, \mathrm{N})$ system. It was apparently introduced by Göppert-Mayer[101] in 1931.

The ladder system is a natural outgrowth of the harmonic oscillator. The harmonic oscillator has an (infinite) sequence of equally spaced energy levels, with transitions occurring only between adjacent levels.[102] If anharmonicities are introduced, then the energy level spacing is altered and other (probably weak) transitions appear. We will refer to any system which can be indexed in such a way that only adjacent states are connected by transitions as a "ladder system". This terminology would not be acceptable to many investigators who would insist that (in addition to these requirements) the energies of the states must increase as one moves "up" the ladder. For example, many (see the references in §2.6) would distinguish between a three-level ladder system and a three-level "lambda"system, in which the middle level is at a higher energy than the extreme levels. We will not make this distinction. By its very nature, the ladder system is particularly suited for modeling multi-photon transitions.

In a theoretical sense, the ladder system of N levels is less tractable than the $(1, \mathrm{N})$ system. There are no satisfactory approaches to solving it, in spite of the fact that the eigenvalues are theoretically "known". What is the meaning of this cryptic statement? According to Eberly *et al.*,[103] Bialynicka-Birula *et al.*,[104] and Cantrell *et al.*,[105] the eigenvalues of the N-level ladder system can be found by the following procedure: The matrix elements of the Hamiltonian can be used as recursion coefficients to generate a degree-N characteristic polynomial whose roots (of course) are the eigenvalues. In the usual

[98] J. L. Pietenpol, *Phys. Rev.* **162**, 1301 (1967).
[99] L. A. Khalfin, *Sov. Phys. Dokl.* **1**, 671 (1956); L. A. Khalfin, *Sov. Phys. Dokl.* **2**, 340 (1957); L. A. Khalfin, *Sov. Phys. JETP* **6**, 1053 (1958).
[100] L. Fonda and G. C. Ghirardi, *Nuovo Cimento* **7A**, 180 (1972); L. Fonda and G. C. Ghirardi, *Nuovo Cimento* **10A**, 850 (1972).
[101] M. Göppert-Mayer, *Ann. Phys.* **9**, 273 (1931).
[102] W. Heisenberg, *Z. Phys.* **33**, 879 (1925); M. Born and P. Jordan, *Z. Phys.* **34**, 858 (1925).
[103] J. H. Eberly, B. W. Shore, Z. Bialynicka-Birula, I. Bialynicki-Birula, *Phys. Rev. A* **16**, 2038.
[104] Z. Bialynicka-Birula, I. Bialynicki-Birula, J. H. Eberly, and B. W. Shore, *Phys. Rev. A* **16**, 2048.
[105] C. D. Cantrell, V. S. Letokhov, and A. A. Makarov, in *Coherent Nonlinear Optics: Recent Advances*, ed. by M. S. Feld and V. S. Letokhov (Springer-Verlag, Berlin, 1980), Chap. 5.

model cases, these recursion coefficients are often such that one of the standard orthogonal polynomials is generated, and the eigenvalues can thus be looked up (for example,in AMS-55[106]). In this sense, the eigenvalues are "known". On the other hand, any slight change in the Hamiltonian produces a polynomial other than a known orthogonal polynomial, and thus brings one no closer to knowing the true solution to the problem. This is also a problem with some of our work in Chapter VI and in Ref. 66.

The Laplace transform technique can also be of some use in solving these systems. For example, Kyrölä[107] has investigated a ladder system in which each ladder level is coupled to a background continuum.

Of course, as for the $(1, \mathrm{N})$ system, one can generate computer solutions either to the eigenvalue/eigenvector problem or to the time-dependent Schrödinger equation problem. There are also numerous other (more restricted) methods in use, of which we might mention just one. There is a method (based very loosely on the ideas in Ref. 76) which Hioe[108] has applied to the solution of a three-level ladder system and, in principle, to more general cases.

Our interest in the ladder system [unlike that in the $(1, \mathrm{N})$ system] will not go beyond these few aspects. Thus, there is no need to go beyond this and present any more general history of the applications of the ladder system.

2.5. Studies of Continua

Other than studies which are outgrowths of the approaches mentioned in §2.3, approaches to solving continuum problems can be roughly categorized as follows:

1. Weisskopf-Wigner (Markov) approximations.
2. Perturbation theory (Golden Rule) approximations.
3. Fano-type eigenvalue solutions.
4. Approximations involving the quantum theory of damping.

We will briefly consider these in turn.

The approximation of Weisskopf and Wigner is generally attributed to a Weisskopf and Wigner publication of 1931 (Ref. 4). Actually, this approximation is due to a 1927 publication of Landau, Ref. 43. In either case, the approximation certainly has a distinguished parentage and history. The method derives from the ability to express Schrödinger's equations for the $(1, \mathsf{CONTINUUM})$ or $(1, \mathrm{N})$ system as an integro-differential equation (see previous section), and to apply a Markov approximation destroying the system's "memory". In so doing, one derives an exponential decay law for the probability amplitudes. This method has been employed by far too many authors to mention, including many of those

[106] U. Hochstrasser in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), Chap. 22.
[107] E. Kyrölä, "N Levels and the Continuum", preprint (1985).
[108] F. T. Hioe, *Phys. Lett.* **99A**, 150 (1983).

cited above. The Weisskopf-Wigner approximation may be generalized somewhat by viewing it in the context of the Langevin equation.[109,110] It will also be generalized somewhat in our Chap. V.

Applying perturbation theory to the $(1, \mathsf{CONTINUUM})$ system results in a derivation of the Golden Rule (or "Golden Rule #2"), so called by Fermi because of its great importance.[111] This rule allows us to calculate transition rates from an energy level to a background of levels in a weakly interacting system. The Golden Rule is a special case of the Weisskopf-Wigner formula (in the case of a very weak interaction), though it is traditionally derived very differently. Like the Weisskopf-Wigner approximation, it has been used by far too many authors to cite.

For problems of autoionization (in which a discrete level has an energy placing it within the range of a continuum to which it is coupled), these methods are inadequate. Fano[112] has presented a method for finding the lineshapes of autoionized energy levels in continuous absorption spectra. A simple-minded solution for the "eigenvalues" and "eigenvectors" of the $(1, \mathsf{CONTINUUM})$ system is actually quite straightforward, but the results exhibit a number of peculiarities. First, rather than having an infinite number of eigenstates (as one might expect in analogy with the discrete case), the $(1, \mathsf{CONTINUUM})$ system has only a small finite set of eigenstates. Moreover, these states tend to be unnormalizable, being mathematically singular when considered as functions of energy. Fano circumvented this problem in 1935 (Ref. 112) by *approximating* the $(1, \mathsf{CONTINUUM})$ system in terms of a discrete analog, and then allowing the set of discrete states to become very dense (approaching the continuum limit) at the end of the calculation. In 1961 (Ref. 112), following Dirac,[113] Fano dispensed with this procedure and dealt with the system in an entirely continuous fashion. He also considered the case of a single discrete state interacting with two continua, and the case of a number of discrete states interacting with a single continuum. The results of Chapter IV provide a generalized means of carrying out these calculations, and similar calculations for more complex systems.

The work of Fano has been continued by a number of investigators. These include Armstrong *et al.*[114] Beers and Armstrong,[115] Heller and Popov,[116] Knight,[117] Coleman and Knight,[118] and Coleman *et al.*,[119] who studied the problem of two-photon ionization. Strong-field effects and autoionization effects were investigated by Lambropoulos and

[109] M. Lax, *Phys. Rev.* **145**, 110 (1966).
[110] A good text (unfortunately somewhat marred by typographical errors) is W. H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973).
[111] E. Fermi, *Nuclear Physics* (U. of Chicago Press, Chicago, 1950), p. 142.
[112] U. Fano, *Nuovo Cimento* **12**, 156 (1935); U. Fano, *Phys. Rev.* **124**, 1866 (1961).
[113] P. A. M. Dirac, *Z. Physik* **44**, 585 (1927).
[114] L. Armstrong, Jr., B. L. Beers, and S. Feneuille, *Phys. Rev. A* **12**, 1903 (1975).
[115] B. L. Beers and L. Armstrong, Jr., *Phys. Rev. A* **12**, 2447 (1975).
[116] Y. I. Heller and A. K. Popov, *Opt. Commun.* **18**, 449 (1976).
[117] P. L. Knight in *Laser Physics*, ed. by D. F. Walls and J. D. Harvey (Academic Press, Sydney, 1980), pp. 63-97.
[118] P. E. Coleman and P. L. Knight, *J. Phys. B* **14**, 2139 (1981); P. E. Coleman and P. L. Knight, *J. Phys. B* **15**, 1957 (1982).
[119] P. E. Coleman, P. L. Knight, and K. Burnett, *Opt. Commun.* **42**, 171 (1982).

Zoller[120] and by Rzazewski and Eberly.[121] Several authors cited in the next section have also employed this method.

Finally, we may mention the master-equation or "coarse-grained" approach to the quantum theory of damping (see Ref. 110.) Unlike the Langevin approach, which introduces damping at the level of Heisenberg's operator equations of motion, the master-equation approach introduces it at the density-matrix level. Nevertheless, the effect of both is to carry out a Markov approximation which destroys the "memory" of the system. In this approach, the quantum system is coupled to a large reservoir whose behavior does not really concern us. The master equation is obtained by averaging the density-matrix form of Schrödinger's equation over all reservoir states. In this way, an equation of motion (the "master equation") is obtained which refers explicitly only to the states of the system of interest, and not the reservoir. A simplified form of the master equation is often employed in which the density matrix is diagonal (hence eliminating all coherence in the quantum system). These simplified equations are the "rate equations" commonly found in Kinetic Theory.[122] The master equation was apparently introduced by Pauli[123] in order to deal with the problem of atomic linewidths. See also the work of Lax[124] and Louisell and co-workers.[125]

2.6. Coherent Population Trapping

The problem of coherent population trapping is this: in a complex quantum system, it can happen that the system becomes "trapped" in a state from which it seemingly should make transitions to other allowed states, but doesn't. That is, the population is trapped in a single state, or small set of states, which can *apparently* be strongly coupled to other states that (in spite of this) never become significantly populated. One would like to determine the conditions under which this occurs. A number of studies have been directed towards this end. These studies may be characterized as: those dealing with purely discrete quantum models; those dealing with interacting discrete states and continua; and those dealing with purely continuous quantum models.

Several studies have addressed the problem of purely discrete quantum models. In an interesting study, Whitley and Stroud[126] considered a three-level ladder atom interacting with a quantized electromagnetic field. They derived a density-matrix equation of motion for the atomic system, in which they showed that even in the case of a very strong incident field, the steady-state populations need not be equally divided among the atomic levels. In particular, population could be somewhat inverted in some cases. *A priori*, one would

[120] P. Lambropoulos and P. Zoller, *Phys. Rev. A* **24**, 379 (1981).
[121] K. Rzazewski and J. H. Eberly, *Phys. Rev. Lett.* **47**, 408 (1981); K. Rzazewski and J. H. Eberly, *Phys. Rev. A* **27**, 1866 (1983).
[122] for example, W. V. Smith and P. P. Sorokin, *The Laser* (McGraw-Hill, New York, 1940).
[123] W. Pauli in *Festschrift zum 60. Geburtstage A. Sommerfelds* (Hirzel, Leipzig, 1928).
[124] M. Lax, *J. Phys. Chem. Solid* **25**, 487 (1964).
[125] W. H. Louisell and L. R. Walker, *Phys. Rev.* **137**, B204 (1965); W. H. Louisell in *International School of Physics "Enrico Fermi" XLII Course in Quantum Optics* (Varenna, Italy, 1967); W. H. Louisell and J. H. Marburger, *J. Quantum Electron.* **QE-3**, 348 (1967).
[126] R. M. Whitley and C. R. Stroud, Jr., *Phys. Rev. A* **14**, 1498 (1976).

think it more likely that at high field strengths one-third of the population would reside in each atomic level, on the average. In no case would one expect a steady-state inversion, since this is non-thermal. Swain[127] has also studied this problem from the pure rate-equation perspective. Radmore and Knight[128] list numerous authors who have studied similar problems. Experimentally, population-trapping in the lambda configuration has been observed by Alzetta *et al.*[129] and Gray *et al.*[130]

Stettler *et al.*[131] solved a two-level system in which each of the levels was split into two (*i.e.*, they really solved a four-level system), in which the upper manifold could lose population because of dissociation of the atomic system. In the large-field case, population was split among the levels of the lower manifold, and no population appeared in the upper manifold. Thus, there was population trapping but no inversion. Deng[132] has studied a different four-level system, formed by splitting the middle level of a three-level lambda system. He showed that under certain conditions on the system parameters, there is a similarity transformation (independent of field strength) in which the system consists of two decoupled manifolds of two levels each. Consequently, population would be trapped in either of these blocks, even at quite large field strengths. Nevertheless, because of the restriction on the system parameters, this result seems to depend in some sense on numerical coincidences.

Cardimona *et al.*[133] have taken the opposite approach to the authors above, in that they studied trapping in the $(1, \mathrm{N})$ system rather than ladder-like systems. Trapping in a $(1, \mathrm{N})$ system cannot easily be attributed to multiphoton effects.

Several studies concern the effects of an (ionization) continuum, in addition to discrete levels. Lami and Rahman[134] have found that population trapping can occur in the two-photon autoionization model described in the preceding section, using a non-Hermitian, discrete effective Hamiltonian. Other authors, including all those below, have performed their calculations using true (albeit highly trivial) continuum models. Coleman and Knight[135] have studied a system of two discrete levels coupled only through an intermediate (non-auto) ionization continuum. They have found that there are combinations of system parameters and/or experimental conditions leading to minimal ion formation (*i.e.*, a small population in the continuum). Deng[136] has formed the same conclusions regarding a similar model system in which the two discrete energy levels of Coleman and Knight are coupled to a third discrete level, and[137] a model system in which the three discrete states and continuum form a ladder configuration rather than a diamond configuration. All of these results fall into the category of "numerical coincidences" described above.

[127] S. Swain, *J. Phys. B* **15**, 3405 (1982).
[128] P. M. Radmore and P. L. Knight, *J. Phys. B* **15**, 561 (1982).
[129] G. Alzetta, L. Gozzini, L. Moi, and G. Orriols, *Nuovo Cimento* **36B**, 5 (1976).
[130] H. R. Gray, R. M. Whitley, and C. R. Stroud, Jr., *Opt. Lett.* **3**, 218 (1978).
[131] J. D. Stettler, C. M. Bowden, N. M Witriol, and J. H. Eberly, *Phys. Lett.* **73A**, 171 (1979).
[132] Z. Deng, *Opt. Commun.* **48**, 284 (1983).
[133] D. A. Cardimona, M. G. Raymer, and C. R. Stroud, Jr., *J. Phys. B* **15**, 55 (1982).
[134] A. Lami and N. K. Rahman, *Phys. Rev. A* **33**, 782 (1986).
[135] P. E. Coleman and P. L. Knight, *J. Phys. B* **15**, L235 (1982).
[136] Z. Deng, *J. Opt. Soc. Am . B* **1**, 874 (1984).
[137] Z. Deng, *Phys. Lett.* **105A**, 43 (1984).

To my knowledge, there is only one published report (at the time of this writing) on trapping in a purely continuous quantum model. This is the work of Deng and Eberly,[138] which demonstrated that trapping can occur in a system consisting of an infinite ladder of broad, featureless continua. In this model, the trapping becomes more complete the higher the degree of apparent coupling among the continua, and not as a result of numerical coincidences. This work actually generated a certain amount of controversy, drawing a response by Arimondo and Rahman,[139] and a subsequent reply by the original authors.[140]

The present author has also been in position to contribute to this discussion,[141] by investigating the problem of population-trapping in continuum-continuum interactions. Other investigators of the strong-field continuum-continuum problem (though not necessarily in this context) include Karule,[142] Klarsfeld and Maquet,[143] and Gontier *et al.*[144]

[138] Z. Deng and J. H. Eberly, *Phys. Rev. A* **34**, 2492 (1986).
[139] E. Arimondo and N. K. Rahman, *Phys. Rev. A* **37**, 2706 (1988).
[140] Z. Deng and J. H. Eberly, *Phys. Rev. A* **37**, 2708 (1988).
[141] R. S. Burkey, A. Glosson, and C. D. Cantrell, accepted for publication in *Phys. Rev. A*, March 1, 1989 issue.
[142] E. Karule, *J. Phys. B* **11**, 441 (1978).
[143] S. Klarsfeld and A. Maquet, *J. Phys. B* **12**, L553 (1979).
[144] Y. Gontier, M. Poirier, and M. Trahin, *J. Phys. B* **13**, 1381 (1980).

CHAPTER III
BASIC DEFINITIONS AND NOTATION

3.1. Schrödinger's Equation

Below, we will concern ourselves entirely with various new techniques for solving the time-dependent Schrödinger Equation. It is convenient at this point to settle on a consistent notation, and to set out any recurring assumptions to be used later.

Schrödinger's equation can be written in various ways, including:

- A partial differential equation in space and time.
- Coupled ordinary differential equations in time.
- A matrix eigenvalue equation.
- Coupled integral equations.

The first case will not be dealt with, but all of the latter three possibilities will be considered.

In our thinking, the differential form of Schrödinger's equation is somehow fundamental, but we find in some cases that it is convenient to consider an alternative matrix or integral form. This is very reasonable in thinking about the time evolution of quantum systems. Schrödinger's *differential* equation will always appear in one of the following ways:

$$i\frac{d}{dt}\psi(t) = H(t)\psi(t) \tag{3.1}$$

$$i\frac{d}{dt}\psi(t) = \left(H_0 + H'(t)\right)\psi(t) \tag{3.2}$$

$$i\frac{d}{dt}\psi(t) = \left(H_0 + E_1(t)\mu_1 + ... + E_n(t)\mu_n\right)\psi(t) \tag{3.2'}$$

$$i\frac{d}{dt}\psi(t) = \left(H_0 + E(t)\mu\right)\psi(t). \tag{3.3}$$

These equations appear in order of decreasing generality. Sometimes, we will deal with the more general equations (3.1)-(3.2'), but mostly we will have eq. (3.3) in mind.

The meanings of the symbols in eqs. (3.1)-(3.3) are:

$\psi(t)$	the "state" of the system, a vector not necessarily in Hilbert space (see below).
$H(t)$	a matrix operator, proportional to the Hamiltonian.
H_0	a time-independent matrix operator, proportional to the Hamiltonian in the absence of "driving".
$H'(t)$	a matrix operator providing that part of the Hamiltonian responsible for external driving of the system.
μ	a time-independent matrix operator.
$E(t)$	a scalar (real) function representing some field applied to the system externally.

By saying that $H(t)$ is "proportional" to the Hamiltonian operator, we mean to imply that constant factors such as -1 or $\hbar$ may have been conveniently absorbed into the operator. The reason such absorption is convenient is that all of the results we will derive have no dependence on the particular values of any such constants.

A useful way of thinking about some of these quantities is to imagine we are dealing with, say, a molecule being driven by an external electric field $E(t)$, through an interaction mediated by the dipole operator μ. Such an interpretation is not necessary to our discussion, but at least provides some motivation. We will consider the case in which $E(t)$ is constant, but our main concern will be with time-varying Hamiltonians.

Note that, for us, the Hamiltonian is functionally dependent on time only in a parametrical sense. That is, the time variation occurs because some externally controlled parameter is being changed. For example, $E(t)$ may be controlled by the experimenter if $E(t)$ is the electric field, or the envelope of a quasi-monochromatic electric field. Nevertheless, $H(t)$ is a Schrödinger operator. We will never employ the Heisenberg or the Interaction picture,[1] except where specifically stated.

It is important to emphasize that we avoid perturbation theory (Ref. 2, Chs. 17 and 18) entirely, so $H'(t)$ is not assumed to be "small" in relation to H_0. Moreover, we choose not to rely on either the sudden or the adiabatic approximations,[2] because we wish to make no assumptions about the rate of change of $H'(t)$. The driving term may vary quickly or slowly. It may vary at an intermediate rate. It may vary quickly part of the time, and slowly other times.

We adopt a matrix representation for all operators and states, and thereby eliminate the spatial dependence of all quantities we use. $\psi(t)$ is simply regarded as a vector in some linear space, and has no spatial dependence whatever. As a notational convenience, the "first" element of the vector $\psi(t)$ will be called $a(t)$. The corresponding energy level

[1] Merzbacher, *Quantum Mechanics*, second edition (Wiley, New York, 1970), §15.3, §15.7, and §18.7.
[2] A. Messiah, *Quantum Mechanics*, trans. by G. Temmer (Wiley, New York, 1958) Ch. XVII, part II.

will be called the *ground state*, even though it will not necessarily be the state of lowest energy. Thus, $a(t)$ is the ground-state probability amplitude.

Note that the underlying linear space is not necessarily Hilbert space. Even if $\psi(t)$ itself is in Hilbert space[3] (*i.e.*, $\mid \psi(t) \mid^2 = 1$) we may still be forced to allow other vectors involved in the calculation of $\psi(t)$ to be non-normalizable. This kind of situation arises if μ is an *unbounded* operator.[4] Many sample problems in the literature employ unbounded operators. For the moment, we'll try to avoid restricting ourselves to using only bounded operators. Thus, the underlying linear space may have either countably or uncountably infinite dimension.[5]

Another assumption we avoid is that of the Rotating-Wave Approximation (RWA). (See the review in Chap. II and the brief outline of the RWA in §3.7.) The RWA is used to remove high-frequency components from the right-hand side of eq. (3.3). It also changes various multiplicative constants, signs, $E(t)$, and H_0. However, the basic form of eq. (3.3) is not affected by the RWA. Consequently, by suitable re-interpretation of the operators, we can assume the the RWA has been made or has not been made, as takes our fancy. Nor do we particularly care about any other approximations that may or may not have been applied in order to supply us with eqs. (3.1)-(3.3).

3.2 Low Driver-Rank

The foregoing discussion seems to deny almost all restrictive assumptions. Nothing seems to be needed other than a (presumably) semi-classical Schrödinger equation. The decompositions shown in eqs. (3.1)-(3.3) are only slightly constricting.

We need more than this: Only trivial results can be derived without assumptions. Our trick will be to introduce an assumption that heretofore has played little or no explicit role in Quantum Theory. Our new assumption is based on a concept outlined as follows:

> **Definition:** A quantum system with Hamiltonian $H_0 + H'(t)$ has *low driver-rank* if the matrix rank of $H'(t)$ (or μ) is small.

Recall that the rank of a matrix is defined to be the number of linearly independent rows (or columns) of the matrix.[6] For a non-singular matrix, the rank is equal to the dimension and (in practice) "most" matrices are non-singular.[7] Therefore, most matrices

[3] J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, translated by R. T. Beyer (Princeton University Press, Princeton, 1955); N. Akhiezer and I. Glazman, *Theory of Linear Operators*, vols. I and II, translated by N. Nestell (F. Ungar, New York, 1961 and 1963).

[4] A bounded operator is one which, when acting on a normalizable vector, returns a normalizable vector. See G. Hellwig, *Differential Operators of Mathematical Physics* (Addison-Wesley, Reading, Mass., 1967), Ch. 7.

[5] The dimension of a Hilbert Space is finite or countably infinite. The concepts of "countable" and "uncountable" infinities are explained, for example, in E. Hewitt and K. Stromberg, *Real and Abstract Analysis* (Springer-Verlag, New York, 1975), §1.4.

[6] G. Birkhoff and S. MacLane, *A Survey of Modern Algebra* (Macmillan, New York, 1965), §7.6.

[7] I would like to assert that the set of singular matrices of any given dimension N is of measure zero, but I have not found any reference to support this assertion.

have a rank equal to their dimension. In the case of the dipole operator μ this is equal to the number of energy levels which, in turn, is generally infinite. (A bounded system has only discrete energy levels, and consequently has at most a countable infinity of them. An unbounded system has an uncountable infinity of energy levels.[8]) All other things being equal, one would therefore *not* expect μ to have a "small" rank in any sense. Some further rationale must be given for assuming that the rank is a small (finite) number.

One justification for the low-driver-rank assumption is that many solved problems in the literature involve low driver-rank systems. (For example, almost every solved problem mentioned in Chapter II is of low-driver-rank, except for those involving general ladder systems.) However, low driver-rank has not been previously recognized as an important criterion in analytically solvable problems. In the literature, we find problems that could be solved by low driver-rank methods—but which are actually solved under more restrictive assumptions. Many such solutions are generalizable. For example, we will see shortly that the $(1, \mathrm{N})$ system (§3.3) has a driver-rank of 2, and most of the methods used in the past for dealing with the $(1, \mathrm{N})$ system are successful because of this. Many $(1, \mathrm{N})$ system results are consequently generalizable to other systems with driver-rank 2. Similarly, many results concerning two-level systems are generalizable to a certain type of $(1, \mathsf{CONTINUUM})$ system. An underlying explanatory picture of many past investigations will therefore be revealed.

There are some new possibilities of practical use as well. As mentioned, the condition of low driver-rank cannot be expected to hold generally for real systems, even if it frequently holds for sample systems in the literature. However, we will see in Chapters VII and VIII that (for systems with continuous bands of levels) the assumption of low driver-rank can be an excellent approximation.

Because the notion of low driver-rank will prove to be important for us, it is convenient to introduce a special symbol for the driver-rank:

$$\mathrm{M} = \operatorname{rank} \mu. \tag{3.4}$$

This notation is used continually throughout the paper.

3.3. $(1, \mathrm{N})$ and $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ Systems

The $(1, \mathrm{N})$ system is the prototype (though not the simplest example) of a low driver-rank system. We often use $(1, \mathrm{N})$ systems for illustrative purposes, so it is a good idea to explain in detail what they are.

A $(1, \mathrm{N})$ system has $\mathrm{N} + 1$ energy levels. One level is called the *ground state*. It has probability amplitude $a(t)$. The other N levels form a *band*. Transitions take place only between the ground state and the band. There are no direct transitions between any two levels of the band itself. Normally, the $(1, \mathrm{N})$ Hamiltonian is something like this:

[8] L. Landau and E. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory*, third edition (Pergamon Press, Oxford, 1977), §10.

$$H(t) = \begin{bmatrix} 0 & E(t)\mu_1 & E(t)\mu_2 & \cdots & E(t)\mu_{\mathrm{N}} \\ E(t)\mu_1 & \delta_1 & 0 & \cdots & 0 \\ E(t)\mu_2 & 0 & \delta_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ E(t)\mu_{\mathrm{N}} & 0 & 0 & \cdots & \delta_{\mathrm{N}} \end{bmatrix}. \tag{3.5}$$

The notation δ_n is intended to call to mind the possibility that δ_n is the detuning of the level from the frequency of an applied laser field. This interpretation holds only if the RWA has been made. [In fact, if the RWA has been made, then δ_n must be the negative detuning.] It is *not* to be assumed in general that the differences $\delta_2 - \delta_1$, $\delta_3 - \delta_2$, ..., $\delta_{\mathrm{N}} - \delta_{\mathrm{N}-1}$ are all the same, although we'll very briefly talk about this special case. This equal-spacing assumption is, however, very commonly applied in the literature as indicated in Chap. II.

It is easy to see that the $(1, \mathrm{N})$ Hamiltonian is consistent with eq. (3.3). We take H_0 to be

$$H_0 = \mathrm{diag}\,(0, \delta_1, ..., \delta_{\mathrm{N}})\,. \tag{3.6}$$

Moreover, the dipole matrix μ is of low rank, with $\mathrm{M} = 2$. This can be seen by defining the vectors $\psi_0 = (1, 0, ..., 0)^\dagger$ and $\psi_1 = (0, \mu_1, ..., \mu_{\mathrm{N}})^\dagger$. Then,

$$\mu = \psi_0\psi_1^\dagger + \psi_1\psi_0^\dagger. \tag{3.7}$$

ψ_0, ψ_1, and all other vectors are, by convention, column vectors. This accounts for the appearance of the Hermitian conjugate operator $\dagger$ in their definitions.

It is amusing to note that $\mathrm{M} = 2$ regardless of the number of energy levels in the band. Indeed, this is so even if $\mathrm{N} \to \infty$ and we attain a continuum of levels in the band. In later chapters, it will be shown that, in a sense, the complexity of computation depends on M rather than on the number of energy levels. If so, it is really no harder to compute accurately the solution to Schrödinger's equation for continua than for discrete bands.

The $(1, \mathrm{N})$ system is a particular case of the $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ system.[9] An $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ system consists of a series of bands of energy levels. There is a band of N levels, a band of N' levels, a band of N'' levels, *etc*. Transitions occur only between adjacent bands. For example, there are transitions between the N levels of the first band and the N' levels of the second band. There are no transitions between the first and third bands. Also, there are no transitions within any single band. For example, the so-called *ladder* system is a $(1, 1, 1, ...)$ system. Figure (3.1) illustrates these ideas.

This definition of the pure $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ system as given above does not allow any transitions within a given band of energy levels. It therefore does not represent the most general possible quantum system. In some cases, we may want to allow transitions within a certain band (say, the N' band). We will indicate this by the addition of an underline. For instance, an $(\mathrm{N}, \underline{\mathrm{N}'}, \mathrm{N}'', ...)$ system is an $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ system with allowed transitions within the N' band. This addition to the more common notation renders it

[9] C. D. Cantrell, V. S. Letokhov, and A. A. Makarov, in *Coherent Nonlinear Optics: Recent Advances*, ed. by M. S. Feld and V. S. Letokhov (Springer-Verlag, Berlin, 1980).

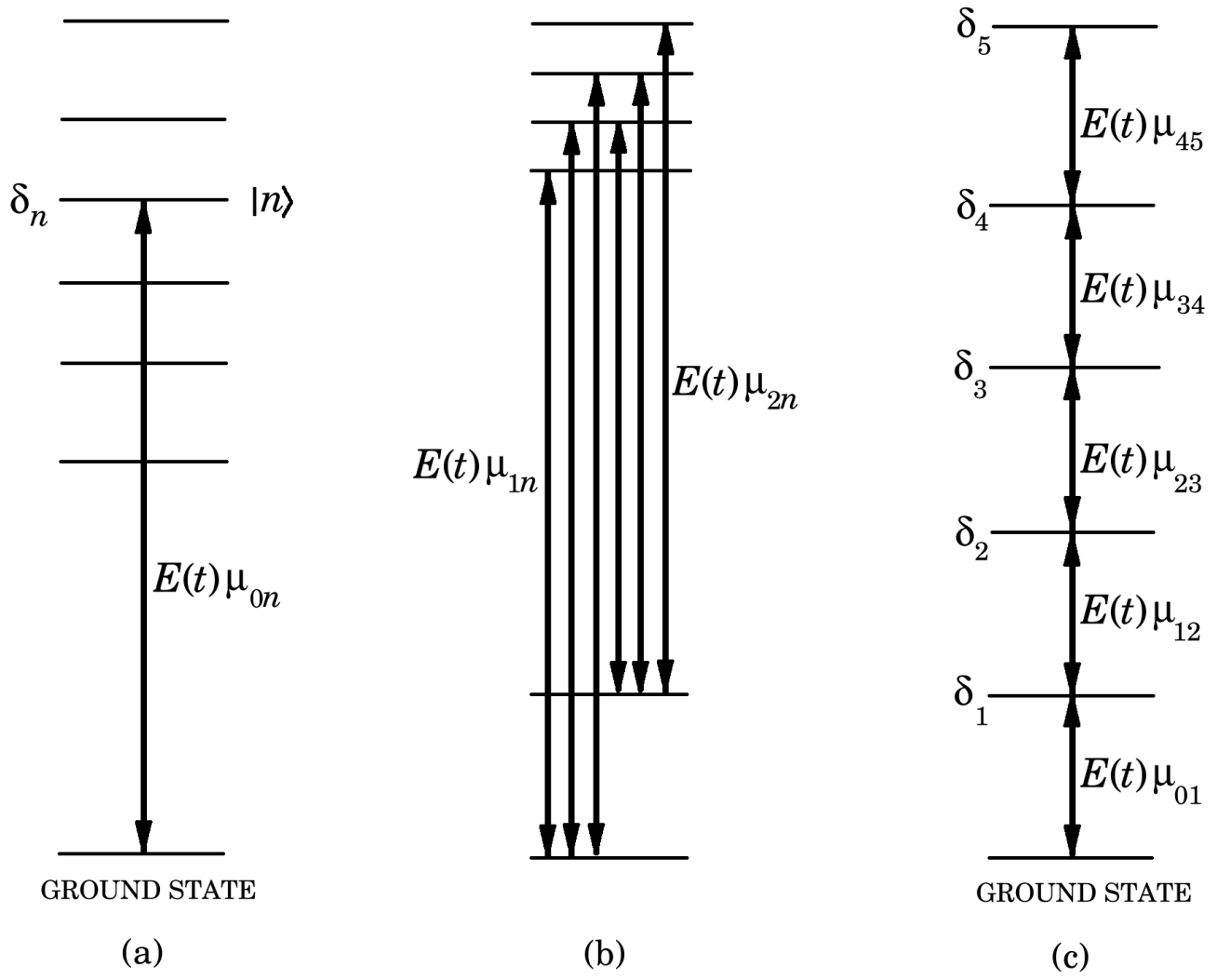

FIGURE 3.1

(a) A generic $(1, \mathrm{N})$ system, with $\mathrm{N} = 6$. Although the levels are shown equally spaced, this is not a requirement. (b) A $(2, 4)$ system. (c) A generic ladder system, with 6 levels. The "detuning" δ_0 of the lowest level is generally chosen to be zero. Again, the levels need not be equally spaced.

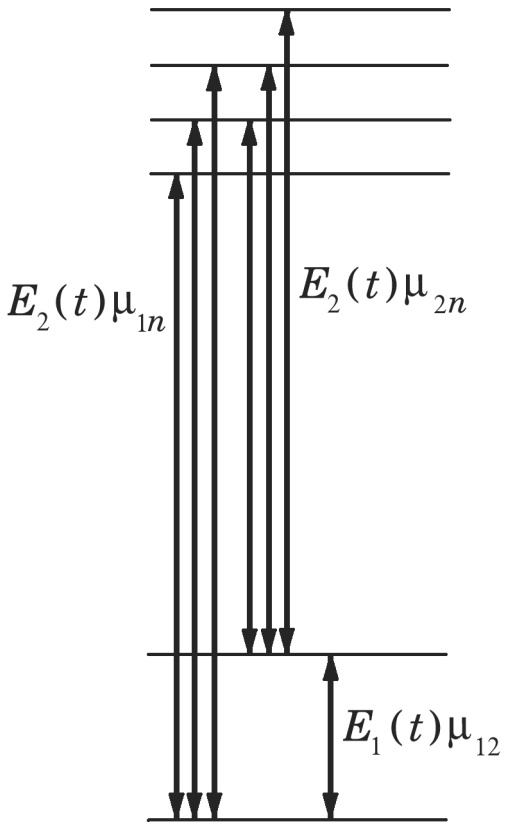

FIGURE 3.2

The (2,4) system of figure (3.1), with an added transition between the two lowest levels, making it a ($\underline{2}$,4) system. Since the separation between these two levels is presumably very different than their separation from the 4-level band, stimulating this transition generally requires a driving field of a different frequency.

perfectly general. An $(\underline{\mathrm{N}})$ system is the most general N-level system. The extension also destroys the notation's uniqueness. A $(1, \mathrm{N}, \mathrm{N}', \mathrm{N}'', \mathrm{N}''', ...)$ system could be expressed as a $(1, \underline{\mathrm{N} + \mathrm{N}' + \mathrm{N}''}, \mathrm{N}''', ...)$ system with equal ease. The latter point will not be too troubling. Ours is a problem of computation, and not of classification. Figure (3.2) illustrates this concept.

3.4. "Continuous Matrix" Notation

The notation "$(1, \mathrm{N})$" implies that the upper band of the $(1, \mathrm{N})$ system consists of a finite number N of discrete energy levels. However, there is no particular reason why N cannot approach infinity. This can happen in two ways. We could end up with an infinite but discrete sequence of levels in the band. We could also end up with a continuous band of levels. Indeed, in Chapters VII and VIII we will insist on having continuous bands. The latter case is described as a "$(1, \mathsf{CONTINUUM})$" system. On the other hand, we call the former a "$(1, \mathsf{DISCRETE})$" system. Some cases arise in which just don't care too much whether the band is continuous, discrete, or even finite. These systems are called "$(1, \mathsf{BAND})$" systems. Other obvious variants will be introduced as needed, without explanation.

Moreover, just as we have $(\mathrm{N}, \mathrm{N}', \mathrm{N}'', ...)$ systems, we might like to have $(\mathrm{N}, \mathrm{N}', \mathsf{CONTINUUM}, \mathrm{N}'', ...)$ systems, or $(\mathsf{CONTINUUM}, \mathrm{N}, \underline{\mathsf{CONTINUUM}}, ...)$ systems, and so forth.

Some extension to normal matrix notation is needed for dealing conveniently with continuous bands. For routine calculations or for description of a model system, it is an unnecessary hardship to write down the various coupled differential equations implied by eq. (3.3) when, for fully discrete systems, we can often summarize most of the interesting transitions in terms of the pictorial appearance of the Hamiltonian matrix. For example, the $(1, \mathrm{N})$ system has a row-column bordering Hamiltonian—that is, it has a single row and column at the "edge" of the matrix governing the transitions. A description like this tells us almost everything we need to know about the structure of the system (for our purposes). Yet there is no similar kind of simple description for continuous systems such as the $(1, \mathsf{CONTINUUM})$ system, which has an identical structure.

In this section, an extension to matrix notation is introduced for the $(1, \mathsf{CONTINUUM})$ system. Higher-order systems can be accommodated as well, but these generalizations will prove too simple to require further comment. Please note that certain dangers are implicit in extending the prevailing matrix notation. Certain results applying only to finite matrices could be plausibly but incorrectly applied to these new continuous matrices. In order to avoid this, for us continuous matrix notation must remain a mere bookkeeping tool—a way of easily writing down and keeping track of operator algebra. We make no further use of it beyond that, and check results independently in dubious cases.

How does continuous matrix notation work? Let's write down a Schrödinger equation and see how we would have to define continuous matrices and continuous matrix multiplication in order to simplify our mathematical manipulations.

Consider a $(1, \mathsf{CONTINUUM})$ system. A discrete band of energy levels is typically indexed by an integer parameter such as n. A continuous band, on the other hand, is indexed by a continuous variable, such as the energy of the level, or the detuning of the

level from some laser frequency. For convenience, we will usually choose as such an index the value appearing along the diagonal of H_0. This value is indeed usually something like the energy or the detuning of the energy level. Discrete values like $\delta_1, \ldots, \delta_N$ appear along the diagonal of H_0 in the discrete $(1, \mathrm{N})$ system. The continuous range of values $-\infty < \Delta < \infty$ or $\Delta_{\min} < \Delta < \Delta_{\max}$ appears along the diagonal of H_0 in a continuous system. The row-column-bordering elements of the dipole matrix μ are denoted by $\mu_1, \ldots, \mu_{\mathrm{N}}$ in the discrete system. Presumably, they would be denoted by something like $\mu(\Delta)$ in the continuous system. Various $(1, \mathsf{CONTINUUM})$ systems are illustrated in figure (3.3) of §3.5.

Schrödinger's equation (3.3) for a $(1, \mathsf{CONTINUUM})$ system thus takes the form

$$\left.\begin{aligned} i\,\frac{d}{dt}\,a(t) &= E(t)\int_{\Delta_{\min}}^{\Delta_{\max}} \mu(\Delta')\,b(\Delta',t)\,d\Delta' \\ i\,\frac{d}{dt}\,b(\Delta,t) &= \Delta\,b(\Delta,t) + E(t)\,\mu(\Delta)\,a(t). \end{aligned}\right\} \tag{3.8}$$

$b(\Delta, t)$ is intended to represent the probability amplitude at time t of the Δth level of the continuous band. For a corresponding discrete system, the equations would read:

$$\left.\begin{aligned} i\,\frac{d}{dt}\,a(t) &= E(t)\sum_{m=1}^{\mathrm{N}} \mu_m\,b_m(t) \\ i\,\frac{d}{dt}\,b_n(t) &= \delta_n\,b_n(t) + E(t)\,\mu_n\,a(t). \end{aligned}\right\} \tag{3.9}$$

In a set of equations like (3.8), one often sees an additional factor $g(\Delta)$ inside the integral.[10] $g(\Delta)$ is a function describing the density of states—*i.e.*, the number of states per unit Δ-interval. This procedure is familiar from statistical mechanics.[11] However, by slightly redefining the quantities $\mu(\Delta)$ and $b(\Delta, t)$ [specifically, by substituting $\mu(\Delta) \to \sqrt{g(\Delta)}\mu(\Delta)$ and $b(\Delta, t) \to \sqrt{g(\Delta)}b(\Delta, t)$], we can assume without any loss of generality that $g(\Delta) = 1$. Hence, omission of this factor does not reduce the generality of the equations in any way.

As pointed out above, these equations are somewhat painful to write down, even though we are so far considering only the simplest case of a continuous system. Moreover, we are required to write down both the discrete and the continuous forms since the notations for the two cases are different. We have already seen the Hamiltonian of eq. (3.9) expressed pictorially as a matrix in eq. (3.5). How might eq. (3.8) be "matricized"? In such a continuous matrix notation, one might index rows of the matrix by Δ, and columns by Δ'. Rather than write out all of the matrix elements, the continuous elements might simply be represented by their functional form. Thus, we might write the state vector $\psi(t)$ of a $(1, \mathsf{CONTINUUM})$ system as

[10] D. Marcuse, *Principles of Quantum Electronics* (Academic Press, New York, 1980), §5.3.
[11] F. Reif, *Fundamentals of Statistical and Termal Physics* (McGraw-Hill, 1974), §9.9.

$$\psi(t) \;=\; \left[\begin{array}{c} a(t) \\ b(\Delta,t) \end{array}\right]. \tag{3.10}$$

Similarly, we might write out the Hamiltonian as

$$H(t) \;=\; \left[\begin{array}{cc} 0 & E(t)\mu(\Delta') \\ E(t)\mu(\Delta) & \Delta\,\delta(\Delta-\Delta') \end{array}\right]. \tag{3.11}$$

The Dirac delta appears in eq. (3.11) because matrix multiplication will involve an integration over Δ. For example, the product of two matrices

$$\left[\begin{array}{cc} a_0 & a_1(\Delta') \\ a_2(\Delta) & a_3(\Delta,\Delta') \end{array}\right] \left[\begin{array}{cc} b_0 & b_1(\Delta') \\ b_2(\Delta) & b_3(\Delta,\Delta') \end{array}\right]$$

would be

$$\left[\begin{array}{cc} a_0b_0+\displaystyle\int a_1(\Delta'')b_2(\Delta'')d\Delta'' & a_0b_1(\Delta')+\displaystyle\int a_1(\Delta'')b_3(\Delta'',\Delta')d\Delta'' \\ a_2(\Delta)b_0+\displaystyle\int a_3(\Delta,\Delta'')b_2(\Delta'')d\Delta'' & a_2(\Delta)b_1(\Delta')+\displaystyle\int a_3(\Delta,\Delta'')b_3(\Delta'',\Delta)d\Delta'' \end{array}\right].$$

This result was arrived at by replacing $\Delta' \to \Delta''$ in the first matrix, $\Delta \to \Delta''$ in the second matrix, performing a normal matrix multiplication, and then integrating over Δ''. It is readily ascertained that this definition of matrix multiplication does indeed produce eq. (3.8) from eqs. (3.10) and (3.11).

A novelty of this notation is that not all elements of these matrices are dimensionally the same. Consider, for example, eq. (3.10). The first element of the vector ψ is $a(t)$, which is a pure number. That is, $a(t)$ has no units. On the other hand, the second element $b(t)$ must dimensionally be $\sqrt{\text{time}}$, since Δ is dimensionally time^{-1} and since

$$1 = \mid a(t) \mid^2 + \int \mid b(\Delta,t) \mid^2 d\Delta$$

While this inconsistency of dimensionality is uncommon in purely matrix operations, it is familiar in other contexts, such as the matrix-like algebra of tensors.[12] Algebraically, we will not find that matrix elements of incompatible dimension inconvenience us, if we simply insure that any matrices or vectors we multiply according to the prescription in the previous paragraph are compatible with each other. That is, in a matrix product like the one illustrated above, each element is a sum of several terms which must have the *same* dimensionality. This will always happen for us. However, if we try to carry out matrix operations not involving matrix multiplication (such as taking the determinant), more care is required to insure dimensional compatibility.

[12] For example, in the spherical polar coordinate system, the r coordinate has dimensions of length, while the θ and φ coordinates are dimensionless. See I. Sokolnikoff, *Tensor Analysis Theory and Applications to Geometry and the Mechanics of Continua*, second edition (Wiley, New York, 1964), Chap. 2.

Allowing "continuous" matrices such as that in eq. (3.11), and keeping in mind the definition of matrix multiplication just advanced, will simplify our discussion considerably. In the $(1, \mathsf{BAND})$ example just discussed, we were able to represent concisely and manipulate infinite-dimensional continuous operators simply by considering their simple "matricized" forms. In more complicated examples, the advantage of this notation is even greater.

The continua we have described here are one-dimensional, in the sense that they are indexed by a single real variable Δ. It is also possible to have multi-dimensional continua, indexed by more than one continuous variable. An example of this is the free particle. A free particle has a continuum of possible states, indexed by the wave-vector $\mathrm{k} = (k_{\mathrm{x}}, k_y, k_{\mathrm{z}})$. All of the methods developed in this paper apply to such systems, but we deal with them only briefly (in §7.7). All continuous bands will have a single index variable throughout the rest of the paper. In any case, as mentioned above such multi-dimensional continua are usually approximated as one-dimensional continua by introducing the density-of-states function $g(\Delta)$, and lumping together all degenerate states.

3.5. Some Commonly Employed $(1, \mathsf{BAND})$ Systems

Let's see some examples of specific $(1, \mathsf{BAND})$ systems. These systems appear in the literature as model systems, and in the remainder of this paper as illustrative examples. We are not, however, interested merely in conducting exhaustive calculations on the systems mentioned below, and will not do so.

$(1, \mathsf{BAND})$ systems are characterized by their *bandshape*. The bandshape is the functional form of $\mu(\Delta)$ or μ_n. [See eq. (3.11).] With one exception, all of the systems outlined in this section will have symmetric bandshapes. That is, they will be symmetric about some particular value of their indexing quantities Δ or δ_n. We'll call this center point s. The symmetry is not a condition for the results that will be derived later, but is mere happenstance. The bands have some characteristic band width, called σ. That is, the non-small matrix elements are confined to the range $s - \sigma < \Delta < s + \sigma$ or to the range $s - \sigma < \delta_n < s + \sigma$. Additionally, there is some overall normalization factor, which we will call γ. The normalization factor will be defined by

$$\gamma^2 = \int \mu(\Delta)^2 d\Delta. \tag{3.12}$$

(Or by the discrete equivalent of this formula.) This normalization is not what would be natural from, for example, Fermi's Golden Rule (Ref. 1, §18.8), but will nevertheless prove useful. [From Fermi's Golden Rule, it would be natural to accept the normalization $\gamma = \mu(0)$.]

The *Uniform Rectangular Band* is probably the simplest continuous band shape to understand. It has the following functional form:

$$\mu(\Delta)^2 \;=\; \begin{cases} \dfrac{\gamma^2}{2\sigma} & ,\mid \Delta - s \mid < \sigma \\ 0 & ,\mid \Delta - s \mid \geq \sigma \end{cases}. \tag{3.13}$$

Numerous authors (see Chap. II) have employed a form of the rectangular band which is unlimited (*i.e.*, $\sigma \to \infty$), calling it the *Broad Featureless Continuum*. When we have occasion to consider this case we will let $\mu(\Delta) \equiv \gamma$, since the broad featureless continuum is not normalizable by integration.

The *Discrete Lorentzian Band* has infinitely many discrete energy levels, with the detunings

$$\delta_n = s + n\,\omega. \tag{3.14}$$

ω is the (equal) spacing between the energy levels. In addition, the dipole matrix elements (given in terms of their squares) are

$$\mu_n^2 = \frac{\gamma^2\,\dfrac{\sigma\omega}{\pi}}{n^2\omega^2 + \sigma^2}\,\tanh\left(\frac{\sigma}{\omega}\right). \tag{3.15}$$

(Notice that almost all of the complexity of this expression is due to the normalization.) In this case, the band is not confined to the interval $\delta_n \in [s-\sigma, s+\sigma]$, but simply has its largest matrix elements here. The Discrete Lorentzian band has appeared notably in Makarov *et al*.[13]

The *Continuous Lorentzian Band* is the limit of the discrete Lorentzian in case $\frac{\omega}{\sigma} \to 0$. It is the continuous analog of discrete Lorentzian. Both the $(1, \mathsf{CONTINUOUS\,LORENTZIAN})$ and the $(1, \mathsf{DISCRETE\,LORENTZIAN})$ systems can be solved fairly completely. Together they give some idea of the differences between the true continuum and the so-called quasi-continuum, consisting of a large number of densely packed discrete states.[14] For $\mu(\Delta)$ we have simply

$$\mu(\Delta)^2 = \frac{\gamma^2\,\dfrac{\sigma}{\pi}}{(\Delta - s)^2 + \sigma^2}\,. \tag{3.16}$$

Note that the center detuning s is absent in eq. (3.15). This is a consequence of our indexing discrete levels by n and continuous levels by Δ. We will find that this continuous Lorentzian bandshape has a significance that transcends its use in simple analytical calculations. Note, however, that Lorentzian (Ref. 9) spectral lineshapes have to do with spontaneous emission. Spectral lineshapes are not immediately relevant to our discussion. Similarly, Doppler-broadened lineshapes are not to be analyzed by introducing a Gaussian bandshape.[15]

The *Rational Band* is a valuable generalization of the Continuous Lorentzian. In this case, $\mu(\Delta)^2$ is a rational function: a ratio of two polynomials:

$$\mu(\Delta)^2 = \gamma^2\,\frac{p(\Delta)}{q(\Delta)}\,. \tag{3.17}$$

[13] A. Makarov, V. Platonenko, and V. Tyakht, *Sov. Phys. JETP* **48(6)**, 1044 (1978).
[14] See the review by N. Bloembergen, C. D. Cantrell, and D. Larsen, in *Tunable Lasers and Applications*, ed. by A. Mooradian, T. Jaeger, and P. Stokseth (Springer, Heidelberg, 1976).
[15] *Ibid.*, §5.5.

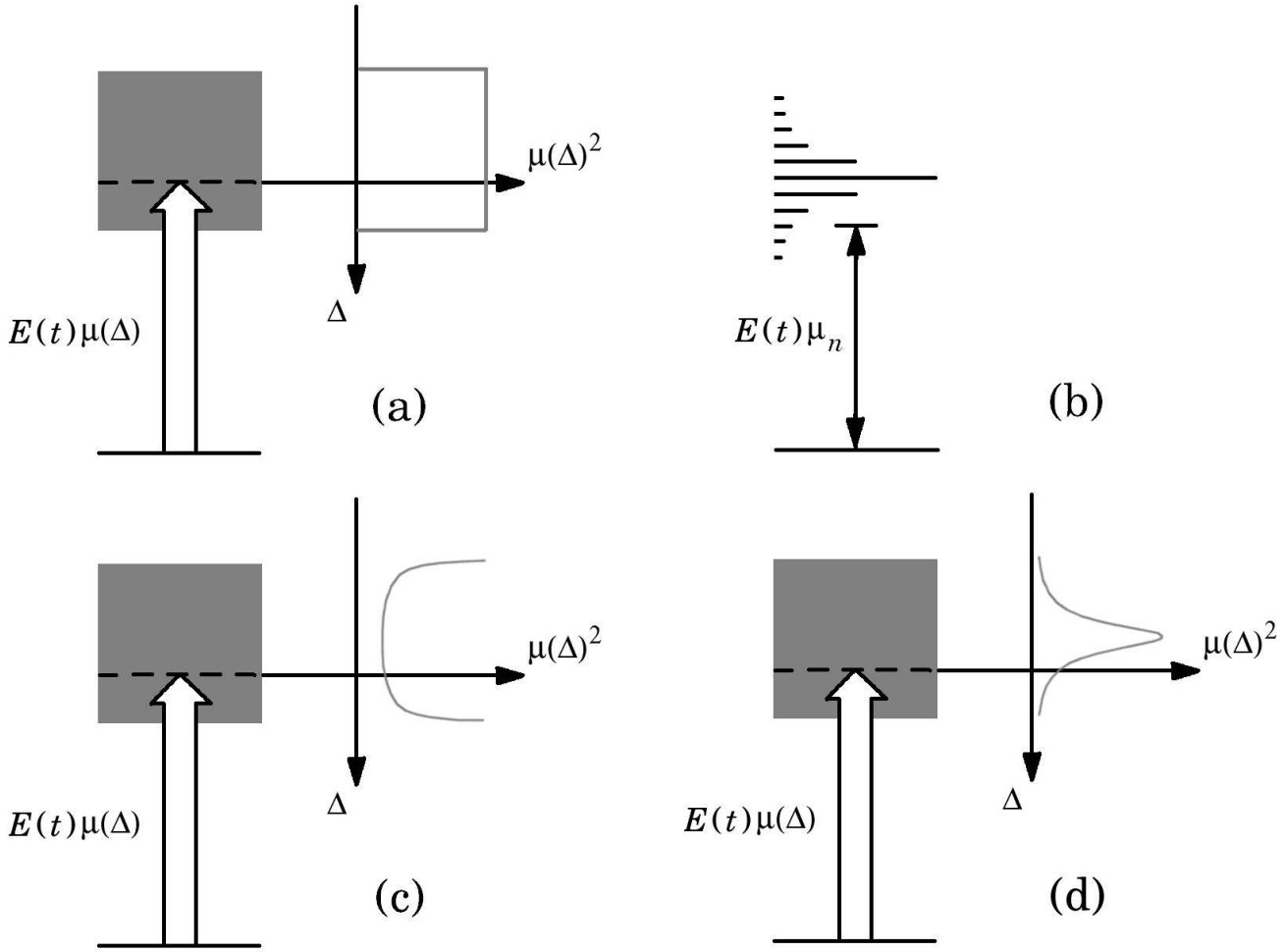

FIGURE 3.3

(a) The $(1, \text{UNIFORM BAND})$ system. (b) The $(1, \text{DISCRETE LORENTZIAN})$ system. (c) The $(1, \text{CHEBYCHEV 1ST KIND})$ system. (d) The $(1, \text{CONTINUOUS LORENTZIAN})$ system.

The polynomials $p(\Delta)$ and $q(\Delta)$ are constrained in some obvious ways by the problem at hand. For example, for a real system (with a Hermitian Hamiltonian) we need to require that both $p(\Delta)$ and $q(\Delta)$ be real polynomials, with the degree of $q(\Delta)$ at least 2 greater than the degree of $p(\Delta)$. In Chapter V, we will need the additional requirement that $\mu(\Delta)^2$ has only simple poles—or equivalently that $q(\Delta)$ has no repeated roots. Rational bands are interesting not merely in that we will find something to do with them. More than that, we can use them to approximate many other bandshapes.[16]

The *Chebychev Band* is of great significance in understanding the behaviors of continua in general,[17] but is relatively (if not entirely) unknown. The Chebychev bandshape

[16] W. Press, B. Flannery, S. Teukolsky, and W. Vetterling, *Numerical Recipes: The Art of Scientific Computing* (Cambridge University Press, Cambridge, 1986), §3.2.
[17] R. S. Burkey and C. D. Cantrell, *J. Opt. Soc. Am. B* **2**, 451 (1985).

is continuous. It is like the uniform rectangular band, but unlike the Lorentzian bands, in that it is strictly limited to the interval $\Delta \in [s-\sigma, s+\sigma]$. Its functional form is

$$\mu(\Delta)^2 = \frac{\gamma^2}{\pi\sigma}\left(1 - \frac{(\Delta - s)^2}{\sigma^2}\right)^{-\frac{1}{2}}. \tag{3.18}$$

This happens to be the weight function for Chebychev polynomials of the first kind, with a somewhat modified normalization, and over a somewhat different interval than usual.[18] Weight functions for other sets of orthogonal polynomials are sometimes interesting when used as bandshapes. None prove to have the fundamental importance of expression (3.18). Note that $\mu(\Delta)^2$ becomes singular at the points $\Delta = s \pm \sigma$. Another bandshape that we will have cause to consider is related to the weight function for Chebychev polynomials of the *second* kind:

$$\mu(\Delta)^2 = \frac{2\gamma^2}{\pi\sigma}\left(1 - \frac{(\Delta - s)^2}{\sigma^2}\right)^{\frac{1}{2}}. \tag{3.18'}$$

Unlike the other Chebychev bandshape (but like the continuous Lorentzian), this band has its maximum matrix elements at the center and goes to zero at the edges.

Several of these bandshapes shown in figure (3.3).

3.6. Some Simple Factorizations

Recall that our primary concern below will be with systems whose dipole matrix μ is of low rank M. Obviously, cases will arise in which μ is not of low rank, but in which we wish to approximate it as being of low rank. In later chapters, we'll see (for continua, at least) approximations that are highly accurate. For the purposes of exposition, on the other hand, we'll sometimes be more concerned with getting a simple, reasonable approximation. Therefore, let's look at some simple low-rank approximations.

Several such approximations are worth collecting here. All deal with continuum-continuum transitions. Such transitions, say between the Δth and Δ'th level, are governed by dipole matrix elements of the form $\mu(\Delta, \Delta')$. In order for the matrix μ to have a low rank, this function will have to be approximated as a finite sum of products of functions (of a single variable) of Δ and of Δ'. We'll assume that it is highly desirable to make this approximation accurate in the neighborhood of $\Delta = 0$ and $\Delta' = 0$. This is reasonable if Δ and Δ' represent detunings, since the point $\Delta = 0$ then represents resonance with transitions from discrete states outside of the continuum. Most of the population should bunch up there. With one exception (presented in Chapter IV), we'll therefore insist that any simple approximations to be introduced be exact for $\mu(\Delta, 0)$ and $\mu(0, \Delta')$. There are two essentially different cases to be considered:

Inter-Band Transitions. The simpler case is if $\mu(\Delta, \Delta')$ represents a transition from the Δth level of one band to the Δ'th level of a different band. If so, $\mu(\Delta, \Delta')$ has no special properties to be accounted for. In particular, there is no special reason to fear that

[18] U. Hochstrasser in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and A. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), Chap. 22.

$\mu(0,0)$ vanishes. If we can assume that $\mu(0,0)$ is non-zero, a very simple approximation is available:

$$\mu(\Delta,\Delta') \approx \frac{\mu(\Delta,0)\mu(0,\Delta')}{\mu(0,0)}. \tag{3.19}$$

Verifying that eq. (3.19) is exact for $\mu(\Delta,0)$ and $\mu(0,\Delta')$ is trivial. Eq. (3.19) represents a rank 2 approximation for this set of transitions. (*I.e.*, the matrix μ would have rank 2 in this approximation, if we did not have to account for transitions in the system other than those connecting these two bands.) The simple approximation to be presented in Chapter IV is also of rank 2, but departs from the conditions we have set. Instead, it will be accurate in the *neighborhoods* $\Delta \approx \Delta'$ for all Δ.

If $\mu(0,0)$ just happens to be zero, the alternate approximation

$$\mu(\Delta,\Delta') \approx \mu(\Delta,0)\iota(\Delta') + \iota(\Delta)\mu(0,\Delta'). \tag{3.20}$$

can be employed. Here, $\iota(\Delta)$ is intended to be a function which is identically unity. Eq. (3.20) is an approximation of rank 4.

Intra-band transitions. If $\mu(\Delta,\Delta')$ refers to transitions between the Δth and Δ'th levels of the same band, slightly more work is involved. For one thing, because of Hermiticity the condition

$$\mu(\Delta,\Delta') = \mu(\Delta',\Delta)^\star \tag{3.21}$$

must be obeyed. For another, we would often require that

$$\mu(\Delta,\Delta) \equiv 0. \tag{3.22}$$

At first sight, the latter condition seems difficult to accommodate. Actually, it is not so difficult. Note first that, without loss of generality, we can assume that $\mu(\Delta,0)$ and $\mu(0,\Delta')$ are both real and non-negative, and consequently that $\mu(\Delta,0) = \mu(0,\Delta)$. (We can always assure this with similarity transformations if μ is Hermitian.) Consider the following expression:

$$\mu(\Delta,\Delta') \approx \mu(\Delta,0)\iota(\Delta') + \iota(\Delta)\mu(0,\Delta') - 2\sqrt{\mu(\Delta,0)\mu(0,\Delta')}. \tag{3.23}$$

Eq. (3.23) clearly satisfies all of the conditions we've imposed. If it happens that $\mu(\Delta,\Delta')$ is not Hermitian (being, say, part of an effective Hamiltonian with damping or coupling to a reservoir), then eq. (3.23) can still be employed. However, in such a case eq. (3.22) is probably also unnecessary, and eq. (3.20) is perhaps a more reasonable approximation. As it stands, eq. (3.23) is an approximation of rank 3.

Eq. (3.23) is globally exact for the function

$$\mu(\Delta,\Delta') = \alpha\,(\Delta-\Delta')^2.$$

with α some constant. This is significant in that it implies that functions of the form $\mu(\Delta-\Delta')$ can have low rank. Actually, one can show that any function $\mu(\Delta,\Delta')$ satisfying eqs. (3.21) and (3.22) is of the form $\mu(\Delta-\Delta') = \alpha\,(\Delta-\Delta')^2 + \mathrm{O}(\Delta^4, \Delta^3\Delta', ..., \Delta'^4)$. Hence, we can conclude that eq. (3.23) matches also all partial derivatives of up to third order of

$\mu(\Delta, \Delta')$ in the neighborhood of $\Delta \approx \Delta'$ (for all Δ). Consequently, we expect approximation (3.23) to be very good indeed for nearly resonant transitions.

Of course, if the requirement $\mu(\Delta, \Delta) \equiv 0$ is not needed, then we can consider lower-rank alternative approximations. The simplest reasonable approximation in the neighborhood of $\Delta = 0,\ \Delta' = 0$ is eq. (3.19), which has a rank of 1.

Let's just briefly verify that the assertions about the "ranks" of these approximations are correct. Consider a $(1, \underline{\mathsf{CONTINUUM}})$ system with the Hamiltonian

$$H(t) = \begin{bmatrix} 0 & E(t)\mu(\Delta') \\ E(t)\mu(\Delta) & \Delta\,\delta(\Delta - \Delta') + E(t)\mu(\Delta, \Delta') \end{bmatrix}. \tag{3.24}$$

[Compare eq. (3.11).] The function $\mu(\Delta, \Delta')$, governing transitions within the continuum, is not to be confused with $\mu(\Delta)$, governing transitions between the ground state and the continuum. Then

$$\mu = \begin{bmatrix} 0 & \mu(\Delta') \\ \mu(\Delta) & \mu(\Delta, \Delta') \end{bmatrix}. \tag{3.25}$$

Supposing we applied the simplest possible approximation, namely eq. (3.19), how could we express μ as a finite sum of outer products of vectors? Well, if we introduced the vectors

$$e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix},\ e_2 = \begin{bmatrix} 0 \\ \mu(\Delta) \end{bmatrix},\ e_3 = \begin{bmatrix} 0 \\ \mu(\Delta, 0) \end{bmatrix}, \tag{3.26}$$

then we could write (non-uniquely)

$$\mu \approx e_1\, e_2^\dagger + e_2\, e_1^\dagger + \frac{e_3\, e_3^\dagger}{\mu(0,0)}, \tag{3.27}$$

so long as we accepted the notion that the Hermitian conjugate operator $\dagger$ can convert $\Delta \to \Delta'$ and $\Delta' \to \Delta$. (Since the Hermitian conjugate takes the matrix transpose, and since Δ and Δ' are used for row and column indices respectively, this conversion of Δ to Δ' should be fairly obvious.) Since there are three terms in the sum, the approximated μ is clearly of rank 3. Of course, the $(1, \mathsf{CONTINUUM})$ system already has driver-rank 2, so the additional rank introduced by the approximate intra-continuum coupling is only 1, as stated earlier.

If we had employed the approximation (3.23) rather than (3.19), we would need a couple of additional vectors:

$$e_4 = \begin{bmatrix} 0 \\ \iota(\Delta) \end{bmatrix},\ e_5 = \begin{bmatrix} 0 \\ \sqrt{\mu(\Delta, 0)} \end{bmatrix}. \tag{3.28}$$

Then we could write

$$\mu \approx e_1\, e_2^\dagger + e_2\, e_1^\dagger + e_3\, e_4^\dagger + e_4\, e_3^\dagger - 2e_5\, e_5^\dagger. \tag{3.29}$$

Since this sum has five outer-product terms, μ has a total rank of 5, which is 3 more than that of the μ for a $(1, \mathsf{CONTINUUM})$ system alone.

3.7. The Rotating-Wave Approximation (RWA)

The Rotating-Wave Approximation (RWA) has no necessary rôle in our investigation, but will nevertheless be mentioned rather often. Since the RWA is more familiar in the field of Quantum Optics than in physics generally, we will give a very short description of it here. In order to make the discussion look more familiar, we will explicitly retain all the usual constants (like $\hbar$) and algebraic signs.

Basically, the RWA is a way to remove certain contributions (due to very rapidly varying driving terms) from Schrödinger's equation. (See the review in Chap. II for conditions of validity of the RWA.) Consider, for example, a two-level system driven by a quasi-monochromatic optical laser field: [19]

$$i\hbar \frac{d}{dt} \begin{bmatrix} a(t) \\ b(t) \end{bmatrix} = \begin{bmatrix} 0 & -E_0(t)\cos(\omega t)\mu_{01} \\ -E_0(t)\cos(\omega t)\mu_{10} & \varepsilon \end{bmatrix} \begin{bmatrix} a(t) \\ b(t) \end{bmatrix}. \tag{3.30}$$

Here, the laser field is supposed to be approximately resonant with the transition—*i.e.*, $\varepsilon \approx \hbar\omega$. Also, $E_0(t)$ is supposed to be some slowly varying (compared to the optical frequency ω) envelope of the laser field. Eq. (3.30) implies a Hamiltonian of the form required by eq. (3.3), but with a problem. The problem is this: the vast difference in time scales in eq. (3.30) between the behavior of $E_0(t)$ and the behavior of $\cos(\omega t)$ makes eq. (3.30) very difficult to solve (particularly numerically). We need some way to specially account for that part of the state vector varying at an optical frequency.

The Rotating-Wave Approximation proceeds to do this as follows: first, instead of using the probability amplitude $b(t)$ of the second level as shown above, introduce a modified probability amplitude of the form

$$b(t) = \widetilde{b}(t)e^{-i\omega t}. \tag{3.31}$$

This results in the Schrödinger equation

$$i\hbar \frac{d}{dt} \begin{bmatrix} a(t) \\ \widetilde{b}(t) \end{bmatrix} = \begin{bmatrix} 0 & -E_0(t)\mu_{01}\dfrac{1+e^{-2i\omega t}}{2} \\ -E_0(t)\mu_{10}\dfrac{1+e^{2i\omega t}}{2} & \varepsilon - \hbar\omega \end{bmatrix} \begin{bmatrix} a(t) \\ \widetilde{b}(t) \end{bmatrix}. \tag{3.32}$$

In eq. (3.30), the element ε in the Hamiltonian is so large the it dominates all of the other matrix elements. In eq. (3.32), ε has been removed, and only much smaller matrix elements remain. Therefore, we expect this new state-vector to vary much less rapidly than $e^{-i\omega t}$. Consequently, when eq. (3.32) is integrated, the contributions to the state vector due to the rapidly varying exponentials $e^{2i\omega t}$ and $e^{-2i\omega t}$ will tend very strongly to zero. We may as well remove them from the equation, leaving just

$$i\hbar \frac{d}{dt} \begin{bmatrix} a(t) \\ \widetilde{b}(t) \end{bmatrix} \approx \begin{bmatrix} 0 & -E_0(t)\dfrac{\mu_{01}}{2} \\ -E_0(t)\dfrac{\mu_{10}}{2} & \varepsilon - \hbar\omega \end{bmatrix} \begin{bmatrix} a(t) \\ \widetilde{b}(t) \end{bmatrix}. \tag{3.33}$$

Approximations of this kind are collectively known as the Rotating-Wave Approximation. As expected, eq. (3.33) is once again of the form dictated by eq. (3.3). As mentioned, the

[19] L. Allen and J. Eberly, *Optical Resonance and Two-Level Atoms* (Wiley, New York, 1975).

techniques to be developed in the succeeding chapters depend only on this form, and not (in principle) on numerical or scale differences like those between eq. (3.30) and eq. (3.33).

CHAPTER IV
SYSTEMS WITH CONSTANT DRIVING

4.1. Introduction

Consider Schrödinger's equation (3.3). Though our main interest will generally be the case of a time-varying Hamiltonian, we will begin our results with a chapter concerning the more usual case of a time-independent Hamiltonian. In the notation of eq. (3.3), we will assume that $E(t)$ is constant in time:

$$H = H_0 + E\mu. \tag{4.1}$$

(Recall that E represents the electric field, and not the energy.)

At least four different types of constant-field problems are of general interest. These are:

Sudden-switching problems. Here, the driving field E has just two possible values. It flip-flops between these values instantaneously. However, the techniques for solving these problems are essentially identical to those used if E were constant for all time. Before time $t = 0$, the field is "off". After time $t = 0$, the field is "on". The "off" value of the field is $E = 0$. The "on" value is anything you like. Typically, the system is taken to be initially in an eigenstate. When the field flips on, the eigenstates of the system are no longer the same, and the new eigenstates are superpositions of the old ones. Population is scattered into the various new eigenstates. Tracking the population may be done by explicitly computing the eigenstates (perhaps by perturbation theory[1]), by computing the time-development operator e^{-iHt} (see review in Chap. II), or by other means. Unfortunately, this is done conveniently only for discrete (indeed, finite) systems. For a system with continuous bands of levels, other approaches must be employed.

Adiabatic-following problems. Here, the driving field E is allowed to vary in time. However, $E(t)$ must vary very slowly in comparison to other characteristic times scales in the problem. This is just the opposite of the sudden-switching case. Once again, we assume that the system is initially in an eigenstate. Again, as $E(t)$ changes, the eigenstates change. Unlike the sudden-switching case, the old eigenstates change smoothly (and con-

[1] L. Landau and E. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)*, third ed. (Pergamon, Oxford, 1977), Ch. VI.

tinuously) into the new ones. Moreover, in some sense the population is not scattered: It can be shown that the system always stays in the driven eigenstate that evolves smoothly from the initial state.[2] We say that the system stays in the eigenstate "correlated" with the initial eigenstate. The "adiabaticity" comes from the fact that the time-evolution is reversible. If the field is returned slowly to its original value, the system returns to its original state. As with sudden switching, this technique is usually applied only with finite systems, although there have been exceptions.[3] Again, constant-field techniques are used to solve for the eigenvalues and eigenvectors.

Decay problems are similar to sudden-switching problems, except that the number of energy levels is very large. In such a case, populations of isolated states appear to decay exponentially. For a discrete system, the appearance is illusory. After a certain (long) time, the populations build up again. This characteristic time is called the system's *recurrence time*. The re-buildup of population itself is called a *recurrence*.[4] For a continuous system, the decay can be real. In a $(1, \mathrm{CONTINUUM})$ system, for example, the continuous band typically absorbs all of the ground state population. The population is never returned so, in a sense, the ground state population "decays".[5] (See Chapter VIII, however, in which it is shown that this does not happen in all cases.) In this "decay", there is no loss of energy from the system as there would be in a true decay process such as spontaneous emission. For the most part, eigenvalue-eigenvector approaches cannot be used to analyze this. Three other approaches are commonly used. (See the review in Chap. II.) First, analytic approximations are very commonly used to estimate ground-state decay rates. These analytic approximations include Fermi's Golden Rule (in which the ground-state population decay rate is estimated) and the Weisskopf-Wigner approximation (in which the ground-state probability amplitude itself is estimated). The latter includes the former as a special case. A second common approach is to calculate probability amplitudes *via* the Laplace transform. Even if the Laplace transform of the ground-state probability amplitude can be found, the inverse-transform problem is relatively difficult. Consequently, the Laplace transform is sometimes used to estimate decay rates, rather than to compute an exact solution. The third common approach is just to eliminate the multitude of inconvenient energy levels. This is done by introducing an "effective" non-Hermitian Hamiltonian with built-in damping. Sometimes this is thought of as coupling the system to a reservoir.

Spectrum problems. These problems, of course, explicitly require finding the eigenvalues of the Hamiltonian.

The discussion above might be summarized as follows. If we would like to use the traditional methods of investigating constant-field driving, it is good to be able to:

- Calculate eigenvalues and eigenvectors.
- Calculate (and invert) Laplace Transforms.

[2] A. Messiah, *Quantum Mechanics*, trans. by G. Temmer (Wiley, New York, 1958), Ch. XVII, part II.
[3] J. Eberly, J. Yeh, and C. Bowden, *Chem. Phys. Lett.* **86**, 76 (1982).
[4] M. Quack, *J. Chem. Phys.* **69**, 1282 (1978); also, the preceding and the following reference.
[5] A. A. Makarov, V. T. Platonenko, and V. V. Tyakht, *Zh. Eksp. Teor. Fiz.* **75**, 2075-2091 (1978) [*Sov. Phys. JETP* **48**, 1044-1051 (1978)][1].

- Find appropriate generalized Weisskopf-Wigner and Golden Rule approximations.
- Find reasonable ways of producing non-Hermitian reservoir coupling.
- Compute the time development operator $U = e^{-iHt}$.

In fact, the low-driver-rank assumption aids every one of these activities except the inversion of Laplace transforms and (as far as we know) the computation of the time-development operator. The calculation of eigenvalues and eigenvectors is briefly discussed in §4.2. Laplace transforms are covered extensively in §4.3 *et seq*. Generalized Weisskopf-Wigner and Golden Rule approximations, as well as reservoir coupling, are also dealt with extensively in Chapter V, in the context of a time-varying $H(t)$.

The assumptions we will need in this chapter are quite simple. First, the operator $(\lambda - H_0)^{-1}$ (often called the *resolvent*) must exist and must be known analytically for any given scalar λ not an eigenvalue of H_0. This is clearly true if, for example, the operator H_0 has a convenient diagonal matrix representation. Second, the operator H_0 must be of low rank M. Third, we will suppose that the underlying vector space is Hilbert space and consequently that all vectors can be normalized.

The second assumption implies that μ has a known factorization as

$$\mu = D\,F, \tag{4.2}$$

where F is an operator mapping the Hilbert space of the system onto some space of small dimension M, and D is an operator from this small space back to the full Hilbert space. Though expressible in terms of projection operators, D and F are not themselves projection operators. In matrix terms, F has row-dimension M and D has column dimension M. In saying that D and F are "known" quantities (which is not obvious for a realistic Hamiltonian), we are simply acknowledging the fact that D and F can normally be obtained by inspection from μ when dealing with simple analytical models.

4.2. Eigenvalues and Eigenvectors

In an eigenvector/eigenvalue calculation, we are interested in finding scalars λ and associated vectors ψ_λ such that

$$H(E)\,\psi_\lambda(E) = \lambda(E)\,\psi_\lambda(E). \tag{4.3}$$

Since the Hamiltonian operator is supposed to depend parametrically on the quantity E, both λ and ψ_λ must also depend parametrically on E, as shown. Recall that E represents the electric field; the eigenvalue λ then represents an energy. The difficulty with a calculation of this kind, of course, is that the effort required to diagonalize the H operator tends to rise dramatically as the number of energy levels goes up. Consequently, we would like some method of drastically reducing the dimensionality of the problem.

Substituting from eqs. (4.1) and (4.2) and rearranging gives

$$\psi_\lambda(E) = E\,\left(\lambda - H_0\right)^{-1} D\,\phi_E(\lambda), \tag{4.4}$$

where we have defined

$$\phi_E(\lambda) = F\,\psi_\lambda(E). \tag{4.5}$$

The purpose of defining the quantity $\phi_E(\lambda)$ is that it is an M-dimensional vector (where M is much smaller than the number of levels in the system), and yet can be used according to eq. (4.4) to generate the full eigenvector set. All we need is a method for calculating $\phi_E(\lambda)$. This is easily accomplished by multiplying eq. (4.4) by F, which gives:

$$\phi_E(\lambda) = E(\lambda)\,K(\lambda)\,\phi_E(\lambda), \tag{4.6}$$

where we define

$$K(\lambda) = F\ (\lambda - H_0)^{-1}\,D. \tag{4.7}$$

Since by hypothesis the values of D, F, and $(\lambda - H_0)^{-1}$ are known, the $\mathrm{M} \times \mathrm{M}$ matrix $K(\lambda)$ is also known. Note that the electric field E (normally a given parameter) has somehow gained a functional dependence on λ. This is discussed below.

Eq. (4.6) is quite interesting. Notice that it is mathmatically an eigenequation for the M-dimensional matrix $K(\lambda)$. The eigenvalues are given by $\frac{1}{E(\lambda)}$, while the associated eigenvectors are given by $\phi_E(\lambda)$. Since we have already seen that $\phi_E(\lambda)$ can be used to compute $\psi_\lambda(E)$ in a straightforward way using eq. (4.4), and since $\phi_E(\lambda)$ itself can be computed "easily" by diagonalizing the $\mathrm{M} \times \mathrm{M}$ matrix $K(\lambda)$, this is the desired simplification of the problem.

The original eigenvalue problem, which was given by eq. (4.3) and was of possibly very high dimension, has been converted to an eigenvalue problem of small dimension. Admittedly, the matrix to be diagonalized in eq. (4.3) was Hermitian, while $K(\lambda)$ is non-Hermitian. This is only a slight complication and, if $M \leq 4$, we are actually guaranteed that the entire problem can be solved *analytically*—for the characteristic polynomial of the matrix $K(\lambda)$ is then at most a quartic, and quartic polynomials can be solved in closed form.[6] Incidentally, though $K(\lambda)$ is non-Hermitian, the characteristic polynomial of $K(\lambda)$ [whose roots are $\frac{1}{E(\lambda)}$] has entirely real coefficients. This fact is demonstrated in Appendix A.

However, there is an odd side-effect of the reduction of dimension in this problem. Note that in moving from eq. (4.3) to eq. (4.6) the quantities E (the electric field) and λ (the energy) have in some sense changed rôles. Physically, E represents an external parameter, perhaps adjustable by the experimenter while $\lambda(E)$ is the resulting energy, *usually* computed as an eigenvalue of the Hamiltonian matrix. In the reduced eigenvalue equation (4.6), on the other hand, λ now mathematically takes on the appearance of an adjustable parameter, while $\frac{1}{E(\lambda)}$ is the resulting eigenvalue. Thus, the result of any such calculation must be knowledge of the electric field $E(\lambda)$ rather than the energy $\lambda(E)$.

[6] The analytic formula for the roots of a quartic polynomial can be found in *CRC Standard Mathematical Tables*, 22nd Edition, edited by Samual M. Selby, (Cleveland, Ohio, CRC Press, 1974), pp. 103-106. A demonstration of the impossibility of general analytic solution by radicals for higher-degree polynomials can be found in I. Herstein, *Topics in Algebra* (Lexington, Massachusetts, Xerox College Publishing, 1975), pp. 250-256.

Whether this is aproblem depends largely on the application. Of course all characteristic equations are implicit relations defining the eigenvalues; their advantage is not that they are explicit but rather that they are single equations instead of coupled sets of equations like eq. (4.3).

Here is a brief list of possible applications:

Quantitative Results. The intuitive implications of eq. (4.6) are unlike those of eq. (4.3). Thus eq. (4.6) can provide odd insights into system behavior. We'll see an example of this in §4.6.1.

Drawing Energy Level Diagrams. These are plots of $\lambda(E)$ *vs.* E. Except in regions of avoided crossings (in which two eigenvalue curves approach each other closely), it is just as easy for a computer to plot λ *vs.* $E(\lambda)$. (From a computer programmer's standpoint, the only difference is that more care needs to be taken in the vicinity of avoided crossings.)

Finding Just One Eigenvalue/Eigenvector. The normal eigenvalue approach (diagonalizing the Hamiltonian) computes all eigenvalues and eigenvectors simultaneously. This is efficient if all that information is truly needed. If not, it is very wasteful of computer resources. Eq. (4.6) computes just one eigenvalue/eigenvector (at M different field values). The only problem is that one cannot simply choose the desired E-value. Therefore, a computer approach to computing the eigenvalues needs to allow some "hunting" for the proper value of the electric field. Even so, eq. (4.6) is more efficient than diagonalization of the true Hamiltonian at finding a single eigenvalue.

Tracking an Eigenvalue/Eigenvector. In this case, a single eigenvector/eigenvalue is tracked as the electric field E is changed. This happens, for example, in the Adiabatic approximation. This is efficient for reasons similar to those given in the previous paragraph.

Measuring the Electric Field. Normal spectroscopic experiments involve measuring the spectral lines (λ) under known external conditions (E). The object of this is to compare measured spectral positions with theoretical ones. One can, however, imagine experiments in which the spectral lines are instead measured in order to determine the (unknown) intensity of the electric field. This, of course, is precisely the information eq. (4.6) provides.

While our concern in this chapter is mainly with analytical methods for investigating simple model systems, note that eq. (4.6) could also be potentially useful for large-scale numerical processing in a more realistic system. The $\mu = DF$ decomposition for a realistic system could not be known *a priori*. In fact, μ would probably be non-singular. However, an approximate decomposition could be determined numerically, for example, by a Singular Value Decomposition.[7] This is approximately as time-consuming as a single normal eigenvalue evaluation, but would only have to be performed once. Of course, we have not yet actually applied low driver-rank techniques in this way.

[7] G. E. Forsythe, M. A. Malcolm, C. B. Moler, *Computer Methods for Mathematical Computations*, (Englewood Cliffs, NJ, Prentice-Hall, 1977), Chap. 9.

4.3. Laplace Transforms

A similar reduction to M dimensions can be accomplished for Laplace-transform problems. In such problems we are interested in solving the Schrödinger equation with an initial condition:

$$i\,\frac{d}{dt}\,\psi(t) = H\,\psi(t), \tag{4.8a}$$

$$\psi(0) = \psi_0. \tag{4.8b}$$

In order to solve this system of equations using the Laplace transform, two steps are necessary. First, one must be able to compute the Laplace transform $\widetilde{\psi}(s)$ and second, one must then be able to invert the transformed function to get $\psi(t)$. While we have little advice to offer on the latter, the former yields to analysis in the case of low-rank driving.

The Laplace transform of eq. (4.8a) is

$$i\left(s\,\widetilde{\psi}(s) - \psi_0\right) = H\,\widetilde{\psi}(s). \tag{4.8}$$

The difficulty of a problem of this type, of course, is that solving eq. (4.8) in a straightforward way involves inverting the high-dimensional matrix $i\,s - H$, which is generally tricky. It is better to proceed indirectly. Substituting from eqs. (4.1) and (4.2), and rearranging, we find

$$\widetilde{\psi}(s) = E\;(i\,s - H_0)^{-1}\,D\,\widetilde{\phi}(s) + i\;(i\,s - H_0)^{-1}\,\psi_0\,. \tag{4.9}$$

Here, $\phi(t)$ is as defined in eq. (4.5): $\phi = F\psi$. If we had some way of computing $\widetilde{\phi}(s)$, we could find $\widetilde{\psi}(s)$ itself using eq. (4.9). How then to compute $\widetilde{\phi}(s)$? Multiplying eq. (4.9) by F and rearranging,

$$\widetilde{\phi}(s) = i\;(I - E\,K(i\,s))^{-1}\,F\;(i\,s - H_0)^{-1}\,\psi_0. \tag{4.10}$$

Here, I is the M-dimensional identity operator.

Eq. (4.10) is the desired result. Since $I - EK(i\,s)$ is an M-dimensional matrix (where M is assumed be very small), eq. (4.10) is easy to compute, even if the number of energy levels in the system is infinite, or if there are continuous bands of energy levels.

Though it may not be obvious from the definition of $\phi(t)$, the elements of the ϕ-vector are generally the probability amplitudes of the discrete levels in the system, along with other quantities having to do with the presence of continuous bands. Thus, any discrete probability amplitudes can generally be deduced by inspection from eq. (4.10). If not, then the full state-vector must be generated by means of eq. (4.9), giving

$$\widetilde{\psi}(s) = i\,\left(I + E\;(i\,s - H_0)^{-1}\,D\;(I - E\,K(i\,s))^{-1}\,F\right)(i\,s - H_0)^{-1}\,\psi_0. \tag{4.11}$$

One indirect advantage of this approach is that the state vector is clearly seen to be divided into two parts. The first term on the right side of eq. (4.11) is the undriven part of the solution, while the remaining term is the correction due to the presence of the driving term $E\mu$ in the Hamiltonian.

In problems of this type, ψ_0 is often the "ground state" of the system, for which $H_0\psi_0 = 0$. In this case, eq. (4.10) reduces to

$$\widetilde{\phi}(s) = s^{-1}\,(I - E\,K(i\,s))^{-1}\,\phi_0, \tag{4.12}$$

with corresponding simplifications in eq. (4.11).

4.4. Laplace Transform of the Ground State

If ψ_0 is the ground state of the system as in eq. (4.12), one is typically really interested in solving for the value of the ground-state probability amplitude

$$a(t) = \psi_0^\dagger\,\psi(t), \tag{4.13}$$

rather than solving for the full state-vector ψ(t). As mentioned, this quantity can typically be found from eq. (4.10) by inspection but, if not, can be found explicitly by an adaptation of the method just outlined.

It will prove convenient for us to partition matrices and vectors into a part pertaining to the ground state and a part pertaining to the remainder of the states. In such a partitioning scheme, the state vector might be partitioned as

$$\psi(t) = \begin{bmatrix} a(t) \\ b(t) \end{bmatrix},$$

where $b(t)$ is a column vector, and $a(t)$ is, as mentioned, the ground-state probability amplitude. Similarly, the Hamiltonian might be partitioned as

$$H = \begin{bmatrix} 0 & v^\dagger \\ v & h \end{bmatrix}, \tag{4.14}$$

where v is a column vector and h is a matrix. We have eliminated the external parameter E appearing in eq. (4.1), as it is irrelevant to the present problem. However, in the spirit of eq. (4.2), we allow

$$h = h_0 + d\,f, \tag{4.15}$$

where the operators h_0, d (not to be confused with a differential operator), and f have properties analogous to H_0, D, and F (except that $d\,f$ has rank $\mathrm{M} - 2$ whereas $D\,F$ has rank M). Notice that, to this point, we are not restricting the nature of the system in any way except its driver rank. The system maybe discrete or continuous, or may contain many interacting continua or quasi-continua.

From eq. (4.8), it is clear that if ψ_0 is the ground state, then $\widetilde{a}(s)$ is the upper left-hand element of the matrix

$$i\,(i\,s - H)^{-1}.$$

Keeping eq. (4.14) in mind, this is just

$$\widetilde{a}(s) = i\,\frac{\det(i\,s - h)}{\det(i\,s - H)}. \tag{4.16}$$

With the use of various determinantal identities, such as expansion in cofactors,[8] eq. (4.16) can be reduced algebraically to

$$\widetilde{a}(s) = \frac{1}{s + i\,v^\dagger (i\,s - h)^{-1} v}. \tag{4.17}$$

Of course, this is not any improvement *per se* over eq. (4.11) unless we have a reasonable way of calculating $(i\,s - h)^{-1}$, which is a high-dimensional matrix.

Fortunately, a variation of the argument given in the previous section gives us the following formula, known as *Woodbury's Formula*,[9] for $(i\,s - h)^{-1}$:

$$(i\,s - h)^{-1} = \sigma(s) + \sigma(s)\,d\,\left(I - k(i\,s)\right)^{-1} f\,\sigma(s), \tag{4.18}$$

where, for brevity, we have put

$$\sigma(s) = (i\,s - h_0)^{-1}, \tag{4.19}$$

$$k(\lambda) = f\,\left(\lambda - h_0\right)^{-1} d. \tag{4.20}$$

Once again, by our assumptions, $\sigma(s)$ and $k(i\,s)$ are supposed to have known analytical forms, so eq. (4.18) is actually meaningful and useful. Eq. (4.18) may be verified by simple multiplication and is valid whether or not the operators involved are discrete and finite. The matrix inverse in eq. (4.18) is merely $\mathrm{M} - 2$ dimensional and is consequently easy to perform for small M.

With eq. (4.18) in hand, we may rewrite eq. (4.17) entirely in terms of operations which, by our original premises, are easy to carry out:

$$\widetilde{a}(s) = \frac{1}{s + i\,v^\dagger \sigma(s)\,v + i\,v^\dagger \sigma(s)\,d\,\left(I - k(i\,s)\right)^{-1} f\,\sigma(s)\,v}. \tag{4.21}$$

The first term in the denominator represents the undriven solution, with $H \equiv H_0$. The first two terms together represent just the $(1, \mathrm{N})$ part of the solution—*i.e.*, the solution with $h = 0$. Thus, the third term is the correction required to take into account the transitions neither originating nor ending at the ground state. This, then, is not merely our desired result, but actually presents the various contributions in a meaningful way.

4.5. A Simple Algebraic Example

To see how some of these algebraic details work out in practice, we'll use eq. (4.21) to find the Laplace transform of the ground-state probability amplitude in a model quantum

[8] A useful compendium of determinant relations is T. Muir, *A Treatise on the Theory of Determinants* (New York, Dover, 1960).

[9] W. Press, B. Flannery, S. Teukolsky, W. Vetterling, *Numerical Recipes* (Cambridge, Cambridge University Press, 1986), p. 68.

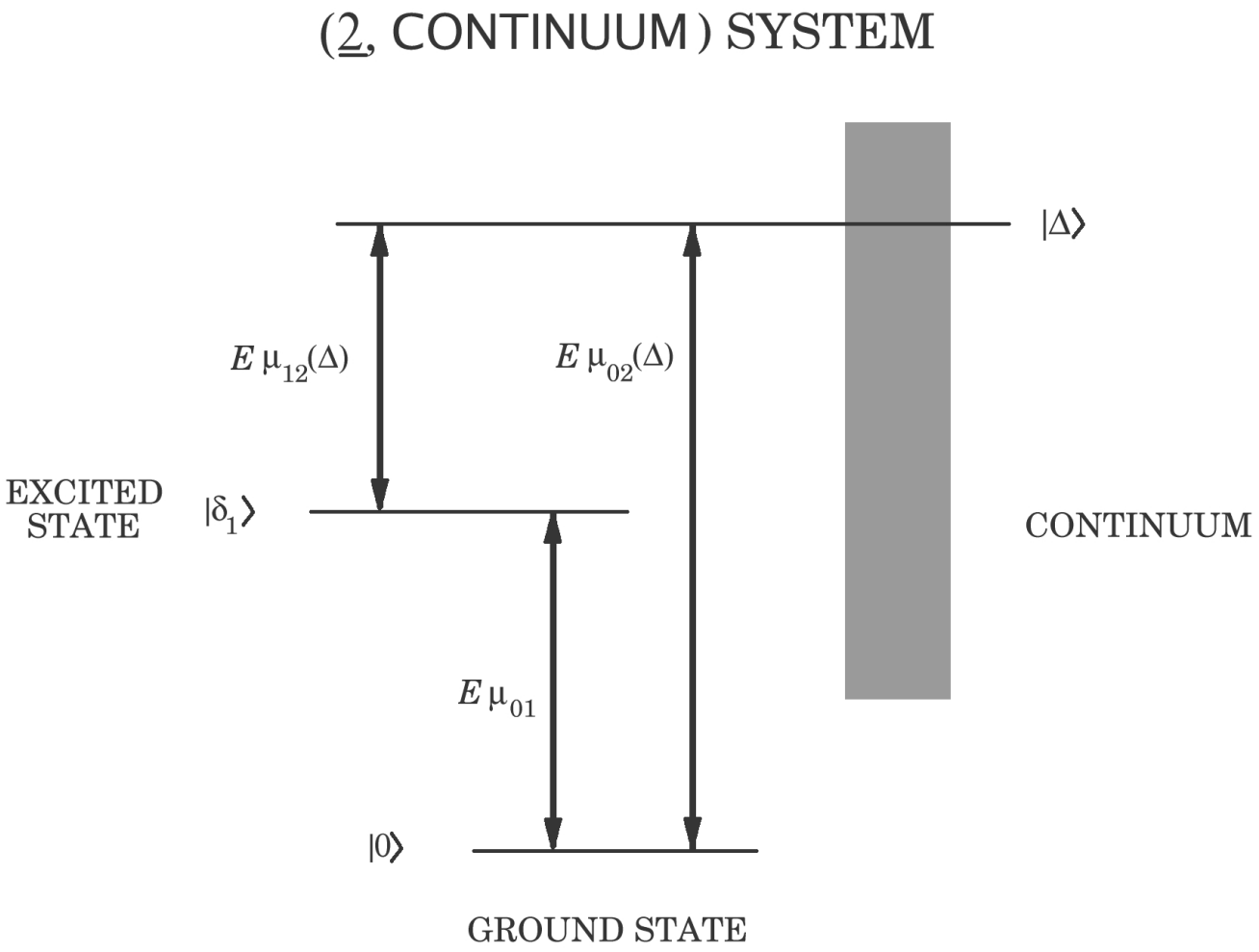

FIGURE 4.1

A (2,*CONTINUUM*) system. Although the second discrete level is shown inside the energy range of the continuum, and the ground state is not, this is not a necessary characteristic of the system. Thus, as shown, the second level is autoionizing. This is the usual case in the literature, but we won't require it.

system. Consider the system of figure (4.1), in which two discrete states (one of which is the ground state) are coupled to a continuum of energy levels *via* a laser field. For the sake of argument, we allow transitions between the discrete states and the continuum states and between the two discrete states, but not between two states in the continuum.

Although this is a relatively simple system, it would not be apparent how we might go about taking its Laplace transform if we had no systematic method for doing so. In fact, a typical approach simply might be to approximate the continuous band with a reservoir, and to use a simplified "effective" Hamiltonian rather than the full Hamiltonian of the system.[10] However, using the approach of eq. (4.21) we encounter no algebraic difficulties at all in attacking the full problem. (Which is not to say that the resulting expression is simple, nor that we necessarily know how to find the inverse transform of it.) For this system $\mathrm{M} = 4$ (if H_0 is taken to be the diagonal of the Hamiltonian), and we consequently know in advance that we will be able to find $\widetilde{a}(s)$ with merely a 2×2 matrix inversion.

Such a system has a Hamiltonian matrix with a double row-column border. Thus, the Hamiltonian matrix might be written as

$$H = \begin{bmatrix} 0 & E\,\mu_{10}^{\star} & E\,\mu_{20}(\Delta')^{\star} \\ E\,\mu_{10} & \delta_1 & E\,\mu_{21}(\Delta')^{\star} \\ E\,\mu_{20}(\Delta) & E\,\mu_{21}(\Delta) & \Delta\,\delta(\Delta-\Delta') \end{bmatrix}. \tag{4.22}$$

From eq. (4.22), we can write down v and h by inspection:

$$v = \begin{bmatrix} E\,\mu_{10} \\ E\,\mu_{20}(\Delta) \end{bmatrix},\ h = \begin{bmatrix} \delta_1 & E\,\mu_{21}(\Delta')^{\star} \\ E\,\mu_{21}(\Delta) & \Delta\,\delta(\Delta-\Delta') \end{bmatrix}. \tag{4.23}$$

While h_0, d, and f are not uniquely defined, by inspection alone we can see that one workable arrangement would be to allow h_0 to be the diagonal of h and

$$d = \begin{bmatrix} 1 & 0 \\ 0(\Delta) & E\,\mu_{21}(\Delta) \end{bmatrix},\ f = \begin{bmatrix} 0 & E\,\mu_{21}(\Delta')^{\star} \\ 1 & 0(\Delta') \end{bmatrix}. \tag{4.24}$$

Note that, as we warned in §3.4, we are using matrices whose various elements have incompatible units. Thus, in the two matrices above, we have elements that are pure numbers (like 1), and elements that are dimensionally energies (or frequencies). This will not prove to be any inconvenience to us, and will in fact simplify our algebra considerably.

The remainder of the calculation is entirely mechanical, once eq. (4.21) is given, and results in:

$$\widetilde{a}(s) = \frac{1}{s + i\,E^2\,(\chi+\chi_{00}) + \dfrac{i\,E^3}{i\,s-\delta_1-E^2\chi_{11}}\left(\mu_{01}\chi_{10}+\mu_{10}\chi_{01}+E\,\left(\chi\chi_{11}+\chi_{01}\chi_{10}\right)\right)}, \tag{4.25}$$

where the following symbols have been introduced for brevity:

[10] A. Lami and N. K. Rahman, *Phys. Rev. A* **33**, 782-785 (1986).

$$\begin{aligned}
\chi(s) &= \frac{\mu_{01}\mu_{10}}{i\,s-\delta_1}\,, \\
\chi_{00}(s) &= \int_{-\infty}^{\infty}\frac{\mu_{02}(\Delta)\mu_{20}(\Delta)}{i\,s-\Delta}\,d\Delta\,, \\
\chi_{01}(s) &= \int_{-\infty}^{\infty}\frac{\mu_{02}(\Delta)\mu_{21}(\Delta)}{i\,s-\Delta}\,d\Delta\,, \\
\chi_{10}(s) &= \int_{\infty}^{\infty}\frac{\mu_{12}(\Delta)\mu_{20}(\Delta)}{i\,s-\Delta}\,d\Delta\,, \\
\chi_{11}(s) &= \int_{-\infty}^{+\infty}\frac{\mu_{12}(\Delta)\mu_{21}(\Delta)}{i\,s-\Delta}\,d\Delta\,.
\end{aligned}$$

Of course, we don't pretend that this expression for $\widetilde{a}(s)$ is simple and easy to invert. In fact, we admit that it is impossible to invert for most (but not *all*) bandshapes $\mu_{21}(\Delta)$ and $\mu_{20}(\Delta)$. Nevertheless, the ease of the routine calculations leading up to $\widetilde{a}(s)$ is impressive, and we are able to take our calculations quite far before adopting any approximations.

4.6. Population Trapping in the Continuum

Recently there has been some interest in the phenomenon of coherent population trapping in quantum systems. Coherent population trapping occurs when the population is confined to some small subset of the entire set of energy levels of the system, even though this subset of energy levels may seem to be strongly coupled to the remainder of the system. Relevant studies include those dealing with discrete systems,[11,12,13,14,15,16,17] those dealing with the interaction of discrete levels and continuous bands of energy levels,[18,19,20,21] and very recently with entirely continuous systems.[22] We[23] have also contributed to this discussion. The population-trapping problem will be discussed in most of the remaining chapters.

Both the eigenvalue and the Laplace-transform methods presented above can sometimes be used to easily obtain some otherwise unobvious qualitative (and quantitative)

[11] R. M. Whitley and C. R. Stroud, Jr., *Phys. Rev. A* **14**, 1498 (1976).
[12] J. D. Stettler, C. M. Bowden, N. M. Witriol, and J. H. Eberly, *Phys. Lett.* **73A**, 171 (1979).
[13] F. T. Hioe and J. H. Eberly, *Phys. Rev. Lett.* **47**, 838 (1981).
[14] P. M. Radmore and P. L. Knight, *J. Phys. B* **15**, 561 (1982).
[15] S. Swain, *J. Phys. B* **15**, 3045 (1982).
[16] Z. Deng, *Opt. Commun.* **48**, 284 (1983).
[17] D. A. Cardimona, M. G. Raymer, and C. R. Stroud, Jr., *J. Phys. B* **15**, 55 (1982).
[18] P. Zoller and P. Lambropoulos, *Phys. Rev.* A **24**, 379 (1981).
[19] P. E. Coleman and P. L. Knight, *J. Phys. B* **15**, L235 (1982).
[20] Z. Deng and J. H. Eberly, *J. Opt. Soc. Am. B* **1**, 874 (1984).
[21] Z. Deng, *Phys. Lett.* **105A**, 43 (1984).
[22] Z. Deng and J. H. Eberly, *Phys. Rev. A* **34**, 2492 (1987).
[23] R. Burkey, A. Glosson, and C. D. Cantrell, *Phys. Rev. A*, in publication.

information about the quantum system under investigation. As an example of this, let's see some applications of these methods to the problem of population trapping.

4.6.1. Odd-Rank Population Trapping

Begin with a trivially derived consequence of our eigenvalue calculation.

Suppose that M is an odd number. Let λ be any real number. As demonstrated in Appendix A, the characteristic polynomial derived from $K(\lambda)$ is a real polynomial in E (of odd degree M). Such polynomials have at least one real root, with all complex roots appearing in conjugate pairs.[24] From this rather trivial reasoning the following appears:

> *Conclusion*: Any system with odd $\mathrm{rank}(\mu)$ has a given real eigenvalue λ for some real value of the external parameter E. That is, the system has a real eigenvalue, and we can choose its value by appropriately choosing E.

This point is hardly surprising for discrete (finite) systems. Finite systems have complete sets of eigenvectors, all with real eigenvalues. (So long as the Hamiltonians are Hermitian.) Because their eigenvalues are real, these systems oscillate. Continuous systems, on the other hand, present a somewhat different picture. (See the review in Chap. II.) Their observed behavior often involves strict absorption of all population into the continuum. This decay can be explained in terms of superposition of (non-eigen) oscillating states.[25] Further, if one succeeds in computing an eigenvalue, the eigenvalue generally has a non-zero imaginary part. Therefore, the population of the eigenstate decays rather than oscillates.

However, it has just been shown that if M is odd, there are always some real eigenvalues. That is, even for a continuum, the population in some states must oscillate rather than decay. Of course, by the very definition of an eigenstate, any population initially prepared to be in the real-eigenvalue eigenstate must be "trapped" there. Thus, we have generically demonstrated coherent population-trapping in all odd-rank quantum systems.

By the way, examination of eq. (4.4) reveals that if the eigenvalue λ is within the energy range of a continuum—*i.e.*, if $\lambda \in (\Delta_{\min}, \Delta_{\max})$—then the eigenvector (for a continuous system) is singular, in the sense that the matrix elements of ψ_λ in the neighborhood of $\Delta = \lambda$ must go to $\pm\infty$. If λ is *not* within the range of a continuum, then (if the operator μ is bounded), the eigenvector is normalizable and well-defined.

More than finding that the system has *some* real eigenvalues, we have found that *any* desired real eigenvalue can be produced by proper manipulation of the value E. Note that this is not true for all systems with *even* driver-rank. For example, for $(1, \mathrm{N})$ systems (of rank 2), there are "forbidden" energy regions in which the system cannot have an eigenvalue λ for any value of E whatever. Let's examine this briefly. For a $(1, \mathrm{N})$ system, eq. (4.6) implies an eigenvalue equation of:

[24] G. Birkhoff and S. MacLane, *A Survey of Modern Algebra* (Macmillan, New York, 1965), Ch. V §4.

[25] This is precisely the case, for example, in the Weisskopf-Wigner approximation.

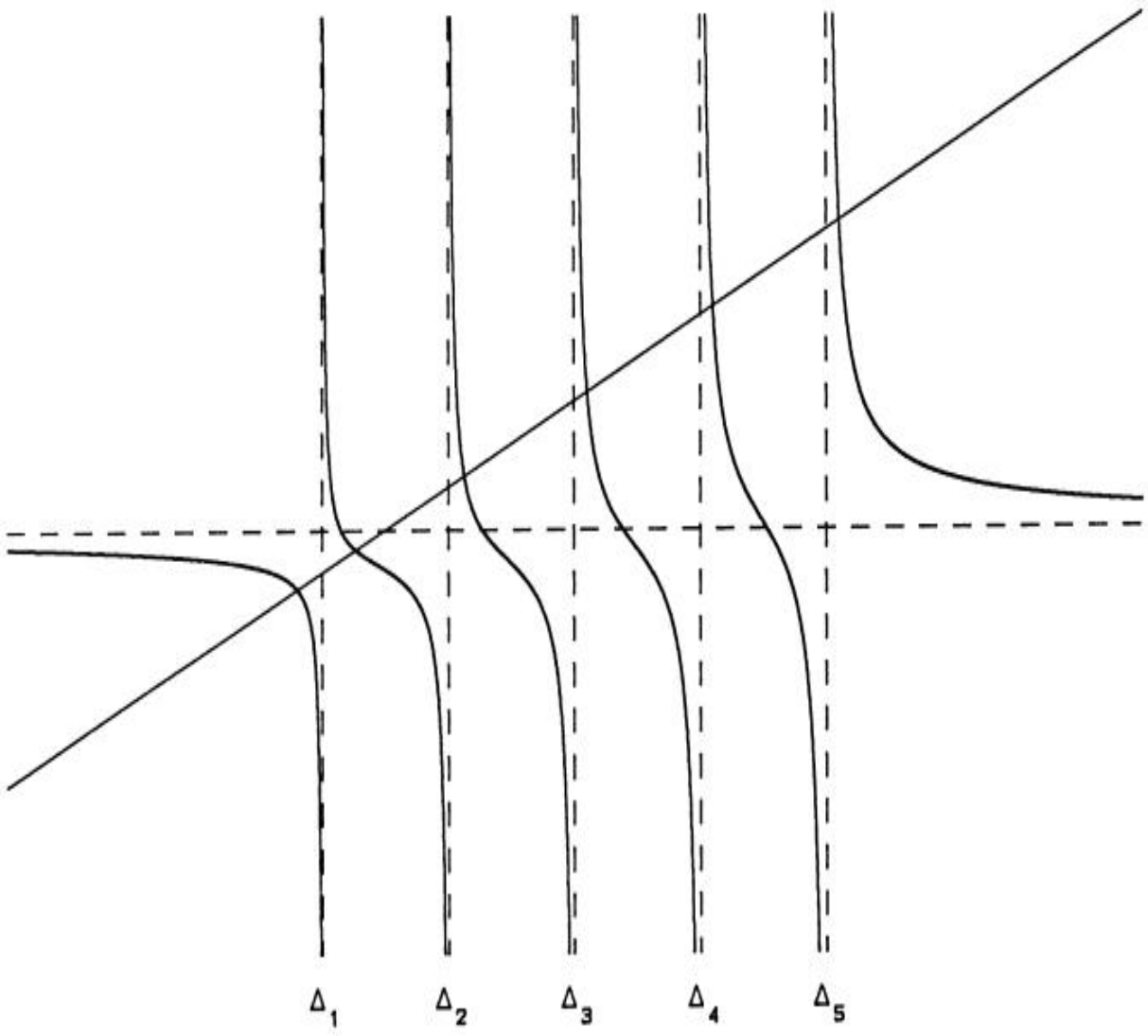

FIGURE 4.2

A depiction of the well-known eigenvalue equation for the $(1, \mathrm{N})$ system, namely eq. (4.26). The eigenvalues occur where the slanted line crosses the broken curve. There is exactly one eigenvalue in each of the regions $(-\infty, \Delta_1)$, (Δ_1, Δ_2), $\ldots$, $(\Delta_{\mathrm{N}}, \infty)$.

$$\lambda = \sum_{n=1}^{\mathrm{N}} \frac{E^2 \mid \mu_n \mid^2}{\lambda - \Delta_n}, \tag{4.26}$$

where Δ_n is the diagonal element of H_0 for the n-th level in the band, and μ_n is the dipole matrix element connecting the ground-state to the n-th level.[26] In figure (4.2) we see both the right-hand and left-hand sides of this equation, plotted against λ. The eigenvalues are at the intersections of the curves. If E is adjusted, the right-hand side of the equation is stretched or compressed in the upwards direction, changing the positions of the intersections (eigenvalues) but never allowing them to cross the λ-axis. Moreover, the zeroes of the right-hand function are not changed by adjustment of E. Therefore, positive-λ eigenvalues can never occur in the regions

$$\sum_{n=1}^{\mathrm{N}} \frac{\mid \mu_n \mid^2}{\lambda - \Delta_n} < 0.$$

Similarly, negative-λ eigenvalues can never appear where this function is positive.

If, as in §3.3, our quantum system consists of various bands of energy levels, we must note that an odd driver-rank M is generally associated with transitions within a single band, rather than with transitions connecting two different bands. To see this, let's imagine adding new low-rank transitions to a system. We'll do this in a way that maintains μ's Hermiticity. Adding some kinds of transitions will increment M by an even number. Adding others will increment M by an odd number.

Obviously, additions to μ representing interband (or, more precisely, non-intraband) transitions are of the form $\psi\phi^\dagger + \phi\psi^\dagger$, where ψ and ϕ are vectors (not to be confused with the vectors ψ and ϕ used above). Consequently, we can only make even additions to M in this way. On the other hand, additions to μ for intraband transitions can be either of this form or of the form $\psi\psi^\dagger$. Intraband transitions can add either an odd or an even number to M. Clearly, from this argument, we do not expect to find $\mathrm{rank}(\mu)$ odd without having intraband transitions. This point is also illustrated by eq. (3.23).

However, population-trapping is not a phenomenon solely of odd-rank systems. We see it in the context of even-rank systems also. In demonstrating this, we will present next a rather extended example of the use of the Laplace transform method.

4.6.2. Continuum-Continuum Population Trapping

Deng and Eberly (Ref. 22, hereafter referred to as DE) investigated population trapping in the system illustrated in Fig. (4.3). In this figure we see an infinite sequence of *featureless* continua, with transitions allowed between adjacent continua. DE demonstrated that the system population could be almost entirely trapped in the continuum initially containing the population, even if this continuum is *apparently* very strongly coupled to all of the other continua. This result is counter-intuitive. Clearly, the stronger the interactions, the more we expect population to spread out among all of the energy levels. Moreover,

[26] For example, J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford U. Press, Cambridge, 1965).

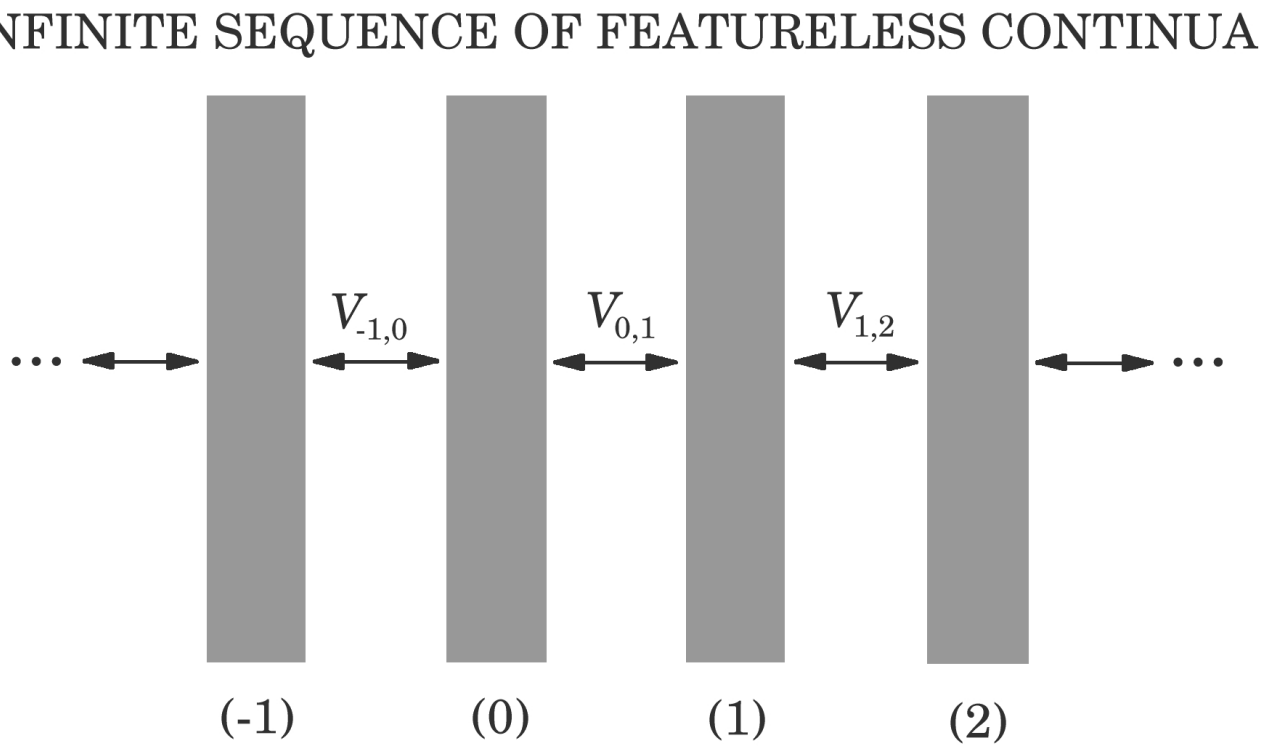

FIGURE 4.3

The system investigated in DE. It has an infinite sequence of featureless continua, with transitions taking place only between adjacent continua.

it is the large-interaction-strength limit which is of interest if the system is coherently stimulated by a laser beam.

We have found that some interesting extensions to this work are possible. In particular, here we would like to consider similar systems with only two or three continua rather than an infinite sequence of continua. However, rather than the featureless continua of DE, we will allow more general continua, and we will not restrict ourselves to the special initial conditions found in DE.

We will find that though this population-trapping occurs, it is really limited to the case of very broad continua. When the continua under consideration are narrower (in energy) than the interaction energy, no such effect occurs. We will show this by example. For broad continua, we will nevertheless find regardless of the initial population distribution that as the interaction strength becomes very large, the two-continuum system's population is trapped (but redistributed) in the continuum initially containing the population. For three-continua systems, the results are similar, but slightly more complex.

Consider the system depicted in Fig. (4.4). In this system, we have two continua interacting with each other through some potential. Unlike DE, we do *not* assume that these are featureless continua. In fact, we do not even commit ourselves as to whether these are infinite continua (characterized by $-\infty < \Delta < \infty$), single-sided continua (characterized by $\Delta_{\min} < \Delta < \infty$), or strictly limited continua (characterized by $\Delta_{\min} < \Delta < \Delta_{\max}$). We will investigate the time-evolution of this system, aided by our systematic Laplace transform technique.

We will suppose that the probability amplitudes of the levels in continuum 0 are denoted by $C_0(\Delta)$. Similarly, continuum 1 will have probability amplitudes $C_1(\Delta)$. (Of course, the probability amplitudes are also functions of time, though not explicitly shown.) The interaction between the Δth level of continuum 0 and the Δ'th level of continuum 1 will be $V_{01}(\Delta, \Delta')$. Thus, Schrödinger's equations will be

$$\left.\begin{aligned} i\,\dot{C}_0(\Delta) &= \Delta\, C_0(\Delta) + \int V_{01}(\Delta, \Delta') C_1(\Delta') d\Delta' \\ i\,\dot{C}_1(\Delta) &= \Delta\, C_1(\Delta) + \int V_{10}(\Delta, \Delta') C_0(\Delta') d\Delta' \end{aligned}\right\}. \tag{4.27}$$

The ranges of integration will be specified later when we make a more specific choice of the interaction $V_{01}(\Delta, \Delta')$.

This system does not have low-rank driving, and consequently needs an approximation (such as those in §3.6) to give the system a low rank. Unfortunately, the approximations of §3.6 were really tailored to be accurate in the neighborhoods $\mid \Delta \mid \approx 0$ and/or $\mid \Delta' \mid \approx 0$. This is appropriate if population is injected into the continua through interaction with a discrete state, but is not appropriate for a purely continuous system. We are still at liberty to retain the simple approximation

$$V_{01}(\Delta, \Delta') \approx V_0(\Delta)\, V_1(\Delta'), \tag{4.28}$$

but a different set of criteria is needed for choosing the functions V_0 and V_1. (We will also discuss more complex approximations at the end of the section). This approximation has the virtue of making $\mathrm{M} = 2$, so that $\phi(t)$ is a 2-vector and $K(i\,s)$ is a 2×2 matrix.

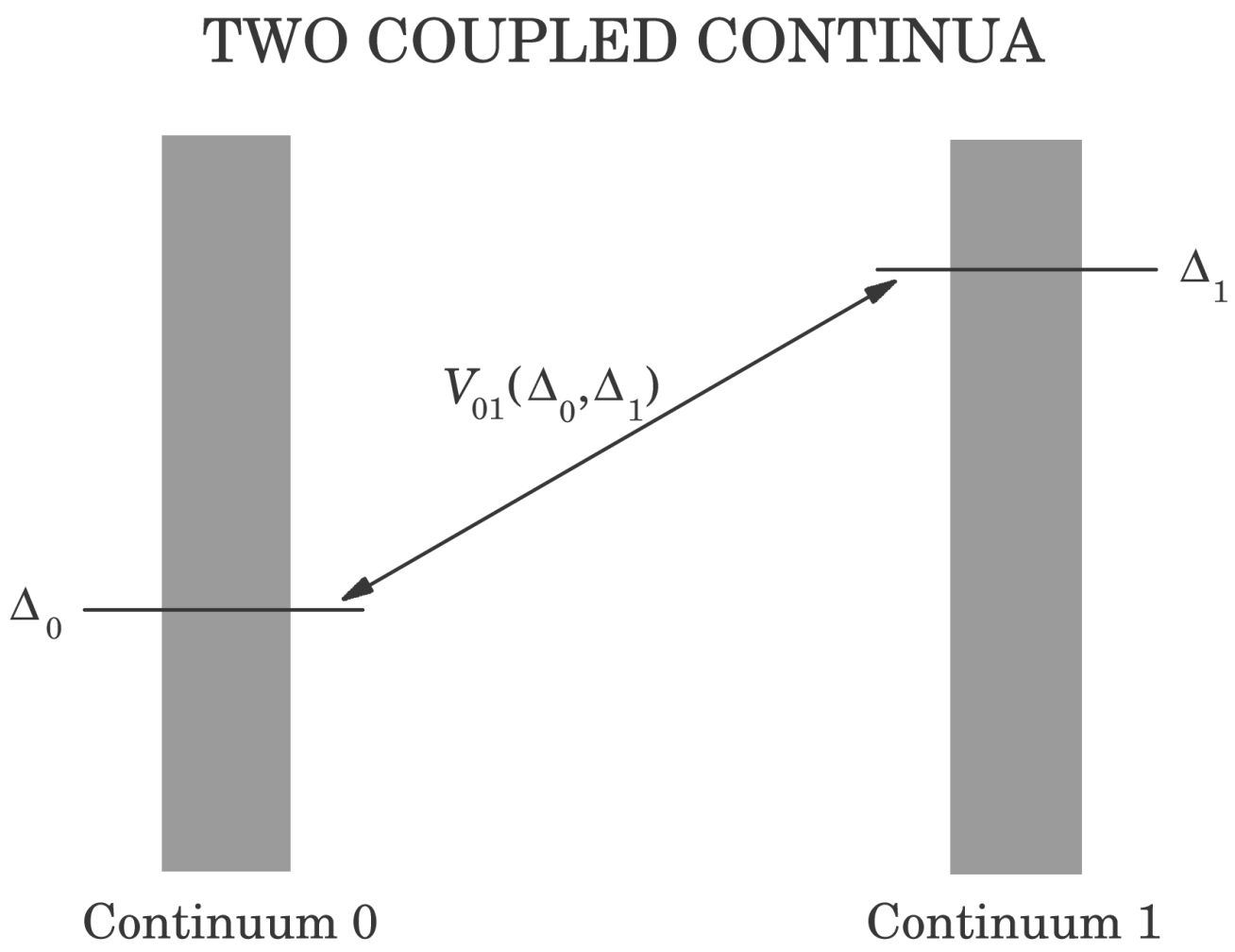

FIGURE 4.4

A system with two continua, labelled 0 and 1. No transitions take place between two levels of the *same* continuum, but transitions from one continuum to the other are controlled by the function $V_{01}(\Delta_0, \Delta_1)$.

In an approximation like eq. (4.28), what characteristics of $V_{01}(\Delta, \Delta')$ must be preserved to physically insure that the time-evolution of the system is not distorted? Basically, we would expect the approximation to be good if the matrix elements in the neighborhood of resonance are approximated well. For our systems, this can be interpreted to mean that $V_{01}(\Delta, \Delta')$ is approximated well for $\Delta \approx \Delta'$. Thus, it would be reasonable to expect any approximating function $V'_{01}(\Delta, \Delta')$ to obey the restrictions

$$V_{01}(\Delta, \Delta) \equiv V'_{01}(\Delta, \Delta), \tag{4.29}$$

$$\frac{\partial}{\partial \Delta'} V_{01}(\Delta, \Delta')\bigg|_{\Delta'=\Delta} \equiv \frac{\partial}{\partial \Delta'} V'_{01}(\Delta, \Delta')\bigg|_{\Delta'=\Delta}. \tag{4.30}$$

By the way, the latter equation automatically guarantees the satisfaction of a similar equation with the rôles of Δ and Δ' reversed.

As it happens, in the approximation $V_{01}(\Delta, \Delta') = V_0(\Delta)\, V_1(\Delta')$, the functions V_0 and V_1 can easily be chosen to satisfy eqs. (4.29) and (4.30). Omitting the (trivial) details, we find that[27]

$$V_1(\Delta) = \exp\left(\int \frac{1}{V_{01}(\Delta, \Delta)} \frac{\partial}{\partial \Delta'} V_{01}(\Delta, \Delta')\bigg|_{\Delta'=\Delta} d\Delta \right), \tag{4.31}$$

$$V_0(\Delta) = \frac{V_{01}(\Delta, \Delta)}{V_1(\Delta)}. \tag{4.32}$$

Consequently, we expect eq. (4.28) to be a rather good approximation.

Without further ado, we can write down the Laplace transforms of the probability amplitudes. If the population of the system is initially distributed in continuum 0 according to the expression

$$C_0(\Delta)|_{t=0} = \alpha(\Delta), \;\; C_1(\Delta)|_{t=0} \equiv 0. \tag{4.33}$$

where $\alpha(\Delta)$ is some given function, then our routine method gives:

$$\widetilde{C}_0(\Delta) = \frac{1}{s + i\,\Delta} \left(\alpha(\Delta) + \frac{\overline{\alpha}(s)}{1 - \chi_0(s)\,\chi_1(s)}\, \chi_1(s)\, V_0(\Delta) \right), \tag{4.34}$$

$$\widetilde{C}_1(\Delta) = \frac{\overline{\alpha}(s)}{1 - \chi_0(s)\,\chi_1(s)}\, \frac{V_1(\Delta)}{s + i\,\Delta}. \tag{4.35}$$

Here

$$\overline{\alpha}(s) = \int \frac{V_0(\Delta)\,\alpha(\Delta)}{i\,s - \Delta}\, d\Delta, \tag{4.36}$$

$$\chi_n(s) = \int \frac{V_n(\Delta)^2}{i\,s - \Delta}\, d\Delta. \tag{4.37}$$

[27] The integral below is an indefinite integral, and therefore unique only up to an additive constant, but it nevertheless uniquely defines $V'_{01}(\Delta, \Delta')$. Of course, it is assumed that $V_{01}(\Delta, \Delta)$ is *never* zero.—RSB, 3/2003.

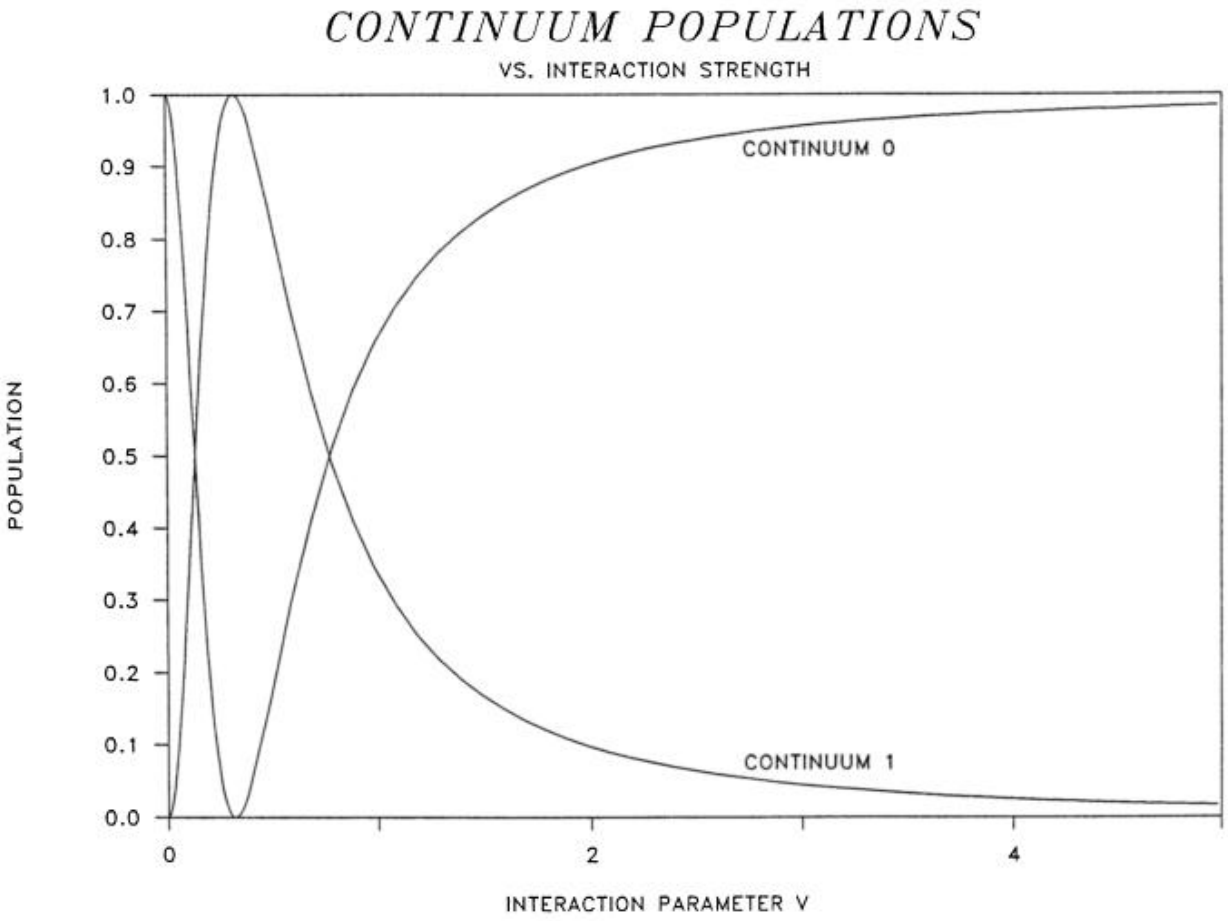

FIGURE 4.5

The steady-state total populations of featureless continua 0 and 1 for various values of the interaction parameter ν. The population is initially in continuum 0 and is trapped there for *either* $\nu \to 0$ *or* $\nu \to \infty$. For $\nu = \frac{1}{\pi}$, the population is entirely transferred to continuum 1.

Up to now, the discussion has been rather general. Let's get more specific. Suppose for the moment that the two continua in this system are *featureless*. To simplify comparison with the results of DE, we will begin by choosing the initial condition

$$C_0(\Delta)|_{t=0} = \sqrt{\frac{\gamma}{\pi}}\,\frac{1}{\Delta + i\,\gamma}\,, \tag{4.38}$$

which describes a Lorentzian population distribution of width γ. The featureless continua are characterized by the equations

$$V_0(\Delta) \equiv 1,\ V_1 \equiv \nu, \tag{4.39}$$

where ν is a dimensionless constant governing the strength of the interaction, similar to E but incorporating some dipole matrix elements. Under these conditions we find that

$$\overline{\alpha}(s) = \frac{-2\sqrt{\gamma\,\pi}}{s+\gamma}, \tag{4.40}$$

with

$$\chi_0(s) \equiv -i\,\pi\,,\ \chi_1(s) \equiv -i\,\pi\,\nu^2. \tag{4.41}$$

Thus,

$$C_1(\Delta) = \frac{-2\sqrt{\gamma\,\pi}\,\nu}{(1+\pi^2\nu^2)\,(\gamma - i\,\Delta)}\left(e^{-i\Delta t} - e^{-\gamma t}\right), \tag{4.42}$$

and, in the limit $t \to \infty$, the total population of continuum 1 goes to

$$\text{Population 1} \to \frac{4\pi^2\nu^2}{\left(1+\pi^2\nu^2\right)^2}\,. \tag{4.43}$$

As noted in DE, this goes to zero in *both* the limits $\nu \to 0$ *and* $\nu \to \infty$. The maximum value is attained at $\nu = \frac{1}{\pi}$, in which all population moves to continuum 1. Interestingly, for the infinite sequence of continua envisaged in DE, the condition for all population to move out of continuum 1 is $\nu = \sqrt{3/4}\,\frac{1}{\pi}$. At the critical interaction strength $\nu = \frac{1}{\pi}$, the probability amplitudes of the levels in continuum 1 at large times t are

$$\widetilde{C}_1(\Delta) = -i\,\widetilde{C}_0(\Delta)\Big|_{t=0} e^{-i\Delta t}. \tag{4.44}$$

Thus, except for a phase shift, it is just as if the population were initially all in continuum 1 and there were no interaction at all. This is not true for the population trapped in continuum 0, which redistributes itself somewhat within the continuum over time. The populations in continua 0 and 1 are shown in Figure (4.5) for various values of ν.

The main qualitative result (that population is trapped incontinuum 0) does not depend on the special initial conditions chosen. We can see this by a simple argument. From eq. (4.35), we find that

$$\widetilde{C}_1(\Delta) = \frac{\overline{\alpha}(s)\,\nu}{1+\nu^2\pi^2}\,\frac{1}{s+i\,\Delta}\,. \tag{4.45}$$

Thus $C_1(t,\Delta)$ is separable into two parts—one depending only on ν, and one only on t and Δ:

$$C_1(t,\Delta) = \frac{\nu}{1+\pi^2\nu^2}\,\mathcal{L}^{-1}\left\{\frac{\widetilde{\alpha}(s)}{s+i\,\Delta}\right\}. \tag{4.46}$$

It is obvious from this that the total population of continuum 1 goes to zero regardless of the exact form of $\alpha(\Delta)$.

On the other hand, we cannot conclude that our qualitative result still holds if we relax the condition that the continua are featureless (or, at least, very broad). In fact, on intuitive grounds we know that if the continua were very narrow, then each of the continua should act something like a single discrete level. The entire $(\mathsf{CONTINUUM},\mathsf{CONTINUUM})$ system should behave like a (weakly damped) two-level system. As ν becomes very large, the population should oscillate rapidly between the two continua (eventually damping down to some steady-state distribution evenly divided between the two continua). We can demonstrate this effect with a model calculation.

For the sake of discussion, suppose that

$$V_0(\Delta) = \frac{1}{\nu}V_1(\Delta) = \alpha(\Delta) = \sqrt{\frac{\dfrac{\sigma}{\pi}}{\Delta^2+\sigma^2}}\,. \tag{4.47}$$

where σ is the "width" of the Lorentzian continua. (Note that this ν is slightly different than the interaction strength used earlier, since rather than being dimensionless it has units of frequency.) In order to perform the inverse Laplace transform, we need to know $\chi_0(s)$, $\chi_1(s)$, and $\overline{a}(s)$ for s having a real part greater than zero. In this case, we find from eqs. (4.36) and (4.37), by contour integration, that

$$\chi_0(s) = \overline{\alpha}(s) = \frac{\chi_1(s)}{\nu^2} = \frac{-i}{s+\sigma},\ (\mathcal{R}\mathsf{e}\ s>0). \tag{4.48}$$

According to eq. (4.35), the Laplace-transformed probability amplitudes in continuum 1 are then

$$\widetilde{C}_1(\Delta,s) = \frac{i\,(s+\sigma)}{(s+\sigma)^2+\nu^2}\,\frac{V_1(\Delta)}{s+i\,\Delta}\,. \tag{4.49}$$

Noting that the roots of the denominator are $-\sigma\pm i\nu$ and $-i\Delta$, this expression is easily inverted to give the probability amplitudes themselves as:

$$C_1(\Delta,t) = \frac{-iV_1(\Delta)}{(\sigma-i\Delta)^2+\nu^2}\left((\sigma-i\Delta)\left(e^{-i\Delta t}-e^{-\sigma t}\cos(\nu t)\right)+e^{-\sigma t}\nu\,\sin(\nu t)\right). \tag{4.50}$$

The steady-state population of level Δ in continuum 1 is thus

$$|C_1(\Delta)|^2_{\mathrm{ss}} = \frac{\dfrac{\nu^2\sigma}{\pi}}{(\sigma^2+\Delta^2-\nu^2)+4\sigma^2\nu^2}\,. \tag{4.51}$$

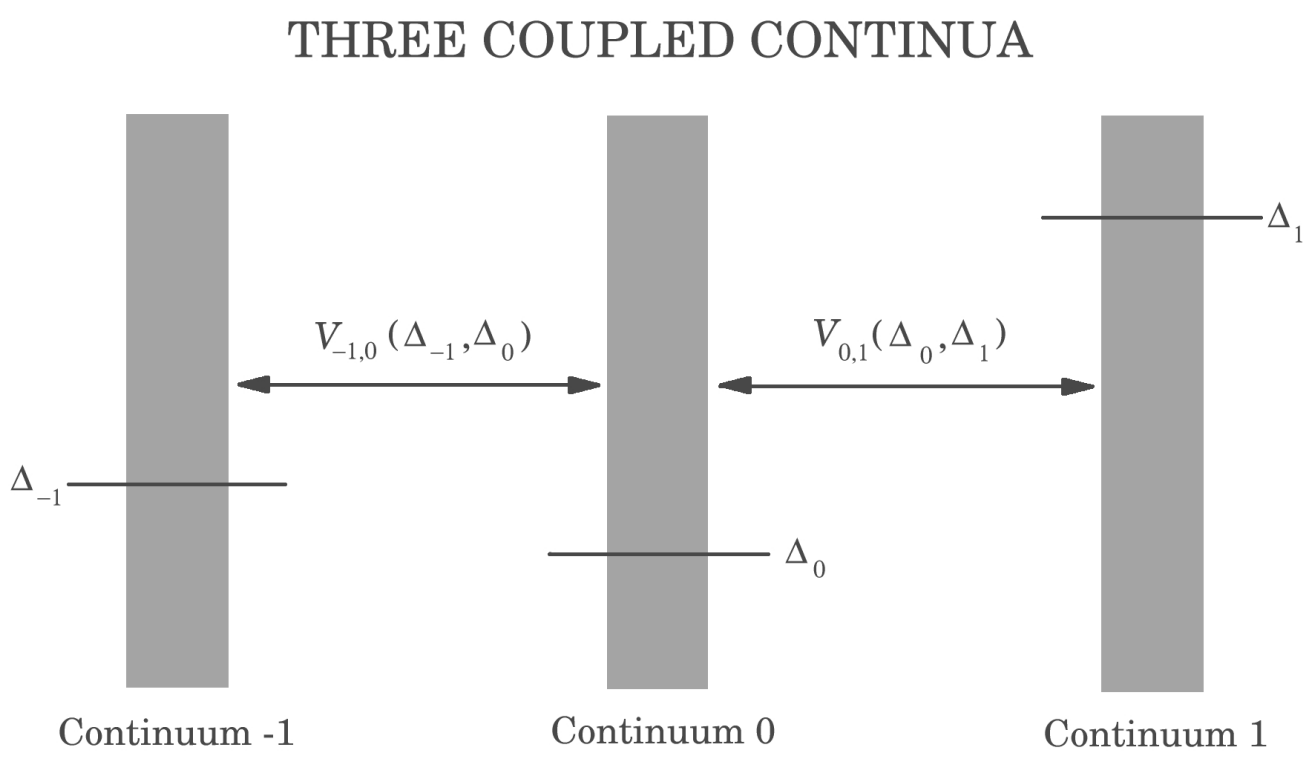

FIGURE 4.6

A system with three continua, labelled -1, 0, and 1. Transitions can take place between continua -1 and 0, and between continua 0 and 1, but not between continua -1 and 1.

This function is very small except for $\Delta \approx \pm\nu$ (for $\sigma \ll \nu$). Thus, the steady-state population is bunched into two sidebands, far from the center of the continuum. The total population of continuum 1 may also be easily computed using contour integration, as

$$\text{Steady state population of continuum 1} = \frac{\nu^2}{2\left(\nu^2+\sigma^2\right)}. \tag{4.52}$$

The steady-state population is therefore evenly distributed between the two continua when $\nu \gg \sigma$, as we had supposed intuitively.

It also is interesting to apply the same reasoning to a system of three continua. Consider the model system shown in Figure (4.6). As before, in order to reduce the driving-rank of the system to a manageable level, we introduce the approximations

$$V_{-10}(\Delta,\Delta') \approx V_{-1}(\Delta)V_0(\Delta'),\ V_{01}(\Delta,\Delta') \approx V_0(\Delta)V_1(\Delta').$$

There are two interesting sets of initial conditions for this system. First, all of the population could initially be confined to continuum 0, as in eqs. (4.33). Second, all of the population could initially be confined to continuum -1.

Consider first the case of all population initially in continuum -1. Our routine Laplace transform calculation gives

$$\widetilde{C}_{-1}(\Delta,s)=\frac{\alpha(\Delta)}{s+i\Delta}+\frac{1}{s+i\Delta}V_{-1}(\Delta)\frac{\chi_0(s)\overline{\alpha}_{-1}(s)}{1-\chi_0(s)\chi_1(s)-\chi_0(s)\chi_{-1}(s)}, \tag{4.53}$$

$$\widetilde{C}_{0}(\Delta,s)=\frac{1}{s+i\Delta}V_{0}(\Delta)\frac{\overline{\alpha}_{-1}(s)}{1-\chi_0(s)\chi_1(s)-\chi_0(s)\chi_{-1}(s)}, \tag{4.54}$$

$$\widetilde{C}_{1}(\Delta,s)=\frac{1}{s+i\Delta}V_{1}(\Delta)\frac{\chi_0(s)\overline{\alpha}_{-1}(s)}{1-\chi_0(s)\chi_1(s)-\chi_0(s)\chi_{-1}(s)}. \tag{4.55}$$

where we have put

$$\overline{\alpha}_n(s)=\int\frac{V_n(\Delta)\,\alpha(\Delta)}{i\,s-\Delta}\,d\Delta. \tag{4.56}$$

If we adopt a Lorentzian initial distribution of population similar to eq. (4.40) (but for continuum -1), and use featureless continua

$$V_{-1}(\Delta)\equiv\nu_{-1},\ V_0(\Delta)\equiv 1,\ V_1(\Delta)\equiv\nu_1,$$

then eqs. (4.53-4.55) can be solved without any particular difficulty. For large times, we find that the total populations of the individual continua are given by

$$\text{Population }-1=\left(\frac{1+\pi^2\left(\nu_1^2-\nu_{-1}^2\right)}{1+\pi^2\left(\nu_1^2+\nu_{-1}^2\right)}\right)^2, \tag{4.57}$$

$$\text{Population }0=\left(\frac{2\pi\nu_{-1}}{1+\pi^2\left(\nu_1^2+\nu_{-1}^2\right)}\right)^2, \tag{4.58}$$

$$\text{Population }1=\left(\frac{2\pi^2\nu_1\nu_{-1}}{1+\pi^2\left(\nu_1^2+\nu_{-1}^2\right)}\right)^2, \tag{4.59}$$

Thus, for large interaction parameters, the population of continuum 0 goes to zero. However, the distribution of population between the two outer continua depends on the ratio of the interaction parameters. In Figure (4.7), the populations of the continua are shown at various values of the interaction parameter ratio. Population is trapped in continuum -1 in both the cases $\nu_{-1}\gg\nu_1$ and $\nu_1\gg\nu_{-1}$. The "worst" case is if the two interaction parameters are equal, in which case all of the population moves from continuum -1 to continuum 1.

As a final case, suppose all of the population is initially in continuum 0, the middle continuum. We find that the Laplace-transformed probability amplitudes are

$$\widetilde{C}_{-1}(\Delta,s)=\frac{1}{s+i\Delta}\,V_{-1}(\Delta)\,\frac{\overline{\alpha}_0(s)}{1-\chi_0(s)\chi_1(s)-\chi_0(s)\chi_{-1}(s)}\,, \tag{4.60}$$

$$\widetilde{C}_{0}(\Delta,s)=\frac{\alpha(\Delta)}{s+i\Delta}+\frac{1}{s+i\Delta}\,V_{0}(\Delta)\,\frac{\overline{\alpha}_0(s)\left(\chi_{-1}(s)+\chi_1(s)\right)}{1-\chi_0(s)\chi_1(s)-\chi_0(s)\chi_{-1}(s)}\,, \tag{4.61}$$

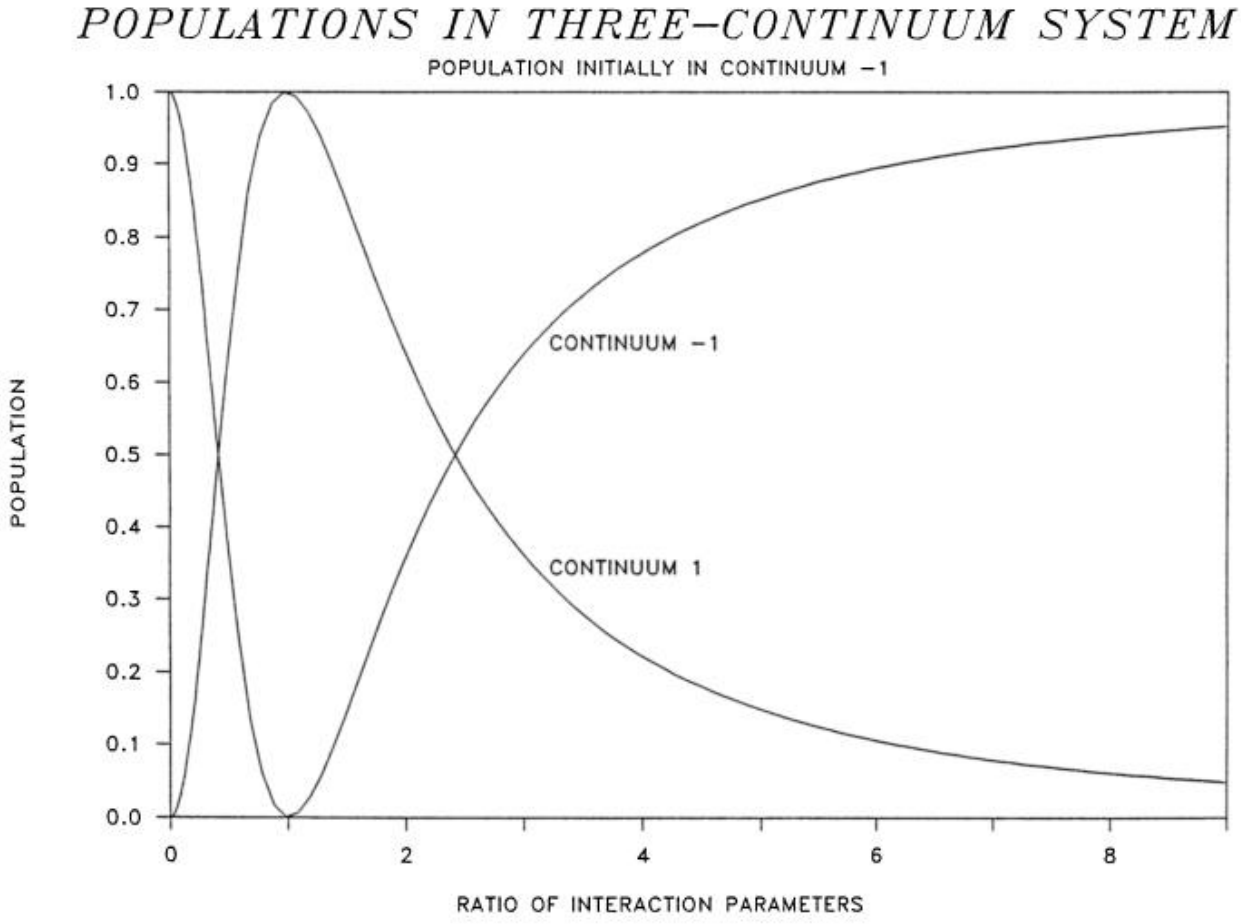

FIGURE 4.7

The steady-state populations in featureless continua -1 and 1 for large interaction parameters ν_1 and ν_{-1}. The population is initially all in continuum -1. Continuum 0 never contains significant population. The distribution of population among continua -1 and 1 varies according to the ratio of the interaction parameters, ν_1/ν_{-1}. The population is trapped in continuum -1 for *either* $\nu_1/\nu_{-1} \to 0$ *or* $\nu_1/\nu_{-1} \to \infty$. If $\nu_1 = \nu_{-1}$, the population is entirely transferred to continuum 1. If $\nu_1 \gg \nu_{-1}$, the system stays in the initial state.

$$\widetilde{C}_1(\Delta, s) = \frac{1}{s + i\Delta} V_1(\Delta) \frac{\overline{\alpha}_0(s)}{1 - \chi_0(s)\chi_1(s) - \chi_0(s)\chi_{-1}(s)}, \tag{4.62}$$

For the featureless continua and Lorentzian initial population distribution we have been using as a test case, the populations of the several continua in the long time limit turn out to be

$$\text{Population } -1 = \left(\frac{2\pi\nu_{-1}}{1 + \pi^2 \left(\nu_1^2 + \nu_{-1}^2\right)} \right)^2, \tag{4.63}$$

$$\text{Population } 0 = \left(\frac{1 - \pi^2 \left(\nu_1^2 + \nu_{-1}^2\right)}{1 + \pi^2 \left(\nu_1^2 + \nu_{-1}^2\right)} \right)^2, \tag{4.64}$$

$$\text{Population } 1 = \left(\frac{2\pi\nu_1}{1 + \pi^2 \left(\nu_1^2 + \nu_{-1}^2\right)} \right)^2, \tag{4.65}$$

Thus, for large interaction parameters the population is trapped in the middle continuum regardless of the ratio of the interaction parameters. The populations in continuum 0 and in the remainder of the system are displayed in Figure (4.5). Actually, Fig. (4.5) represents the populations in a two-continuum system, but if we interpret ν in that figure as

$$\frac{1}{\sqrt{\nu_{-1}^2 + \nu_1^2}}$$

then the curve giving the population in continuum 0 remains correct.

Finally, though no new qualitative results are obtainable, it is interesting to see how our Laplace-transform method deals with approximations for $V_{01}(\Delta, \Delta')$ more accurate than eq. (4.28). For simplicity, we'll confine our discussion to the two-continuum case. Approximation (4.28) produces a system of driver-rank $\mathrm{M} = 2$, while the more accurate approximation

$$V_{01}(\Delta, \Delta') \approx \upsilon_1(\Delta)\zeta_1(\Delta') + ... + \upsilon_{\mathrm{m}}(\Delta)\zeta_{\mathrm{m}}(\Delta') \tag{4.66}$$

produces a system of low (albeit larger) driver-rank $\mathrm{M} = 2\mathrm{m}$. Note that approximation (4.66) can always be made as accurate as desired. This is easily seen by noting that a truncated two-dimensional Taylor series is of the same form as eq. (4.66).

Routinely, we find that

$$\widetilde{C}_0(\Delta) = \frac{\alpha(\Delta)}{s + i\Delta} + \frac{1}{s + i\Delta} \upsilon(\Delta) \left(I - k_1(s)k_0(s)\right)^{-1} k_1(s)\, \overline{\alpha}(s), \tag{4.67}$$

$$\widetilde{C}_1(\Delta) = \frac{1}{s + i\Delta} \zeta(\Delta) \left(I - k_0(s)k_1(s)\right)^{-1} \overline{\alpha}(s), \tag{4.68}$$

In these expressions, $\upsilon(\Delta)$, $\zeta(\Delta)$, and $\overline{\alpha}(s)$ are m-vectors, respectively having elements $\upsilon_n(\Delta)$, $\zeta_n(\Delta)$, and

$$\left[\overline{\alpha}(s)\right]_n = \int \frac{\upsilon_n(\Delta)\alpha(\Delta)}{i\, s - \Delta} d\Delta. \tag{4.69}$$

$\alpha(\Delta)$ is, as usual, the initial probability amplitude distribution in continuum 0. I is the $\mathrm{m} \times \mathrm{m}$ identity matrix, and k_0 and k_1 $\mathrm{m} \times \mathrm{m}$ matrices with the matrix elements

$$[k_0(s)]_{nm} = \int \frac{\upsilon_n(\Delta)\upsilon_m(\Delta)}{i\,s-\Delta} d\Delta,\ [k_1(s)]_{nm} = \int \frac{\zeta_n(\Delta)\zeta_m(\Delta)}{i\,s-\Delta} d\Delta. \tag{4.70}$$

4.7. Laplace Inversion for Rational Bands

While it is wonderful to have a simple method for computing the Laplace transform of the state vector for a quantum system, it is unfortunate that we are then usually unable to invert this transform exactly. There are special cases, of course, in which we are able to say something about the inversion process. Thus in the previous section we were able to completely solve systems containing only featureless continua and Lorentzian continua. A generalization of these special cases is that in which the continuous bands in the system have *rational* bandshapes, as outlined in §3.5. For rational bands, the matrices $K(is)$ and $k(is)$ [and the various ancillary functions $\nu^\dagger\sigma(s)\,d$, $f\,\sigma(s)\,\nu$, $\nu^\dagger\sigma(s)\,\nu$] will be rational functions (*i.e.*, ratios of polynomials) of the variable s. This is so because any integrals over continua appearing in these expressions can be computed by complex residue techniques.[28] Of course, general smooth functions can be approximated by rational functions[29] in any case, so we could alternately just assume (as an approximation) that $K(is)$ and/or $k(is)$ (and the ancillary quantities) are approximately rational.

If this is so, then $\widetilde{\psi}(s)$ [as given by eq. (4.11)] and $\widetilde{a}(s)$ [as given by eq. (4.21)] are also rational functions, by inspection. All rational functions can be Laplace-inverted in a straightforward way *via* the Heaviside expansion theorem.[30] Thus, systems with only rational bands can in principle be exactly solved, and other systems can be approximately solved to the extent that they can be approximated with rational bands.

To see how this is done, consider the very simple case of the ground-state probability amplitude $\widetilde{a}(s)$ in the $(1, \mathsf{RATIONAL\,BAND})$ system of§3.5. This is a special case of the $(\underline{2}, \mathsf{CONTINUUM})$ example done in §4.5, with the quantities μ_{01} and $\mu_{12}(\Delta)$ being zero, and with

$$\mu_{00}(\Delta)^2 = \frac{p(\Delta)}{q(\Delta)}, \tag{4.71}$$

for some polynomials $p(\Delta)$ and $q(\Delta)$. In this case, eq. (4.25) reduces to

$$\widetilde{a}(s) = \frac{1}{s + i\,E^2\,\chi_{00}(s)}\,, \tag{4.72}$$

with

[28] G. Polya and G. Latta, *Complex Variables* (Wiley, New York, 1974), Ch. 5.

[29] Software for the purpose of approximating arbitrary functions by rational functions is readily available. For example, the routines ARAT and DARAT in the IBM Scientific Subroutine Package can produce the coefficients for an approximating rational function.

[30] V. Bush, *Operational Circuit Analysis* (Wiley, New York, 1946), Ch. VII.

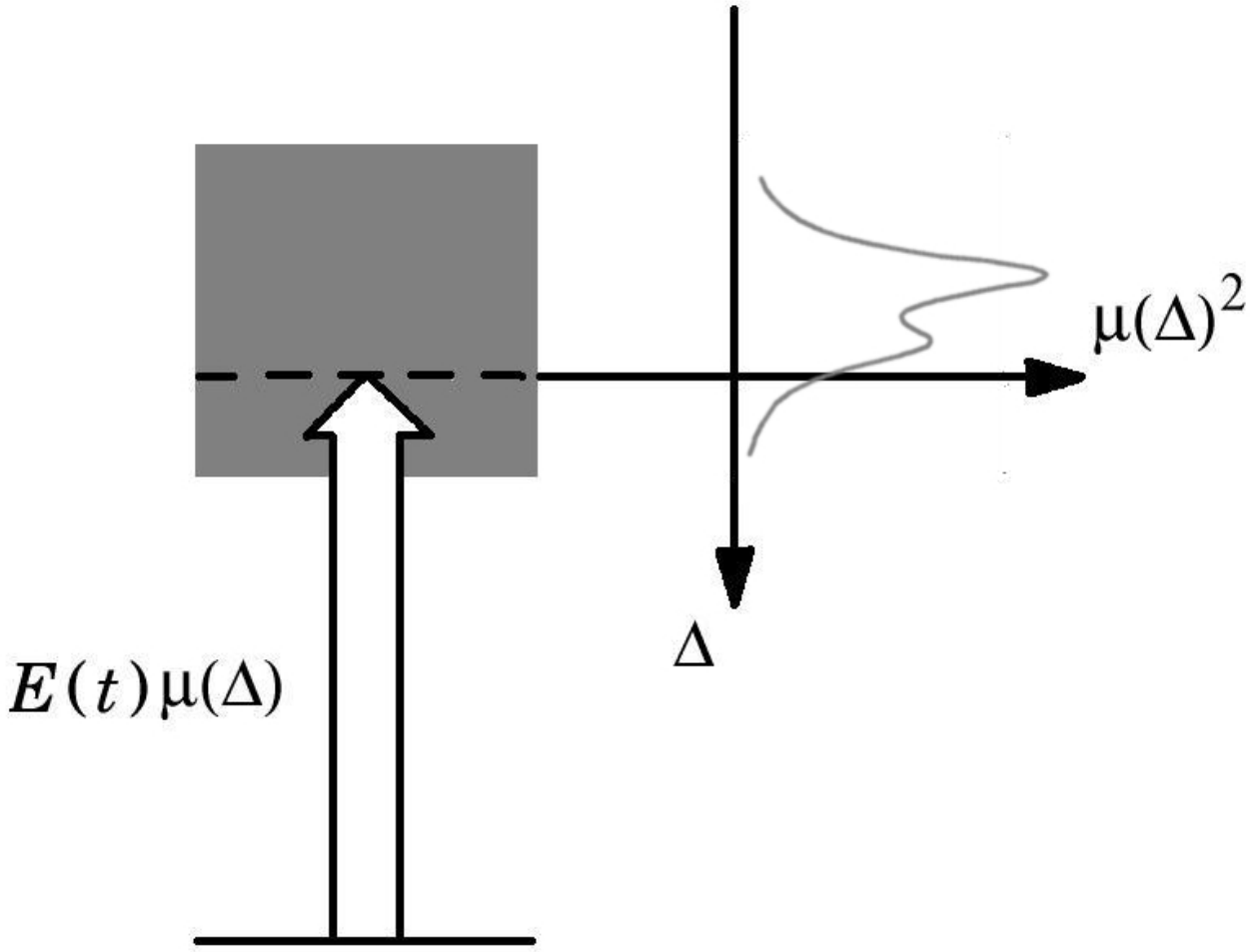

FIGURE 4.8

$(1, \text{CONTINUUM})$ system, where the continuum has the shape of two Lorentzian humps.

$$\chi_{00}(s) = \int_{-\infty}^{\infty} \frac{p(\Delta)}{(i\,s - \Delta)\,q(\Delta)}\,d\Delta\,. \tag{4.73}$$

Suppose, just for the sake of discussion, that the continuous band has the shape of two Lorentzian humps [see eq. (3.16)] as in figure (4.8):

$$\frac{p(\Delta)}{q(\Delta)} = \frac{\frac{\gamma_1^2\sigma_1}{\pi}}{(\Delta - s_1)^2 + \sigma_1^2} + \frac{\frac{\gamma_2^2\sigma_2}{\pi}}{(\Delta - s_2)^2 + \sigma_2^2}\,. \tag{4.74}$$

Then from eq. (4.73) we find

$$\chi_{00}(s) = \frac{\gamma_1^2}{i\,s - (s_1 - i\sigma_1)} + \frac{\gamma_2^2}{i\,s - (s_2 - i\sigma_2)}\,. \tag{4.75}$$

Then,

$$\widetilde{a}(s) = \frac{(s + i\beta_1)\,(s + i\beta_2)}{s^3 + i\,(\beta_1 + \beta_2)\,s^2 + (\alpha_1 + \alpha_2 - \beta_1\beta_2)\,s + i\,(\alpha_1\beta_2 + \alpha_2\beta_1)}\,. \tag{4.76}$$

where we use the abbreviations

$$\alpha_n = E^2\gamma_n^2\,,\ \beta_n = s_n - i\sigma_n.$$

By the Heaviside expansion theorem, a function $a(t)$ whose Laplace transform $\widetilde{a}(s)$ is rational with only simple poles,

$$\widetilde{a}(s) = \frac{P(s)}{Q(s)},$$

$P(s)$ and $Q(s)$ polynomials, is computed by the formula

$$a(t) = \sum_{\lambda:\,\text{roots of } Q(s)} \frac{P(\lambda)\,e^{\lambda t}}{\frac{d}{ds}Q(s)\big|_{s=\lambda}}. \tag{4.77}$$

If $Q(s)$ instead has repeated roots, a slightly different expression applies.

Since in eq. (4.76) $Q(s)$ is a cubic polynomial we could, of course, go ahead and find its roots and to use eq. (4.77) to write down $a(t)$ as a sum of three exponential terms. In some ways, however, it is actually more interesting to reason *backward* from eq. (4.75) than to reason forward from eq. (4.77). If we do so, it cannot escape our attention that eq. (4.75) is precisely the expression we would have derived for $\psi_{00}(s)$ had we started with the following discrete (but non-Hermitian) "Hamiltonian" operator rather than with eq. (4.22):

$$H_{\text{eff}} = \begin{bmatrix} 0 & E\gamma_1 & E\gamma_2 \\ E\gamma_1 & s_1 - i\sigma_1 & 0 \\ E\gamma_2 & 0 & s_2 - i\sigma_2 \end{bmatrix}. \tag{4.78}$$

Thus, in so far as the ground-state probability amplitude is concerned, the system of figure (4.8) is precisely equivalent *without approximation* to the system of eq. (4.78).

The ability to write down an effective (but *analytically exact*) Hamiltonian like eq. (4.78) is not dependent on the type of model system we have chosen, but only on the system being of low driver-rank and on the ability to approximate $K(is)$ in terms of rational functions. We will defer further discussion of this point until Chapter V, where we will discuss the production of an effective Hamiltonian in the context of a time-varying $E(t)$. Remarkably, we will discover there that an expression like eq. (4.78) is exact even in the time-varying case.

4.8. Conclusion

In this chapter, we have seen that if the driving term of the Hamiltonian of a quantum system has a low rank M (with M much less than the number of energy levels in the system), then by virtue of this alone great shortcuts can be taken in eigenvector/eigenvalue and Laplace-transform calculations.

Determination of the eigenvalues and eigenvectors of the Hamiltonian usually requires diagonalizing a matrix with dimension equal to the number of levels. However, in eq. (4.6) we have managed to replace this calculation with a matrix inversion and a matrix diagonalization of only M dimensions.

Determination of the Laplace transform of the state vector normally requires inversion of a matrix with dimension equal to the number of energy levels. However, in eq. (4.11) we have managed to replace this calculation with a matrix inversion of only M dimensions. If only the Laplace transform of the ground-state probability amplitude is required, we have gone even further, in eq. (4.21) finding $\widetilde{a}(s)$ with a matrix inversion of only $\mathrm{M}-2$ dimensions.

As applications of these methods, we have also seen some remarkable results concerning population-trapping in continuum-continuum transitions. Basically, we saw that for either *very weak* or for *very strong* interactions between two broad (featureless) continua, the population of the system remains in the continuum containing it initially. For some intermediate interaction strength, however, it is totally transferred to the other continuum. For three continua, we found similar but slightly more complex results.

4.9. Appendix A: Reality of Characteristic Polynomial

We wish to demonstrate that the characteristic polynomial of $K(\lambda)$ has real coefficients even if the matrix elements of μ are complex, as long as μ is Hermitian. In order to do this we choose a special decomposition $\mu = DF$ somewhat differently than we would in a physical problem. Recall that D and F are not uniquely determined by μ. Though the way D and F are chosen affects $K(\lambda)$, the particular choice cannot affect the characteristic polynomial of $K(\lambda)$. This is clear simply because the same eigenvalues must be produced in any case (even for complex values of λ and E), so the same polynomial is produced, up to multiplication by a constant.

Since μ is Hermitian, it can be expressed in the form

$$\mu = U^\dagger \Sigma\, U. \tag{4.79}$$

Here, U is a projection operator onto an M-dimensional subspace. Σ is an $\mathrm{M} \times \mathrm{M}$ real diagonal operator. (To obtain these operators, we simply diagonalize the μ operator, discarding the eigenvalues which are zero, along with the associated eigenvectors.) Thus we are at liberty to choose

$$D = U^\dagger,\ F = \Sigma\, U.$$

This is not normally done in a physical problem simply because it is easier to choose D and F by inspection than to calculate the eigenvalues and eigenvectors of μ as implied by the expressions above.

Thus,

$$K(\lambda) = \Sigma\, U\ (\lambda - H_0)^{-1}\, U^\dagger. \tag{4.80}$$

The interesting point about this is that $K(\lambda)$ is seen to be the product of a real diagonal matrix Σ and a Hermitian matrix which we will call χ.

The characteristic polynomial of $K(\lambda)$ can thus be written as

$$\det\, \left(\frac{1}{E} - \Sigma \chi \right),$$

bearing in mind that the eigenvalues of $K(\lambda)$ are $\frac{1}{E(\lambda)}$. By the multiplicative property of determinants, this is equal to

$$\det\, (\Sigma)\ \det\, \left(\frac{1}{E} \Sigma^{-1} - \chi \right).$$

Notice, however, that now each of these determinants is the determinant of a Hermitian matrix. But the determinant of a Hermitian matrix is real.[31] Therefore, the expression we have derived is real. Therefore, the characteristic polynomial of $K(\lambda)$ is real for real μ.

[31] Of course, this follows trivially from the reality of the eigenvalues of a Hermitian matrix, and from the fact that the determinant is the product of the eigenvalues. See E. Brown, *Introduction to the Theory of Matrices and Determinants* (University of North Carolina Press, Chapel Hill, 1958), Ch. VIII.

CHAPTER V
THE INTEGRAL EQUATIONS

5.1. Integral Form of Schrödinger's Equation

Many of the approximate methods given in the literature for solving Schrödinger's equation are based on the ability, in certain instances, to convert Schrödinger's equation from a differential equation (or set of equations) to an integral equation. Typically, this is done for the $(1, \mathsf{BAND})$ system, or a relatively trivial generalization thereof, in the case $E(t) \equiv E_0$. (See the review in Chap. II.) As mentioned before, we are more interested in time-varying fields $E(t)$. Fortunately, the constant-field restriction is unnecessary and, in this chapter, we derive simple integral equations for all low-driver-rank systems in the case of a time-dependent driving field. In general, integral equations and their properties are much less familiar to physicists than are differential equations. Nevertheless, having an integral formulation of Schrödinger's equation must be considered an advantage since various approximations which would be unobvious if the equations remained in differential format offer themselves readily in the integral case.

Three important points are made. First, it will be shown that Schrödinger's equation can always be converted systematically to a simple set of integral equations in the low-driver-rank case. In general, there are $\mathrm{M} = \mathrm{rank}(\mu)$ coupled integral equations. This is significant since if a set of coupled differential equations is *straightforwardly* converted to a set of coupled integral equations, there is generally the same number of integral equations as differential equations. (A set of N differential equations can always be converted to a set of N integral equations, but N integral equations cannot generally be converted to N differential equations.[1]) In the case of a quantum system, we would expect to find as many coupled integral equations as there are energy levels in the system. Ending up with a mere M equations is therefore quite an improvement. Second, we will see that generalizations to the Weisskopf-Wigner approximation (or the Golden Rule) follow naturally from these integral equation formulations. (See Chap. II for a review of the Weisskopf-Wigner approximation.) Third, we will see that certain approximations made to the equations in integral format can readily be interpreted as simplifications of the associated differential formulation of Schrödinger's equation. In terms of numerical calculation, differential equations are easier to deal with than integral equations, which is why the latter point is important. Consequently, having Schrödinger's equation in integral form leads to useful analytical and numerical simplifications.

[1] F. Smithies, *Integral Equations* (Cambridge University Press, New York, 1958).

We will begin with the simplest case: we will use eq. (3.3) for Schrödinger's equation, and restrict ourselves to the case $H'(t) = E(t)\mu$. In §5.2 we will present the integral equations in the more general case of $H'(t) = E_1(t)\mu_1 + ... + E_{\rm K}(t)\mu_{\rm K}$. Naturally, the matrices μ, μ_1, μ_2, etc., are all supposed to be of low rank, with μ having rank $\rm M$. The method may be generalized beyond this point quite easily, but we will not do so here.

As in eq. (4.2) of Chapter IV, a convenient beginning is to adopt the decomposition

$$\mu = DF,$$

where the column dimension of the D operator and the row dimension of the F operator are both $\rm M$.

The problem we are interested in solving is Schrödinger's equation with an initial condition:

$$i\,\frac{d}{dt}\psi(t) = H(t)\,\psi(t), \tag{5.1}$$

$$\psi(0) = \psi_{0.} \tag{5.2}$$

Replacing this problem (a set of coupled differential equations) with a set of coupled integral equations is not difficult—simply time-integrating eq. (5.1) accomplishes this. Unfortunately, the number of integral equations so obtained is equal to the number of energy levels in the system, which may be quite large. If the quantum system includes a continuous spectrum of energy levels, the number of coupled equations so obtained is uncountably infinite. We can, however, use the condition of low driver rank to obtain a much smaller number of integral equations ($\rm M$ of them, actually). How is this done?

Several steps are required. First, with various obvious and trivial (but tedious) analytic and algebraic manipulations that we will omit, eqs. (5.1,5.2) can be integrated once to obtain the set of integral equations

$$\psi(t) = e^{-iH_0 t}\psi_0 - i\int_0^t e^{iH_0(t-t')}H'(t')\,\psi(t')\,dt'. \tag{5.3}$$

The number of coupled integral equations here is equal to the number of energy levels, as mentioned above. This will always be the case so long as ψ itself appears in the equation. If, for example, we would like to have only $\rm M$ integral equations, we need a vector quantity of only $\rm M$ elements to appear in the equations in place of ψ. Following eq. (4.5), we can define such an $\rm M$-vector as follows:

$$\phi(t) = F\,\psi(t).$$

Since F is an operator with row-dimension $\rm M$, $\phi(t)$ must be an $\rm M$-vector.

Eq. (5.3) can be rewritten as

$$\psi(t) = e^{-iH_0 t}\psi_0 - i\int_0^t E(t')\,e^{iH_0(t-t')}D\,\phi(t')\,dt'. \tag{5.4}$$

Eq. (5.4) is interesting because it tells us that knowledge of $\phi(t)$ is sufficient to describe the behavior of the system: given ϕ, we are able to compute ψ via a simple time-integration.

In practical terms, this means that (as in Chapter IV) we can concentrate on calculating just the small vector $\phi(t)$, rather than the large vector $\psi(t)$.

But how to calculate $\phi(t)$? Well, multiplying eq. (5.4) by F, we get the equation

$$\phi(t) = F\, e^{-iH_0 t}\psi_0 - i\int_0^t X(t-t')\, E(t')\, \phi(t')\, dt'. \tag{5.5}$$

where the M-by-M matrix $X(t)$ is defined by the expression

$$X(t) = F\, e^{-iH_0 t} D. \tag{5.6}$$

$X(t)$ can be regarded as a known quantity since H_0 is a diagonal matrix and since D and F are known. Notice that the function $K(s)$ discussed in Chapter IV is closely related to the Fourier transform of $X(t)$.

Eqs. (5.5) are the desired results of our derivation. They form a set of M coupled integral equations for the quantity $\phi(t)$, which can be inserted into eq. (5.4) to give $\psi(t)$ with only an explicit time integration.

If the initial state is the ground state of the system, then

$$H_0\psi_0 = 0. \tag{5.7}$$

In this case, eq. (5.5) reduces to

$$\phi(t) = \phi_0 - i\int_0^t X(t-t')\, E(t')\, \phi(t')\, d\phi. \tag{5.8}$$

If eq. (5.7) holds, it is generally the case that we are *only* interested in solving for the ground-state probability amplitude $a(t)$ and have no real interest in the probability amplitudes of the remaining levels. If so, we can save ourself the effort of applying eq. (5.4) to generate $\psi(t)$ from $\phi(t)$: for, if the initial (ground) state $\psi_0^\dagger$ happens to be one of the rows of the matrix F, then the element of $\phi(t)$ corresponding to that row is the ground-state probability amplitude $a(t)$. If the ground state is *not* one of the rows of F, we can simply adjoin $\psi_0^\dagger$ to F by fiat, adjoining an extra column of zeroes onto D at the same time to preserve relation (4.2).

The most familiar instance of eq. (5.8) is the $(1, \mathsf{BAND})$ system. For example, a $(1, \mathsf{CONTINUUM})$ system [see eq. (3.11)] has

$$\mu = \begin{bmatrix} 0 & \mu(\Delta') \\ \mu(\Delta) & 0(\Delta, \Delta') \end{bmatrix},$$

as expressed in "continuous matrix" notation (§3.4). Though D and F are not uniquely determined, by inspection one workable alternative is to allow

$$D = \begin{bmatrix} 0 & 1 \\ \mu(\Delta) & 0(\Delta) \end{bmatrix},\ F = \begin{bmatrix} 1 & 0(\Delta') \\ 0 & \mu(\Delta') \end{bmatrix}. \tag{5.9}$$

As usual, the various elements of these matrices are dimensionally incompatible, without being of any great concern to us. From eq. (5.9) it follows immediately that

$$X(t) = \begin{bmatrix} 0 & 1 \\ \chi(t) & 0 \end{bmatrix}, \tag{5.10}$$

where

$$\chi(t) = \int \mu(\Delta)^2 e^{-i\Delta t} d\Delta. \tag{5.11}$$

Though there are two integral equations (5.8) in this example, we note that $a(t)$ (the ground-state probability amplitude) is itself the first element of the 2-vector $\phi(t)$. We can trivially combine the two integral equations to give the familiar single integro-differential equation

$$\frac{d}{dt}\, a(t) = -E(t) \int_0^t E(t')\, \chi(t-t')\, a(t')\, dt'. \tag{5.12}$$

In the case of a discrete band, this equation still holds, with the integral replaced by a sum in eq. (5.11). These equations have appeared very often in the literature, as mentioned earlier.

5.2. Several Driving Fields

Now let us consider the more general case of eq. (3.2'), in which

$$H'(t) = E_1(t)\mu_1 + ... + E_{\mathrm{K}}(t)\mu_{\mathrm{K}}. \tag{5.13}$$

This is the kind of driving term we could expect to encounter, for example, in the case of a molecular system being driven by several different quasi-monochromatic laser fields. In such a case, the Rotating-Wave Approximation has probably been made, and the $E_n(t)$ functions presumably represent the envelopes of the individual laser fields.

We must think a little more carefully in defining the driving rank of a system of this kind. Since $H'(t)$ varies in time, the rank of the matrix $H'(t)$ can vary in time as well. Nevertheless, there is still a characteristic overall driving rank M, obeying the constraint

$$\mathrm{M} \leq \mathrm{rank}\, \mu_1 + \mathrm{rank}\, \mu_2 + ... + \mathrm{rank}\, \mu_{\mathrm{K}}. \tag{5.14}$$

For any given matrix, the rank is equal to the number of linearly independent rows (or columns). We will define the overall driving rank of this system to be the total number of linearly independent rows (or columns) of all of the μ_n matrices taken together. Thus, the equality in eq. (5.14) holds only if no column in any of μ matrices is a linear combination of columns appearing in the other μ matrices.

A decomposition principle similar to eq. (4.2) holds: There exists an operator F, and operators D_n, such that each individual μ_n can be decomposed as

$$\mu_n = D_n F. \tag{5.15}$$

Here, F has row-dimension M and each of the D_n has column-dimension M. However, D_n has a rank of only rank(μ_n). This can be seen quite easily: to form F, we simply decompose

each μ_n individually as $D_n F_n$. Then we stack up all of the F_n matrices to form F, and add extra columns of zeroes onto D_n to make the dimensions of the matrices compatible.

Thus, in place of eq. (5.4), we have

$$\psi(t) = e^{-iH_0 t}\psi_0 - i\int_0^t e^{iH_0(t'-t)}\left(E_1(t')D_1 + ... + E_{\rm K}(t')D_{\rm K}\right)\,\phi(t')\,dt', \tag{5.16}$$

and in place of eq. (5.5),

$$\phi(t) = F\,e^{-iH_0 t}\psi_0 - i\int_0^t \left(E_1(t')X_1(t-t') + ... + E_{\rm K}(t')X_{\rm K}(t-t')\right)\,\phi(t')\,dt', \tag{5.17}$$

Naturally, we have defined

$$X_n(t) = F\,e^{-iH_0 t}\,D_n. \tag{5.18}$$

Once again, if the initial state is the ground state, then eq. (5.17) reduces to

$$\phi(t) = \phi_0 - i\int_0^t \left(E_1(t')X_1(t-t') + ... + E_{\rm K}(t')X_{\rm K}(t-t')\right)\,\phi(t')\,dt', \tag{5.19}$$

The use of these equations is naturally similar to the use of those in the previous section: eq. (5.19) [or (5.17)] is used to solve for $\phi(t)$, which is then inserted into eq. (5.16) to give $\psi(t)$ itself. As in the previous section, if our only desire is to find $a(t)$ [and not all of $\psi(t)$], the use of eq. (5.16) can be avoided entirely.

5.3. Generalizing the Weisskopf-Wigner and Golden-Rule Approximations

One advantage in having a set of integral equations like eqs. (5.5) or (5.19) is that since the theory of approximation of integrals is more highly developed than the theory of approximation of derivatives, it is easier for us to write down demonstrably valid approximations to the integral equations. For example: just as the Weisskopf-Wigner approximation and Fermi's Golden Rule can be derived from eq. (5.12), generalizations to these approximations can be derived from the full set of integral equations (5.8) or (5.19).

To get the general idea of how this is done, let us derive the normal Weisskopf-Wigner and Golden-Rule approximations as an exercise. Starting from eq. (5.12), we simply need to approximate the integral using the mean value theorem of the integral calculus.[2] To do this we need first to understand the properties of the $\chi(t)$ function. For a continuum, the function $\chi(t)$ obeys the relations

$$\chi(0) = \gamma^2,$$

(recall definition 3.12), and

[2] J. Todd in *Handbook of Physics*, second edition, ed. by E. Condon and H. Odishaw (McGraw-Hill, New York, 1967), Ch. 3.

$$\chi(t) \xrightarrow{(t\to 0)} 0\,.$$

In fact, this decay of $\chi(t)$ occurs in a time something like $\frac{1}{\sigma}$, where σ is the "width" in frequency space of the continuous band. This may be easily seen by noting that for a continuum $\chi(t)$ is essentially the Fourier transform of the bandshape function $\mu(\Delta)^2$ (except for a normalizing constant). Speaking loosely, the width of a bell-shaped function times the width of its Fourier transform is of order unity.[3]

If this decay time is assumed to be short compared to the characteristic time scales of change of $E(t)$ and $a(t)$, then eq. (5.12) may be approximated

$$\frac{d}{dt}\,a(t) \approx -E(t)^2 \left(\int_0^\infty \chi(t')\,dt'\right) a(t). \tag{5.20}$$

[One could imagine improvements to this approximation by taking the upper limit of the integration as t, by introducing a delay time in $a(t-\delta t)$ and $E(t-\delta t)$, and so forth. The latter step would have importance in a discussion of quantum chaos.[4]] Incidentally, approximations of this kind are generically referred to as Markov Approximations, since a Markov process[5] is one in which the future behavior of the system depends only on its present state and not its past state. The full set of Schrödinger's equations are Markovian since $\frac{d\psi}{dt}$ depends on $\psi(t)$. However, the integro-differential equation (5.12) for $a(t)$ is not Markovian since $\frac{da(t)}{dt}$ depends on the values of $a(t)$ for all past values of t. Thus, in this formulation, the system has some memory of its past. The Markov approximation is said to destroy the system's memory, since in eq. (5.20), $\frac{da(t)}{dt}$ once again depends only on $a(t)$.

As it happens, by inserting eq. (5.11) into the integral in eq. (5.20), we can actually compute the integral, using a Dirac delta function and a Cauchy principal value:[6]

$$\overline{\chi} = \int_0^\infty \chi(t)\,dt = \pi\,\mu(0)^2 + i\,\mathbb{P}\int_{-\infty}^\infty \frac{\mu(\Delta)^2}{\Delta}\,d\Delta, \tag{5.21}$$

where the name $\overline{\chi}$ has been assigned to this quantity for convenience. If eqs. (5.20) and (5.21) are used together with the assumption that $E(t)$ is constant in time, the result is the Weisskopf-Wigner approximation

$$a(t) \approx e^{-E^2\overline{\chi}\,t}. \tag{5.22}$$

If, in addition, eq. (5.22) is specialized to short times [$a(t) \approx 1$], then we arrive at the Golden Rule:

$$\begin{aligned}\frac{d}{dt}\,|a(t)|^2 &\approx -2\,E^2\,\mathcal{R}\mathrm{e}(\overline{\chi})\;|a(t)|^2 \\ &\approx -2\,E^2\,\mathcal{R}\mathrm{e}(\overline{\chi}).\end{aligned} \tag{5.23}$$

---

[3] F. Matsen, *Vector Spaces and Algebras for Chemistry and Physics* (Holt, Rinehart, and Winston, New York, 1970), §3.8.

[4] K. Ikeda, K. Kondo, and O. Akimoto, *Phys. Rev. Lett.* **49**, 1467 (1982); P. W. Milonni, J. Ackerhalt, H. Galbraith, and M.-L. Shih, *Phys. Rev. A* **28**, 32 (1983).

[5] S. Ross, *Stochastic Processes* (Wiley, New York, 1982).

[6] A. Messiah, *Quantum Mechanics*, trans. by G. Temmer (Wiley, New York, 1958).

If

$$E^2 \, |\overline{\chi}| \ll \sigma, \tag{5.24}$$

where σ is the decay rate of $\chi(t)$, then the assumptions used to derive the equations are valid, and hence the equations themselves are valid. These same formulas are often applied as well to systems with densely packed, but still discrete, levels in the band. In such a case, formulas (5.23) and (5.22) remain initially correct. Eventually, however, after a *recurrence time* $\tau_{\rm R}$ characteristic of the system, the ground-state population builds up again.[7] This will be discussed later. [To recognize eq. (5.23) as the Golden Rule, by the way, it is helpful to use units of measurement more standard than ours. For example, in the RWA, our $E^2\mu(0)^2 \rightarrow E^2\mu(0)^2/(2\hbar)$ in terms of more normal notation.]

To illustrate how one can go about generalizing these approximations, let us repeat the corresponding calculations for a $(1, \underline{\text{CONTINUUM}})$ system. Recall from §3.3 that the underline implies that there are transitions within the continuous band. We only want to do simple calculations here, so we will adopt a very simple scheme of intraband transitions. For us, "simple" means "of low dipole rank", so we'll simply add one to the rank of the dipole matrix. In the continuous matrix notation introduced in §3.4, we will convert the $(1, \text{CONTINUUM})$ dipole matrix μ to a $(1, \underline{\text{CONTINUUM}})$ according to the prescription in eq. (3.19):

$$\mu = \begin{bmatrix} 0 & \mu(\Delta')^\star \\ \mu(\Delta) & 0(\Delta, \Delta') \end{bmatrix} \rightarrow \begin{bmatrix} 0 & \mu(\Delta')^\star \\ \mu(\Delta) & \frac{\mu(\Delta,0)\mu(0,\Delta')}{\mu(0,0)} \end{bmatrix}. \tag{5.25}$$

An adequate decomposition of μ for our purposes is

$$\mu = DF = \begin{bmatrix} 0 & 1 & 0 \\ \mu(\Delta) & 0(\Delta) & \mu(\Delta, 0) \end{bmatrix} \begin{bmatrix} 1 & 0(\Delta') \\ 0 & \mu(\Delta')^\star \\ 0 & \frac{\mu(0,\Delta')}{\mu(0,0)} \end{bmatrix}. \tag{5.26}$$

As usual, we have arranged for the first component of the 3-vector $\phi(t)$ to be the ground-state probability amplitude $a(t)$. For simplicity, we will refer to the other elements of $\phi(t)$ as $b(t)$ and $c(t)$. $X(t)$ is seen to be

$$\begin{aligned} X(t) &= \begin{bmatrix} 0 & 1 & 0 \\ \int |\mu(\Delta)|^2 e^{-i\Delta t} d\Delta & 0 & \int \mu(\Delta, 0)\mu(\Delta)^\star e^{-i\Delta t} d\Delta \\ \int \frac{\mu(\Delta)\mu(0,\Delta)}{\mu(0,0)} e^{-i\Delta t} d\Delta & 0 & \int^{-i\Delta t} \frac{|\mu(\Delta,0)|^2}{\mu(0,0)} e^{-i\Delta t} d\Delta \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 & 0 \\ \chi_{\rm ba}(t) & 0 & \chi_{\rm bc}(t) \\ \chi_{\rm ca}(t) & 0 & \chi_{\rm cc}(t) \end{bmatrix}. \end{aligned} \tag{5.27}$$

If we insert $X(t)$ from eq. (5.27) into the set of integral equations (5.8), we unfortunately do not see any obvious way of uncoupling the equations for $a(t)$, $b(t)$, and $c(t)$ [as

[7] A. Makarov, V. Platonenko, and V. Tyakht, *Sov. Phys. JETP* **48**, 1044 (1978).

was quite easily done for the $(1, \mathsf{BAND})$ system]. Nevertheless, we can still carry out a Markov approximation similar to that used with the $(1, \mathsf{BAND})$ system. As before, for a continuum we expect $\chi_{\rm ba}(t)$, ..., $\chi_{\rm cc}(t)$ to decay to zero at some characteristic respective rates $\sigma_{\rm ba}$, ..., $\sigma_{\rm cc}$. Thus, if $E(t)$ and $\phi(t)$ change slowly relative to these quantities, we can once again perform our Markov approximation on eq. (5.8) using the mean value theorem of calculus:

$$a(t) = 1 - i \int_0^t E(t')\, b(t')\, dt' \tag{5.28}$$

$$b(t) \;\approx -E(t)\,(\overline{\chi}_{\rm ba} a(t) + \overline{\chi}_{\rm bc} c(t)) \tag{5.29}$$

$$c(t) \;\approx -E(t)\,(\overline{\chi}_{\rm ca} a(t) + \overline{\chi}_{\rm cc} c(t))\,, \tag{5.30}$$

where the quantities $\overline{\chi}_{\rm ba}$, ..., $\overline{\chi}_{\rm cc}$, are defined in analogy to eq. (5.21). For example,

$$\overline{\chi}_{\rm bc} = \int_0^\infty \chi_{\rm bc}(t)\, dt = \pi\, \mu(0,0)\, \mu(0)^\star + i\, \mathbb{P} \int_{-\infty}^\infty \frac{\mu(\Delta, 0)\, \mu(\Delta)^\star}{\Delta}\, d\Delta,$$

with $\mathbb{P}$ denoting the Cauchy principal value. Now, even though the full set of integral equations could not be decoupled in this example, the approximate eqs. (5.28-5.30) can be decoupled with very little difficulty to give:

$$\frac{d}{dt}\, a(t) = -\left(\overline{\chi}_{\rm ba} - \frac{i\, E(t)\, \overline{\chi}_{\rm bc}\, \overline{\chi}_{\rm ca}}{1 + i\, E(t)\, \overline{\chi}_{\rm cc}}\right) E(t)^2 a(t). \tag{5.31}$$

This expression is the required generalization of the Weisskopf-Wigner approximations. In the earlier equation (5.20) which corresponded to eq. (5.31) for a $(1, \mathsf{CONTINUUM})$ system, we had simply the first term. Therefore, the second term represents a correction for intraband transitions.

Of course, eq. (5.31) is valid only if (as mentioned above) the $\chi(t)$ functions die to zero quickly compared to the times on which $E(t)$ and $a(t)$ change significantly [and to the extent that the approximation in eq. (3.19) is reasonable]. The strength of the method lies in the fact that if some of the $\chi(t)$ functions do *not* die away rapidly enough, we have the option of applying some approximations other than the mean-value theorem on the offending integral equations.

These manipulations are closely related to those used in the quantum theory of damping to derive the Langevin equations[8] of the system. In a Langevin approach, the electromagnetic field is quantized (and time-independent) rather than classical (and time-varying) as in our derivation above. The net result (*i.e.*, Langevin's equation), however, is an integral equation that does not differ from those we have seen above, except for the addition of a random-noise driving term that simulates the effect of the field quantization. The low driver-rank approach can thus probably be used to derive Langevin equations as well as semi-classical integral equations, although we have not yet used it to do so.

[8] W. H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973).

5.4. Reconstructing the Differential Equations, I: Effective Hamiltonian

We can look at the Markov approximation described in the previous section in a different way. Having started with a large set of differential equations (5.1), we passed to a small set of integral equations (5.8), and finally to a small set of differential equations (5.31). In essence, what we have done is to introduce a low-dimensional effective Hamiltonian for the system. (See the survey in Chap. II.)

This point is perhaps more easily appreciated for a more complex system. Consider an $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system, which can be viewed as a completely general N-level discrete system with each level coupled to a set of background energy levels or reservoir. (Again, see the survey in Chap. II.) Such a system has a rank of $2\mathrm{N}$, and we are able to produce an N-level effective Hamiltonian for it under the kinds of manipulations and conditions mentioned in the previous section. Let's see how.

First, we must write down the Hamiltonian for the system. In an obvious notation:

$$H = \begin{bmatrix} \delta_1 & 0 & \cdots & 0 & 0(\Delta') \\ 0 & \delta_2 & \cdots & 0 & 0(\Delta') \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \delta_{\mathrm{N}} & 0(\Delta') \\ 0(\Delta) & 0(\Delta) & \cdots & 0(\Delta) & \Delta\delta(\Delta - \Delta') \end{bmatrix} + E(t) \begin{bmatrix} \mu_{11} & \mu_{12} & \cdots & \mu_{1\mathrm{N}} & \mu_1(\Delta)^\star \\ \mu_{21} & \mu_{22} & \cdots & \mu_{2\mathrm{N}} & \mu_2(\Delta)^\star \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mu_{\mathrm{N}1} & \mu_{\mathrm{N}2} & \cdots & \mu_{\mathrm{NN}} & \mu_{\mathrm{N}}(\Delta)^\star \\ \mu_1(\Delta) & \mu_2(\Delta) & \cdots & \mu_{\mathrm{N}}(\Delta) & 0(\Delta, \Delta') \end{bmatrix}.$$

In practice, of course, we expect the dipole matrix elements μ_{nn} to be zero. Also, without loss of generality, we can insist that $\delta_1 = 0$. By inspection a workable $\mu = DF$ decomposition is

$$D = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ 0(\Delta) & 0(\Delta) & \cdots & 0(\Delta) & \mu_1(\Delta) & \mu_2(\Delta) & \cdots & \mu_{\mathrm{N}}(\Delta) \end{bmatrix}. \tag{5.32}$$

$$F = \begin{bmatrix} \mu_{11} & \mu_{12} & \cdots & \mu_{1\mathrm{N}} & \mu_1(\Delta)^\star \\ \mu_{21} & \mu_{22} & \cdots & \mu_{2\mathrm{N}} & \mu_2(\Delta)^\star \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mu_{\mathrm{N}1} & \mu_{\mathrm{N}2} & \cdots & \mu_{\mathrm{NN}} & \mu_{\mathrm{N}}(\Delta)^\star \\ 1 & 0 & \cdots & 0 & 0(\Delta') \\ 0 & 1 & \cdots & 0 & 0(\Delta') \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0(\Delta') \end{bmatrix}. \tag{5.33}$$

By inspection of F, it is clear that the probability amplitudes of the N discrete levels will be the final N elements of $\phi(t)$. Let us denote the first N elements of $\phi(t)$ by $\Phi_1(t)$, ..., $\Phi_{\mathrm{N}}(t)$ and the N discrete probability amplitudes by $\psi_1^{(\mathrm{D})}(t)$, ..., $\psi_{\mathrm{N}}^{(\mathrm{D})}(t)$. We will find it

convenient in a moment to denote these sets of elements as the N-vectors $\Phi(t)$ and $\psi^{(\mathrm{D})}(t)$, respectively. Thus, $\phi(t)$ consists of the two vectors $\Phi(t)$ and $\psi^{(\mathrm{D})}(t)$ joined "end to end." Also, we will find it convenient to define two $\mathrm{N}\times\mathrm{N}$ matrices: $H_0^{(\mathrm{D})} = \mathrm{diag}(\delta_1, ..., \delta_{\mathrm{N}})$ and $\mu^{(\mathrm{D})} = [\mu_{ij}]$. Of course, the meaning of the superscript "D" is that these are the parts of the state vector and the Hamiltonian pertaining only to the discrete part of the system.

A further trivial calculation shows that the $2\mathrm{N}\times 2\mathrm{N}$ matrix $X(t)$ can be conveniently partitioned into $\mathrm{N}\times\mathrm{N}$ parts:

$$X(t) = \begin{bmatrix} \mu^{(\mathrm{D})} e^{-iH_0^{(\mathrm{D})}t} & \chi(t) \\ e^{-iH_0^{(\mathrm{D})}t} & 0 \end{bmatrix}, \tag{5.34}$$

where the $\mathrm{N}\times\mathrm{N}$ matrix $\chi(t)$ has matrix elements $\chi_{ij}(t)$ given by

$$\chi_{ij}(t) = \int \mu_i(\Delta)^\star \mu_j(\Delta)\, e^{-i\Delta t} d\Delta. \tag{5.35}$$

Writing out the integral equations (5.8) gives us

$$\Phi(t) = \mu^{(\mathrm{D})}\psi^{(\mathrm{D})}(t) - i\int_0^t E(t')\left(\mu^{(\mathrm{D})} e^{-iH_0^{(\mathrm{D})}(t-t')}\Phi(t') + \chi(t-t')\,\psi^{(\mathrm{D})}(t')\right) dt'$$

$$\psi^{(\mathrm{D})}(t) = \psi_0^{(\mathrm{D})} - i\int_0^t e^{-iH_0^{(\mathrm{D})}(t-t')} E(t')\,\Phi(t')\, dt'.$$

If we are interested in $\psi^{(\mathrm{D})}(t)$ alone, and not in $\Phi(t)$, these two sets of equations can be combined into a single set of N integro-differential equations reminiscent of eq. (5.12):

$$i\,\frac{d}{dt}\,\psi^{(\mathrm{D})}(t) = \left(H_0^{(\mathrm{D})} + E(t)\,\mu^{(\mathrm{D})}\right)\psi^{(\mathrm{D})}(t) - E(t)\int_0^t E(t')\,\chi(t-t')\,\psi^{(\mathrm{D})}(t')\,dt'. \tag{5.36}$$

Now, eq. (5.36) is exact, and is interesting in itself as a Schrödinger's N-level equation with corrections. But consider what happens if we make an approximation to the integral in eq. (5.36), of the type discussed in the previous section. The matrix elements of the $\chi(t)$ matrix are expected to die to zero. If the characteristic time scale on which this occurs is short compared to the rate of change of $\psi^{(\mathrm{D})}(t)$ or $E(t)$, then by the mean value theorem of calculus (the Markov approximation),

$$i\,\frac{d}{dt}\,\psi^{(\mathrm{D})}(t) \approx \left(H_0^{(\mathrm{D})} + E(t)\,\mu^{(\mathrm{D})} - E(t)^2\,\overline{\chi}\right)\psi^{(\mathrm{D})}(t). \tag{5.37}$$

Here, is as expected:

$$\overline{\chi} = \int_0^\infty \chi(t)\,dt\,,$$

which can be evaluated using Dirac delta functions and Cauchy principal values, as discussed previously. Thus, we have found an effective Hamiltonian for this system of

$$H_{\mathrm{eff}} = H_0^{(\mathrm{D})} + E(t)\,\mu^{(\mathrm{D})} - E(t)^2\,\overline{\chi}\,. \tag{5.38}$$

Note that in this system of units, $E\mu$ has the dimensionality of a frequency. χ has the dimensionality of μ^2, while $\overline{\chi}$ has the dimensionalityof $\mu^2 \times (\mathrm{time})$. Thus, all of the terms in eq. (5.38) are dimensionally frequency and, as promised, the dimensional incompatibility among the various matrix elements of D, F, X, *etc.*, has not harmed us.

The conditions under which this approximation is good have been discussed in a general way in §5.3. Basically, we expect this to be a good approximation for low values of E, if $E(t)$ is slowly varying (or has been switched on suddenly and then only varies slowly), and if the *width* of the continuum is large.

5.5. Reconstructing the Differential Equations, II: Rational Functions

Another way in which an approximate (and different) set of differential equations can be constructed from the (exact) integral equations involves approximation by rational functions. To put our discussion on more concrete terms, let's restrict ourselves to the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system introduced in the previous section. Everything we have to say will be applicable to any low-dipole rank system (containing continua), but we would not gain any understanding by discussing the more general problem. In line with this, we will aim at simplicity rather than optimization in the following discussion.

Suppose that the products $\mu_n(\Delta)^\star \mu_m(\Delta)$ appearing in eq. (5.35) go to zero (as $|\Delta|$ goes to ∞) as $|\Delta|^{-\mathrm{k}}$ for some integer k. We will refer to continua of this kind as *broad-winged continua* to distinguish them from the more quickly dying *narrow-winged continua* discussed in the next section. Products of this kind can be approximated as quotients of polynomials,

$$\mu_n(\Delta)^\star \mu_m(\Delta) \approx \frac{p_{nm}(\Delta)}{q_{nm}(\Delta)}, \tag{5.39}$$

where the degree $Q_{nm} = \partial q_{nm}$ of q_{nm} is k (or more) greater than the degree ∂p_{nm} of p_{nm}.

Note that if these products are rational functions, then the integrals in eq. (5.35) can actually be evaluated simply, turning out to be sums of Q_{nm} exponentially decaying terms.[9] [This is true if the polynomial q_{nm} has no repeated roots. We will always assume there are no repeated roots since, as an approximation, we could always just separate the two roots by a minuscule amount without altering the numerical value of the function by much.] Suppose, therefore, that we have an expression of the form

$$\chi(t) = \sum_{q=1}^{\mathrm{Q}} \chi_q \, e^{-\lambda_q t}, \tag{5.40}$$

where $\chi(t)$ is the $\mathrm{N} \times \mathrm{N}$ matrix defined in the previous section. Here, the χ_q are constant $\mathrm{N} \times \mathrm{N}$ matrices and Q is some constant less than the sum of all the Q_{nm}. (If this description seems too sketchy, a sample calculation with all of these steps made explicit appears in §5.8.)

[9] G. Polya and G. Latta, *Complex Variables* (Wiley, New York, 1974), Ch. 5.

Leaving this $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system momentarily, for the sake of argument let us consider a discrete system with the following "Hamiltonian":

$$H_{\text{eff}} = \begin{bmatrix} H_0^{(\mathrm{D})} + E(t)\,\mu^{(\mathrm{D})} & E(t)\chi_1 & E(t)\chi_2 & \cdots & E(t)\chi_{\mathrm{Q}} \\ E(t)I & -i\lambda_1 I & 0 & \cdots & 0 \\ E(t)I & 0 & -i\lambda_2 I & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ E(t)I & 0 & 0 & \cdots & -i\lambda_{\mathrm{Q}} I \end{bmatrix}. \tag{5.41}$$

Of course, not being Hermitian, this cannot be a true Hamiltonian. The $\mathrm{N}\times\mathrm{N}$ χ_n matrices are as defined in eq. (5.40), while the I are intended to be $\mathrm{N}\times\mathrm{N}$ identity matrices. This "system" therefore has $(\mathrm{Q}+1)\mathrm{N}$ "energy levels".

It will not escape our attention that, like the original $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system, the system with the Hamiltonian of eq. (5.41) is of rank $2\mathrm{N}$. In fact, we can go further than this. Using eq. (5.40), it is easy to ascertain that this system has a $X(t)$ matrix identical to that of the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system, as given by eq. (5.34). Thus, in so far as the probability amplitudes of the discrete states are concerned, this new system behaves identically to the original system.

In other words, eq. (5.41) is in fact an effective Hamiltonian for the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system. Though having many more levels than the effective Hamiltonian of eq. (5.38), it is accurate under a much wider range of circumstances. If fact, if eq. (5.39) is exact (and the band shapes are describable as rational functions), then eq. (5.41) is *exact*. Unlike the effective Hamiltonian derived in the previous section, this Hamiltonian is then valid in all circumstances.

Note, by the way, that eq. (5.41) is not uniquely determined by eq. (5.40). For example, we could just as easily have put the χ_n in the first column and the I in the first row. In fact, we could have put anything in these rows and columns, just so long as the corresponding elements of the first column and the first row multiply to give the proper χ_n matrix.

One particular case is worth special attention. This is the case of the continuous Lorentzian band, as defined in §3.5. This band-shape is interesting both in that it is widely studied, but also in that it is the simplest example of a rational band.

If we use the shape of the Lorentzian band, as described by eq. (3.16), along with the equations developed earlier in this section, we find that:

$$H_0^{(\mathrm{D})} = 0,\ \chi(t) = \gamma^2 e^{-(\sigma + i\,s)t}.$$

(These are 1×1 matrices.) Thus, according to the foregoing discussion, we can simply write down an effective Hamiltonian of

$$H_{\text{eff}} = \begin{bmatrix} 0 & E(t)\gamma \\ E(t)\gamma & s - i\,\sigma \end{bmatrix}. \tag{5.42}$$

This equation is *exact* for the $(1, \mathsf{LORENTZIAN\ CONTINUUM})$ system. We saw something like this earlier [eq. (4.33)] using Laplace transforms in the case of a constant E-field, but now see it more generally.

Eq. (5.42) is, of course, precisely the Hamiltonian for a 2-level system, with the "slight" modification of a complex detuning in the upper level. Consequently, many analytical

results concerning 2-level systems can be immediately generalized to the $(1,\mathsf{LORENTZIAN})$ system simply by adding a complex part to the detuning.

Examples of failed opportunities for such generalization are easily found in the literature. For example, the ground-state probability amplitude for a 2-level system has been derived analytically for $E(t)$ having a *semi-exponential* pulse shape.[10] A semi-exponential pulse increases from a value of zero at $t = -\infty$ to a limiting value of ε_∞ at $t = \infty$, with most of the actual increase being approximately of the form $e^{\lambda t}$. See figure (5.1) in §5.9. Though the original authors solved only for the ground-state probability amplitude in a 2-level system, they *could* have immediately generalized their result to the $(1, \mathsf{LORENTZIAN\ CONTINUUM})$ system, giving

$$a(\tau) = e^{i\zeta_- t}\mathrm{M}\left(i\,\frac{(s+i\sigma)\zeta_-}{2\lambda\alpha},\, -i\,\frac{s+i\sigma}{\lambda},\, 2i\alpha\tau\right),$$

where

$$\zeta_- = \frac{s+i\sigma}{2\varepsilon_\infty} - \alpha\,,\ \alpha = \sqrt{\left(\frac{s+i\sigma}{2\varepsilon_\infty}\right)^2 + \left(\frac{\mu_{01}}{2}\right)^2}.$$

M here is the confluent hypergeometric function,[11] not to be confused with the rank of the system, which is 2. It is amusing to note that in the same paper proving the result above (for 2-level systems only), the exact solution for the 2-level system and the $(1, \mathsf{LORENTZIAN})$ system was given in terms of Bessel functions for a different pulse shape, namely $E(t) = E_0 e^{\lambda t}$. As we would expect, these solutions differed only in that one had a complex detuning. The authors noted this, but it did not occur to them that the semi-exponential case described above could be similarly extended to the $(1,\mathsf{LORENTZIAN})$ case.

As mentioned above, the rational approximation technique for describing continua will receive some further practical development in §5.8.

5.6. Reconstructing the Differential Equations, III: Gaussian Integration

In the prior two sections we saw two different methods of producing a discrete effective Hamiltonian in a system with low dipole rank. In essence, these methods introduced damping in the form of a non-Hermitian part of the Hamiltonian. In this section, we see yet a third method of getting a discrete set of approximate differential equations from the integral form of Schrödinger's equations. This time there will be a different emphasis. Here, we would like to produce a fully Hermitian effective Hamiltonian. For the sake of discussion, let us again restrict ourselves to the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system, again with the understanding that the approach we will present has general application to low-rank systems (with continua).

[10] R. S. Burkey and C. D. Cantrell, *Opt. Commun.* **43**, 64 (1982).

[11] L. J. Slater in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), Ch. 13.

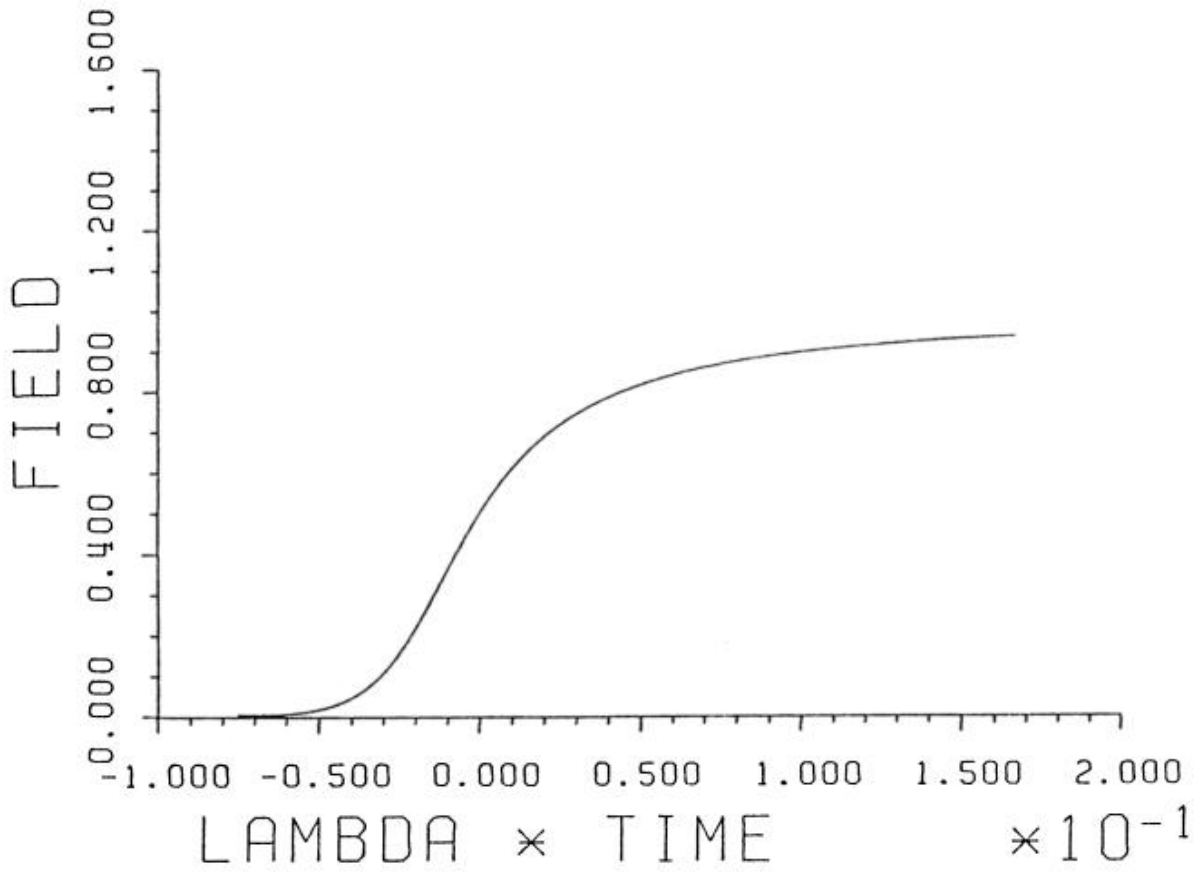

FIGURE 5.1

The shape of a *semi-exponential* pulse. The pulse is approximately exponential ($e^{\lambda t}$) for $t < 0$, but goes to a limit ε_∞ as $t \to \infty$. The shape is defined implicitly by the equation

$$E(\tau) = \frac{1}{1 + \dfrac{\lambda \tau}{\varepsilon_\infty}},$$

where in place of the time t we use the monotonically increasing quantity

$$\tau(t) = \int_{-\infty}^{t} E(t')\, dt'.$$

What we would like to do here is to apply straightforward approximate integration techniques to the evaluation of the individual matrix elements of the kernel $X(t)$, or in the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ case to the evaluation of $\chi(t)$. Thus, we would like to express integrals like those in eq. (5.35) in terms of sums of exponential functions [as in eq. (5.40)], by means of approximate integration formulas.[12]

The need to approximate the integral in eq. (5.35) well at all times t makes things tricky, since the behavior of the function $e^{-i\Delta t}$ is very different at different times. At small times it oscillates slowly, at large times it oscillates rapidly in Δ, and we need a single formula to cover both cases.

We'll suppose that the shape functions $\mu_n(\Delta)$ appearing in the Hamiltonian represent variations on some overall shape $\sqrt{w(\Delta)}$. Thus,

$$\mu_n = \sqrt{w(\Delta)}\rho_n(\Delta), \tag{5.43}$$

where $\rho_n(\Delta)$ is some function relatively constant in Δ. From this standpoint, all of the functions $\chi_{nm}(t)$ are integrals of the form

$$\int w(\Delta)\, f(\Delta)\, d\Delta.$$

Thus, the problem we are left with is really that of how to approximate such integrals effectively.

It is helpful to shift our emphasis from solution of this integral *per se* to the more general problem of approximating the linear functional[13] W defined by

$$W\{f(\Delta)\} = \int w(\Delta)\, f(\Delta)\, d\Delta. \tag{5.44}$$

Such a functional takes a Δ-function as an argument and returns a number as result. Having solved that problem, it would be a simple matter to compute

$$\chi_{nm}(t) = W\left\{\rho_n(\Delta)^\star \rho_m(\Delta)\, e^{-i\Delta t}\right\}.$$

In general, one approximates a linear functional such as that of eq. (5.44) as a weighted sum of the function's values at various sample points, its derivative values at various sample points, *etc*. There is no unique approximation: it is possible to choose the number of sample points, what order derivatives are to be used, and so forth. For this application, we are interested solely in the function values. We would like to have an approximation of the form

$$W\{f(\Delta)\} \approx W_1 f(\Delta_1) + \ldots + W_{\mathrm{Q}} f(\Delta_{\mathrm{Q}}), \tag{5.45}$$

for some reasonably small value of Q, so that

$$\chi_{nm}(t) \approx \sum_{q=1}^{\mathrm{Q}} W_q\, \rho_n(\Delta_q)^\star \rho_m(\Delta_q)\, e^{-i\Delta_q t}. \tag{5.46}$$

[12] P. Davis and I. Polansky in preceding reference, Ch. 25.
[13] J. B. Cooper in Ref. 2, Ch. 6.

This is precisely what we were able to do in the preceding section [in eq. (5.40)] for broad-wing bands, except that here we have oscillating (rather than decaying) χ-functions. The matrix referred to as χ_q in eq. (5.40) is in this case seen to have the elements

$$[\chi_q]_{nm} = W_q \, \rho_n(\Delta_q)^\star \rho_m(\Delta_q), \tag{5.47}$$

while

$$\lambda_q = i\Delta_q. \tag{5.48}$$

Thus, having obtained an approximation like eq. (5.45) we know that it is quite possible to derive an effective Hamiltonian from it, simply by using eq. (5.41) along with the identifications implied by eqs. (5.47,5.48). Of course, we still do not know that such an effective Hamiltonian could be made purely Hermitian.

One reasonable way to get an equation like eq. (5.45) would be merely to employ standard approximate integration formulas such as Gaussian quadrature [if $w(\Delta)$ is literally zero outside of a finite Δ-interval], Gauss-Hermite quadrature [for an infinite interval], or Gauss-Laguerre quadrature [for a semi-infinite interval]. We are at liberty to do this because we can choose the function $w(\Delta)$ however we want. For example, for Gaussian integration we would be choosing $w(\Delta)$ to be constant. All approximate integration formulae of the type mentioned are of the form (5.45), with W_q being $w(\Delta_q)$ times the q-th weight coefficient for the given integration type, and the Δ_n being just the sample points. Since so much is known about these particular techniques, essentially no extra thought is needed to make them work.

Another possibility is that an optimum set of W_q coefficients can be computed specifically to account for $w(\Delta)$ as a weight function. There is actually a standardized technique for this, as outlined by Hamming.[14] The tricky part is in the selection of the sample points Δ_q. If this can be done, computing the W_q is quite easy; one simply matches the known values of $W\{1\}$, $W\{\Delta\}$, ..., $W\left\{\Delta^{\mathrm{Q}-1}\right\}$ to their approximate values according to eq. (5.45), solving for the Q coefficients W_q as unknowns. This ensures that the approximate formula (5.45) is exact at least for all polynomials of degree $\mathrm{Q}-1$ or less.

If $w(\Delta)$ is a non-negative function, one can do considerably better than this by choosing sample points through the use of orthogonal polynomials. One defines polynomials $p_0(\Delta)$, $p_1(\Delta)$, ... so that the relation

$$\delta_{nm} = \int w(\Delta)\, p_n(\Delta)\, p_m(\Delta)\, d\Delta \tag{5.49}$$

holds. This procedure can only be carried out if the function $w(\Delta)$ dies to zero faster than any power of $|\Delta|$, as $|\Delta|$ goes to ∞. We refer to this type of bandshape as a *narrow-winged continuum*, in distinction to the broad-winged continua encountered in the previous section. In any case, one then chooses the sample points to be the roots Δ_1, ..., Δ_{Q} of the polynomial p_{Q}. As stated above, the W_q are calculated from

[14] R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1962).

$$\left.\begin{array}{rcrcl} 1 &=& W\{p_0(\Delta)\} &\approx& W_1 p_0(\Delta_1) + ... + W_{\rm Q} p_0(\Delta_{\rm Q}) \\ 0 &=& W\{p_1(\Delta)\} &\approx& W_1 p_1(\Delta_1) + ... + W_{\rm Q} p_1(\Delta_{\rm Q}) \\ & & \vdots & & \\ 0 &=& W\{p_{\rm Q-1}(\Delta)\} &\approx& W_1 p_{\rm Q-1}(\Delta_1) + ... + W_{\rm Q} p_{\rm Q-1}(\Delta_{\rm Q}). \end{array}\right\} \tag{5.50}$$

Because of eq. (5.50), eq. (5.45) is exact for all $\mathrm{Q}-1$ degree polynomials. Because of the choice of Δ_q, it happens that eq. (5.45) is also exact for all polynomials of degree Q through $2\mathrm{Q}-1$. To see this, simply calculate $W p_n p_{\rm Q}$ for $n = 0, 1, ..., \mathrm{Q}-1$. The values are all zero because of the orthogonality of the polynomials. On the other hand, all sums of the form

$$W_1 p_n(\Delta_1) p_{\rm Q}(\Delta_1) + ... + W_{\rm Q} p_n(\Delta_{\rm Q}) p_{\rm Q}(\Delta_{\rm Q})$$

are also zero, by virtue of the fact that $p_{\rm Q}(\Delta_n) = 0$. Thus Q more equations could be added to eq. (5.50) automatically.

In order to complete the derivation of the effective Hamiltonian, we need to compute the coefficients W_q. Fortunately, this is fairly easy. It turns out (and we will demonstrate in §6.3), that the Q-vectors

$$\begin{bmatrix} p_0(\Delta_q) \\ \vdots \\ p_{\rm Q-1}(\Delta_q) \end{bmatrix}$$

are orthogonal for distinct q. Consequently, the solution for the W_q in eq. (5.50) is immediate:

$$W_r = \frac{1}{\sum_{q=0}^{\rm Q-1} p_q(\Delta_r)^2}. \tag{5.51}$$

It only remains to be seen that we can write a handy Hermitian replacement for eq. (5.41) in this case. Since the W_q are all non-negative, we can do this as follows:

$$H_{\rm eff} = \begin{bmatrix} & & & E(t)\mu_{11} & \cdots & E(t)\mu_{\rm Q1} \\ H_0^{(\rm D)} + E(t)\,\mu^{(\rm D)} & & & \vdots & & \vdots \\ & & & E(t)\mu_{\rm 1N} & \cdots & E(t)\mu_{\rm QN} \\ E(t)\mu^\star_{11} & \cdots & E(t)\mu^\star_{\rm 1N} & \Delta_1 & & \\ \vdots & & \vdots & & \ddots & \\ E(t)\mu^\star_{\rm Q1} & \cdots & E(t)\mu^\star_{\rm QN} & & & \Delta_{\rm Q} \end{bmatrix} \tag{5.52a}$$

where

$$\mu_{nm} = \sqrt{W_n}\rho_m(\Delta_n). \tag{5.52b}$$

Thus, we obtain an effective Hamiltonian with $\mathrm{N}+\mathrm{Q}$ energy levels. Although we won't analyze the error in this approximation in detail until Chapters VI and VIII, it is easy to see that our discretized ($\underline{N}$,Q) system will produce "good" calculations as long as eq. (5.46)

is "good". In this preliminary analysis, let's simply suppose that eq. (5.46) is a fairly good approximation as long as there is at least one sample point per period of $e^{-i\Delta t}$. If ω is defined to be the maximum spacing $\Delta_{n+1} - \Delta_n$ among the sample points, then we expect our approximation to be good for

$$\omega t < 2\pi,$$

or

$$t < \frac{2\pi}{\omega}.$$

We will see in the next section, and in Chapter VIII, that $\frac{2\pi}{\omega}$ represents the *recurrence time* of the system, which happens to be the longest time for which it would be possible to have agreement between a discrete (Hermitian) system and a continuous system. Thus, our integration formula is not only "optimum", but gives us about as much accuracy as we can reasonably hope for, at least with a discretized Hamiltonian that is Hermitian.

Unlike the rational band theory in §5.5, the result we have derived here is purely an approximation (*i.e.*, there is no continuum shape for which it is exact), though one which can be improved at will by increasing Q. However, there are practical difficulties in application. If we decide to employ standard integration formulae (*e.g.*, Gaussian integration) there is no particular problem in doing so, but we do not attain the optimum approximation. If we choose the route of finding an optimized integration formula based on orthogonal polynomials with the weight function $w(\Delta)$, the problems become extreme—the worst difficulty being that we have no good (computer) method for getting the orthogonal polynomials.

We will recall this method in Chapter VI when we derive the effective Hamiltonian of eq. (5.52a-5.52b) in a completely different way, and without any of the associated difficulties just mentioned.

5.7. A Quirky Case: The Discrete-Lorentzian Band

Let's very briefly see one last example of back-conversion of the integral equations to differential Schrödinger equations. The example we are going to give does not fit in well with either the broad-wing or narrow-wing theory presented earlier, but is nevertheless so novel that it must be included. Let us consider the $(1, \mathsf{DISCRETE\,LORENTZIAN})$ system. [See eq. (3.15) and figure (5.2).]

Recall that the discrete Lorentzian bandshape is like the continuous Lorentzian, except that it has discrete levels with a spacing $\delta_{n+1} - \delta_n = \omega$. As mentioned above, it has been shown by Makarov *et al.* (Ref. 7) that the population in this system is absorbed from the ground state by the band (just as for a continuous Lorentzian), except that much of the population is quasi-periodically returned to the ground-state. This population return occurs after a certain time, called the recurrence time, defined by

$$\tau_{\mathrm{R}} = \frac{2\pi}{\omega}. \tag{5.52}$$

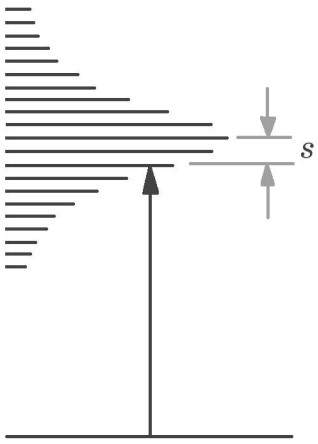

FIGURE 5.2

A $(1, \text{DISCRETE LORENTZIAN})$ system. Although only a finite number of levels is shown in the band, there are actually infinitely many levels

(Recall the appearance of this formula in the previous section.) They have also shown that the $\chi(t)$ function is periodic, with period $\tau_{\rm R}$, and that for times less than $\tau_{\rm R}$

$$\chi(t) = \gamma^2 e^{-ist}\left(\cosh(\sigma t) - \tanh\left(\frac{\pi\sigma}{\omega}\right)\sinh(\sigma t)\right). \tag{5.53}$$

Recall that the hyperbolic sine and cosine functions are defined as sums of exponential functions. It is then clear from eq. (5.53) that for times less than the recurrence time, $\chi(t)$ is a sum of two exponentials, and (as in the prior two sections) is suitable for producing an effective Hamiltonian for the system.

In fact, without further ado, we find that for times less than the recurrence time $\tau_{\rm R}$, the $(1, \textsf{DISCRETE LORENTZIAN})$ system is precisely equivalent (in so far as the ground-state probability amplitude is concerned) to a (1,2) system with Hamiltonian

$$H_{\rm eff} = \begin{bmatrix} 0 & E(t)\,\gamma\,\alpha_+ & E(t)\,\gamma\,\alpha_- \\ E(t)\,\gamma\,\alpha_+ & s - i\,\sigma & 0 \\ E(t)\,\gamma\,\alpha_- & 0 & s + i\,\sigma \end{bmatrix}, \tag{5.54}$$

where

$$\alpha_\pm = \sqrt{\frac{1 \pm \tanh\left(\frac{\pi\sigma}{\omega}\right)}{2}}. \tag{5.55}$$

Actually, eq. (5.54) is just eq. (4.78), the effective (but exact) Hamiltonian of a $(1, \textsf{CONTINUUM})$ system with two continuous Lorentzian humps. By inspection we see that for $t < \tau_{\rm R}$ the discrete Lorentzian behaves (exactly) like two continuous Lorentzians—one of *positive* width and one of *negative* width. When the level spacing ω is narrow, the negative-width Lorentzian has little effect (*i.e.*, $\alpha_- \ll \alpha_+$); when the level spacing is large, the two Lorentzians have similar effect (*i.e.*, $\alpha_- \approx \alpha_+$). The positive-width Lorentzian controls the initial time-evolution, as the ground-state probability amplitude decays. For long periods of time, however, the negative-width Lorentzian causes an exponential buildup of the ground-state population. This exponential buildup ceases at the recurrence time $\tau_{\rm R}$, since eq. (5.54) ceases to be valid at that point.

We will continue the discussion of recurrences in Chapters VII and VIII.

5.8. Numerical Examples

An important facet of the discretization methods described in §5.5 and §5.6 is that they are of adjustable (and potentially unlimited) accuracy. This distinguishes them from (for example) the Weisskopf-Wigner approximation which can be either very bad or very good, but for which there are really no steps that can be taken to improve it. For this reason, some of the numerical examples we will develop in this section are designed more to demonstrate a high level of accuracy, rather than to demonstrate any new physical phenomenon. We will consider numerical examples based on the $(1, \textsf{UNIFORM BAND})$ system, concentrating largely on the discretization scheme introduced in §5.5 [eq. (5.52a-5.52b)]. However, we will also complete our discussion of the rational band approximation.

The uniform rectangular band is defined by eq. (3.13). As a crude qualitative result, we know that for a "wide" band the ground-state probability amplitude decays exponentially (because of the Weisskopf-Wigner approximation), while a "narrow" band acts essentially like a discrete level for small times. As a test case, we will try to compute the ground-state probability amplitude accurately to six figures. (Admittedly, we know of no reason why such an accurate solution to this system would ever be needed. By the same token, however, we know of no other computational method capable of providing such accuracy in an economical way.)

To begin with, let's contrast the fully Hermitian type of discretization discussed in §5.5 with a more straightforward kind of discretization. For concreteness, suppose that the continuous band has width $\sigma = 0.3\,\mathrm{cm.}^{-1}$ and center frequency $s = 0\,\mathrm{cm.}^{-1}$. (Units of $\mathrm{cm.}^{-1}$ are converted to units of $\mathrm{sec.}^{-1}$ by multiplying with $2\pi c$.) The strength of the transitions will be given by

$$E(t)\,\gamma = \begin{cases} 0 & , t < 0 \\ \dfrac{\varepsilon_\infty t}{\tau} & , 0 < t < \tau \\ \varepsilon_\infty & , \tau < t \end{cases} . \tag{5.56}$$

Thus, τ will be the time to turn the field on, which we will set at $\frac{1}{30}$ nanosecond. ε_∞ will be the limiting strength of the interaction, say $0.05\,\mathrm{cm.}^{-1}$. We will suppose that the time interval of interest is $\frac{1}{3}$ nanosecond. Fortunately, when the center of a symmetric band is at resonance in a $(1, \mathsf{BAND})$ system (*i.e.*, $s = 0$), the ground-state probability amplitude is real.

The $(1, \mathsf{UNIFORM\ BAND})$ system is very convenient from the standpoint of the discussion in §5.5, since the effective Hamiltonian [eq. (1,(5.52a-5.52b)] has only a single bordering row and column, so that the discretized system is just a $(1, \mathrm{Q})$ system. Moreover, if we just choose $w(\Delta) \equiv 1$, then the various parameters needed in eq. (5.52a-5.52b) need no calculation, for eq. (5.45) is then just the standard formula for Gaussian integration (see Ref. 12), as adapted to the integration region $(s - \sigma,\ s + \sigma)$ rather than the standard $(0, 1)$, and consequently can be looked up in books. In figure (5.3) we see a representation of the discretized system.

Experimentation (or Chapter VIII) shows that setting $\mathrm{Q} = 16$ provides the specified accuracy on the time interval of interest. It is then a simple matter to numerically integrate the system using the effective Hamiltonian as given by eq. (5.52a-5.52b). The resulting ground-state probability amplitude as a function of time is shown in figure (5.4).

In contrast, let's consider the situation using a more straightforward method of discretizing the continuum. One apparently reasonable procedure is to simply replace the continuum by a series of Q equally spaced levels with equal dipole matrix elements connecting them to the ground state. We refer to this as *Rice discretization* because Rice[15] was the first to investigate $(1, \mathsf{DISCRETE})$ systems with all the levels in the band evenly spaced. Figure (5.5) compares the error in the ground-state probability amplitude for Rice-discretized systems with various numbers of levels against the exact solution [gotten using eq. (5.52a-5.52b) with $\mathrm{Q} = 16$]. For small times, the agreement is quite good even for a small number of levels in the Rice-discretized system. In fact, none of the curves shown

[15] O. Rice, *J. Chem. Phys.* **1**, 375 (1933).

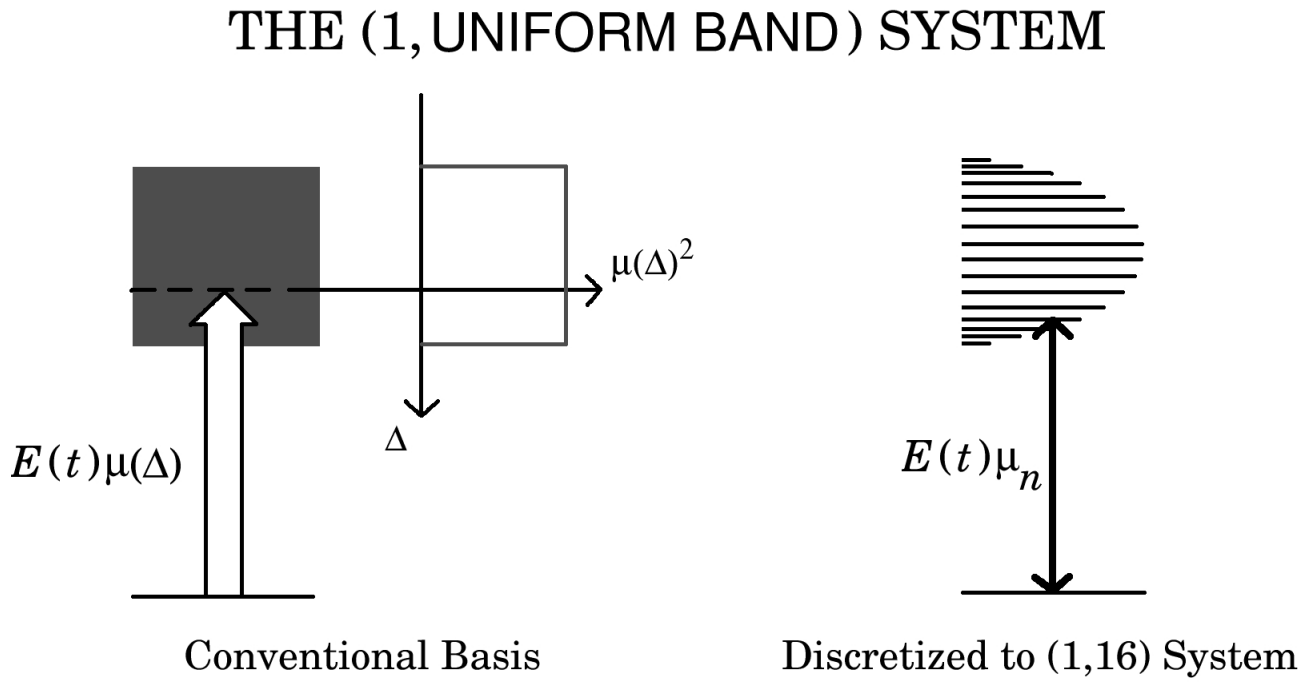

FIGURE 5.3

The $(1, \text{UNIFORM CONTINUUM})$ system in the conventional basis, and its discretized form according to eq. (5.52a-5.52b) with 16 discrete levels replacing the continuum.

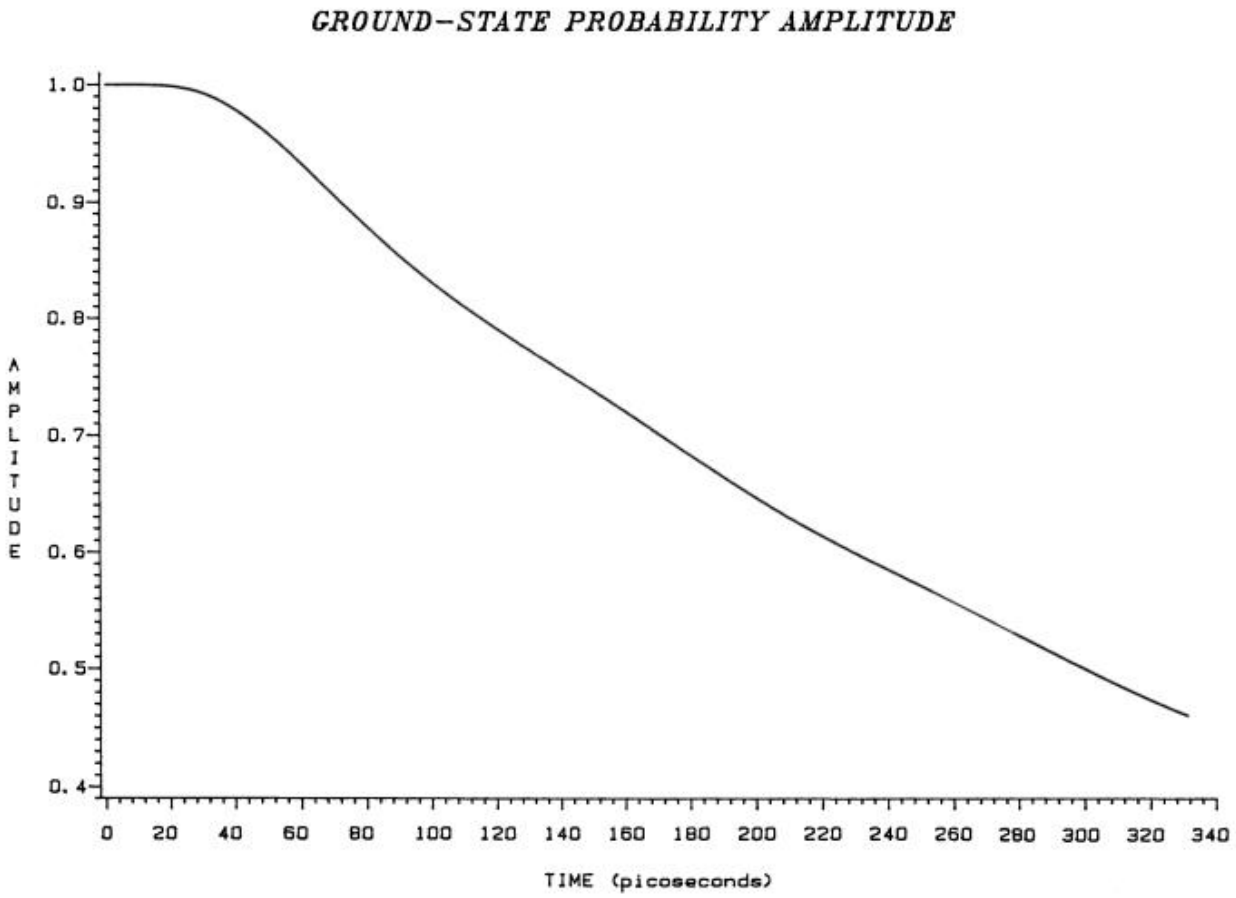

FIGURE 5.4

The ground-state probability amplitude for a $(1, \text{UNIFORM BAND})$ system with $s = 0\,\text{cm.}^{-1}$, $\sigma = 0.3\,\text{cm.}^{-1}$, and with $\gamma E(t)$ ramping linearly from $0\,\text{cm.}^{-1}$ at $t = 0\,\text{psec.}$ to $0.05\,\text{cm.}^{-1}$ at $t = \tau = 33\,\text{psec.}$

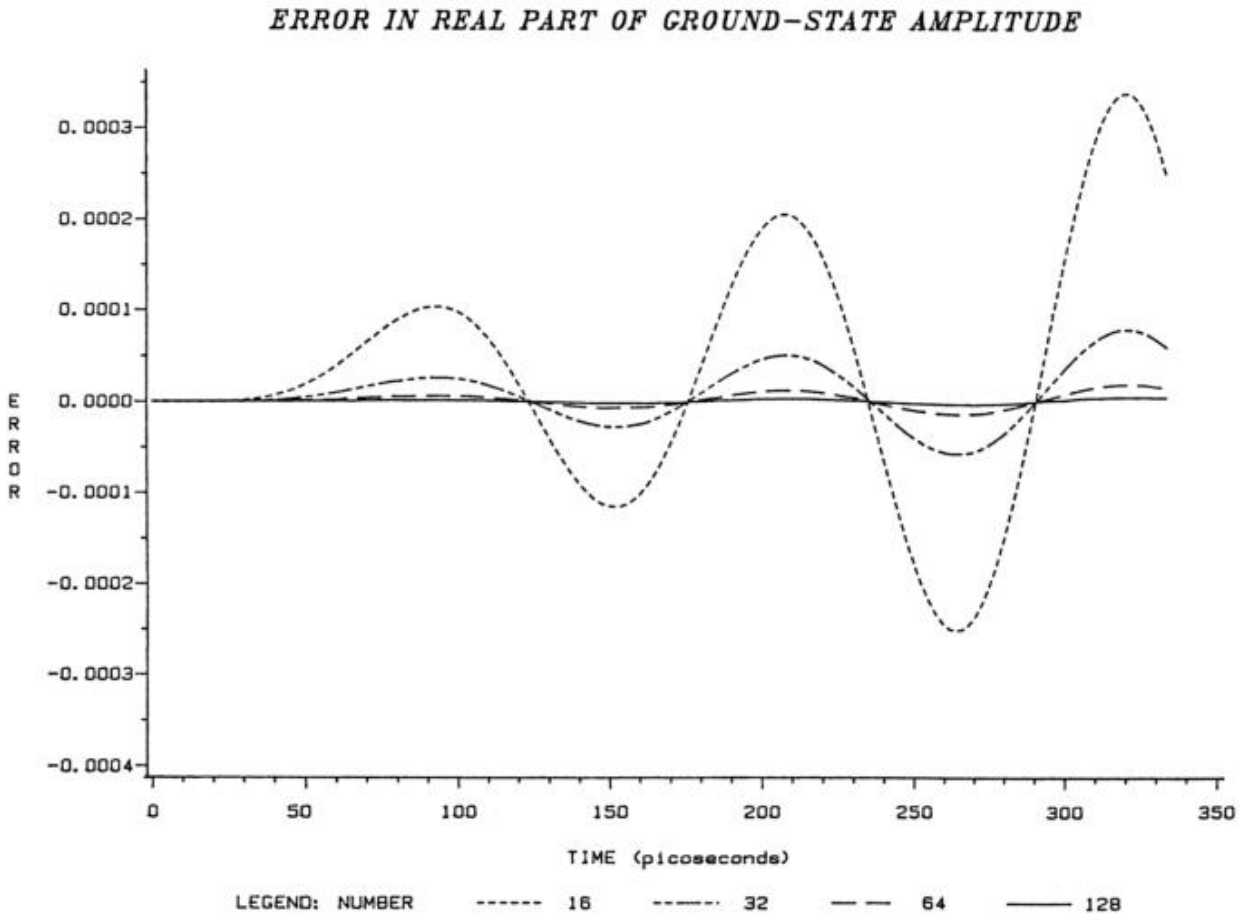

FIGURE 5.5

Error in the straightforward Rice-discretization of a $(1, \text{UNIFORM BAND})$ system using various numbers of equally spaced levels, as opposed to the "exact" ground-state probability amplitude calculated from eq. (5.52a-5.52b). The system has $s = 0\,\text{cm.}^{-1}$, $\sigma = 0.3\,\text{cm.}^{-1}$, and with $\gamma E(t)$ ramping linearly from $0\,\text{cm.}^{-1}$ at $t = 0\,\text{psec.}$ to $0.05\,\text{cm.}^{-1}$ at $t = \tau = 33\,\text{psec.}$ The straightforward method requires many more levels to attain the same degree of accuracy as our method.

has an error over 0.1% in the calculation. Nevertheless, the (1,16) system with Hamiltonian (5.52a-5.52b) has an error 1000 times less than the (1,16) Rice-discretized system, and we must use a (1,128) Rice-discretized system to attain the six-figure accuracy level we have specified.

It is also interesting to compare our solution, which is exact for all practical purposes, against the probability amplitude as predicted by the Weisskopf-Wigner approximation. Since the electric field is changing in time, we cannot directly use eq. (5.22), but must use eq. (5.20) instead, resulting in an approximate probability amplitude of

$$a(t) \approx \exp\left(-\overline{\chi}\int_0^t E(t')^2 dt'\right). \tag{5.57}$$

Hence,

$$\begin{aligned} |a(t)|^2 &\approx \exp\left(-2\mathcal{R}\mathsf{e}\left(\overline{\chi}\right)\int_0^\infty E(t')^2 dt'\right) \\ &= \exp\left(-2\frac{\mathcal{R}\mathsf{e}\left(\overline{\chi}\right)}{\gamma^2}\int_0^\infty \gamma^2 E(t')^2 dt'\right). \end{aligned} \tag{5.58}$$

As mentioned, for $t > \tau$, eq. (5.58) shows strict exponential decay of the ground-state probability amplitude. This misses some of the very interesting qualitative information in figure (5.4), which shows the exact solution. While the exact solution does decay, the appearance (after $t = \frac{1}{30}\,\text{nanosecond}$) is far from exponential. Indeed, the decay appears to be almost a sequence of *linear* decay intervals with different slopes. Each linear decay interval is between 100 and 120 picoseconds in length, corresponding roughly with a time scale relating to the width of the continuous band:

$$\frac{1}{c\,\sigma} = \frac{1}{\left(3\times 10^{10}\,\frac{\text{cm.}}{\text{sec.}}\right)\left(0.3\,\text{cm.}^{-1}\right)} = 111\,\text{picoseconds.}$$

This stepwise change in slope has been predicted by Eberly *et al*.[16] using very different reasoning. Now, from eq. (5.21) we have immediately that

$$2\,\frac{\mathcal{R}\mathsf{e}\left(\overline{\chi}\right)}{\gamma^2} = 2\pi\,\frac{\mu(0)^2}{\gamma^2} = \frac{\pi}{\sigma}.$$

For $t > \tau$, eq. (5.58) therefore evaluates to

$$\begin{aligned} a(t) &\approx \exp\left(-\frac{\pi}{\sigma}\,\varepsilon_\infty^2\,\left(t-\frac{2\tau}{3}\right)\right) \\ &= \exp\left(-4.9339\,\left(t-\frac{2\tau}{3}\right)\,\text{nsec.}^{-1}\right). \end{aligned} \tag{5.59}$$

For the parameters of this system and external field, this expression is actually a fair approximation to the true population of the ground-state (though not of an accuracy comparable to those in the previous paragraphs). See figure (5.6).

[16] J. Eberly, J. Yeh, and C. Bowden, *Chem. Phys. Lett.* **86**, 76 (1982); J. Yeh, C. Bowden, and J. Eberly, *J. Chem. Phys.* **76**, 5936 (1982).

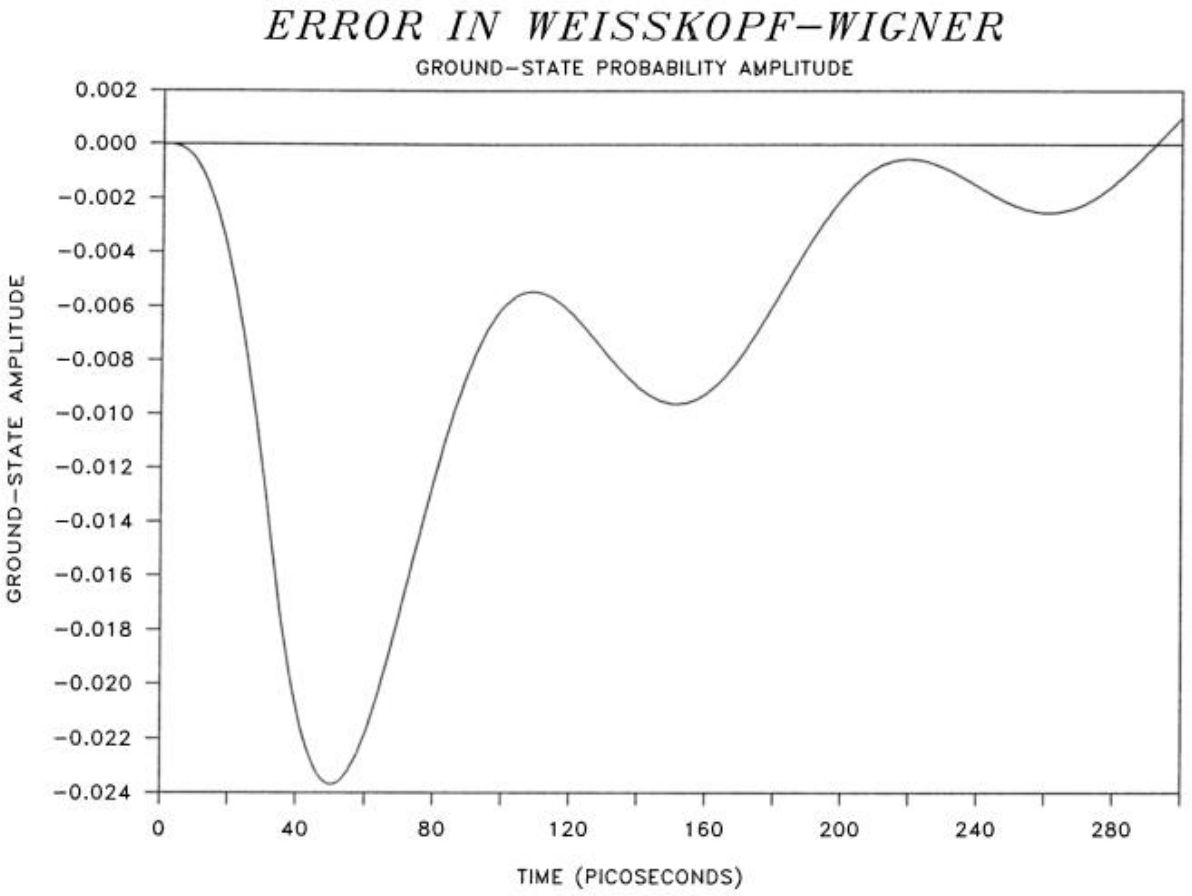

FIGURE 5.6

Error in the Weisskopf-Wigner approximate solution to the $(1, \text{UNIFORM BAND})$ system with $s = 0\,\text{cm.}^{-1}$, $\sigma = 0.3\,\text{cm.}^{-1}$, and with $\gamma E(t)$ ramping linearly from $0\,\text{cm.}^{-1}$ at $t = 0\,\text{psec.}$ to $0.05\,\text{cm.}^{-1}$ at $t = \tau = 33\,\text{psec.}$ Note that the error must approach zero as t increases, simply because both the exact and Weisskopf-Wigner solutions individually go to zero.

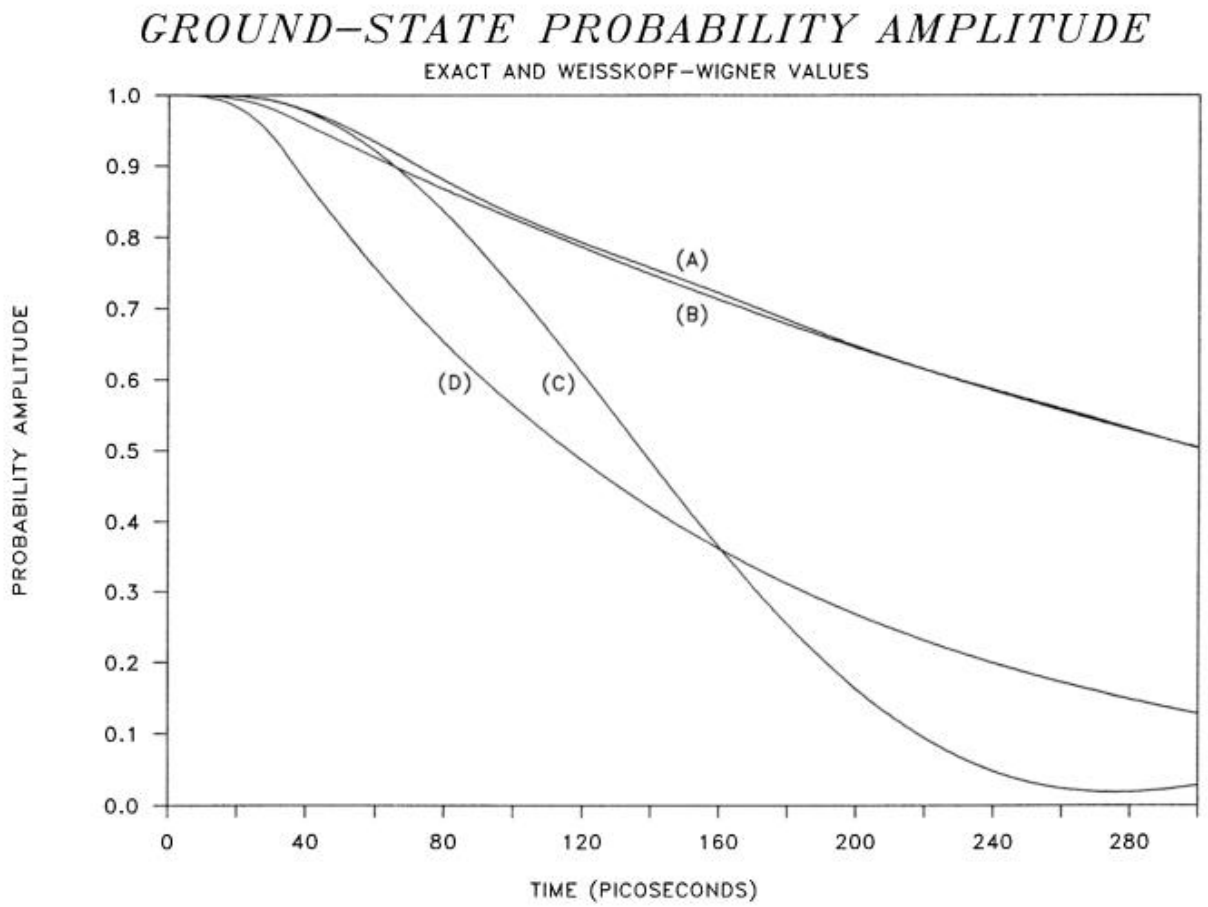

FIGURE 5.7

Weisskopf-Wigner and exact solutions for the ground-state probability amplitude of a $(1, \text{UNIFORM BAND})$ system at two different band-widths, and with $s = 0\,\text{cm.}^{-1}$ and with $\lambda E(t)$ ramping linearly from $0\,\text{cm.}^{-1}$ at $t = 0\,\text{psec.}$ to $0.05\,\text{cm.}^{-1}$ at $t = \tau = 33\,\text{psec.}$ Curve (A) is the "exact" solution [from eq. (5.52a-5.52b)] with $\sigma = 0.3\,\text{cm.}^{-1}$, while curve (B) is the associated Weisskopf-Wigner approximation. Curves (C) and (D), respectively, repeat the calculation for $\sigma = 0.1\,\text{cm.}^{-1}$.

However, we know that the Weisskopf-Wigner approximation is best for small, slowly varying fields $E(t)$, and large band-widths σ. Outside of this range of conditions, the approximation can fail quite badly. For example, in eq. (5.59) above, we see that as σ becomes small the Weisskopf-Wigner approximation would predict that the ground-state population decays instantaneously. Physically, we know that this doesn't happen. For $\sigma \to 0$, the system should behave like a two-level system and oscillate. Thus if we were to repeat our sample numerical calculation for a narrower band, say with $\sigma = 0.1\,\mathrm{cm.}^{-1}$, we would get a less favorable view of the Weisskopf-Wigner approximation. In figure (5.7), we see the exact and Weisskopf-Wigner solutions for both the $\sigma = 0.3\,\mathrm{cm.}^{-1}$ and $\sigma = 0.1\,\mathrm{cm.}^{-1}$ cases. Clearly, the match in the latter case is somewhat worse than in the former. Interestingly, the number of levels needed in our discretization scheme is less (approximately 5) in the latter case as well, so our approximation scheme has become more accurate even as the Weisskopf-Wigner approximation fails. (For the narrower band, the exact population is seen to be increasing at the very end of the integration, so the Weisskopf-Wigner approximation is actually qualitatively wrong at that point.)

Conversely, if we had gone to wider bands rather than narrower ones, we would have seen the Weisskopf-Wigner approximation becoming more accurate, while our discretization scheme would require more and more levels. This is not a true flaw in our scheme, however, since in Chapter VIII we will see a modification of this class of discretization schemes that obviates the necessity for adding any additional levels.

As it happens, we have no particular reason to think that the Weisskopf-Wigner approximation would be especially accurate for this particular example. Our derivation of the Weisskopf-Wigner formula assumed that $\sigma^{-1} \ll \tau$. This is not the case here since (after application of the necessary unit conversion) σ^{-1}=18 picoseconds τ=33 picoseconds. It would be interesting to see a similar calculation with a longer turn-on time for the field. This we have provided in figure (5.8) where we have set the turn-on time τ of the electric field at 300 picoseconds. The agreement between the exact and Weisskopf-Wigner solutions is somewhat better, but still rather inaccurate in the case of the narrower band.

Of course, as mentioned, as the band becomes very narrow, we expect the system to behave somewhat like a two-level system. Therefore, we can also use our method to begin with a very narrow band and to investigate how the behavior of the system differs from that of a two-level system as the band becomes wider. In the resonant ($s = 0$) two-level approximation, Schrödinger's equation becomes simply

$$i\,\frac{d}{dt}\begin{bmatrix} a(t) \\ b(t) \end{bmatrix} = E(t)\,\gamma \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} a(t) \\ b(t) \end{bmatrix}. \tag{5.60}$$

This has the solution

$$a(t) = \cos\left(\gamma \int_0^t E(t')\,dt'\right). \tag{5.61}$$

In our case, therefore, after the turn-on time τ of the field, we expect the ground-state probability amplitude to become

$$a(t) = \cos\left(\varepsilon_\infty\, t + \varphi\right),$$

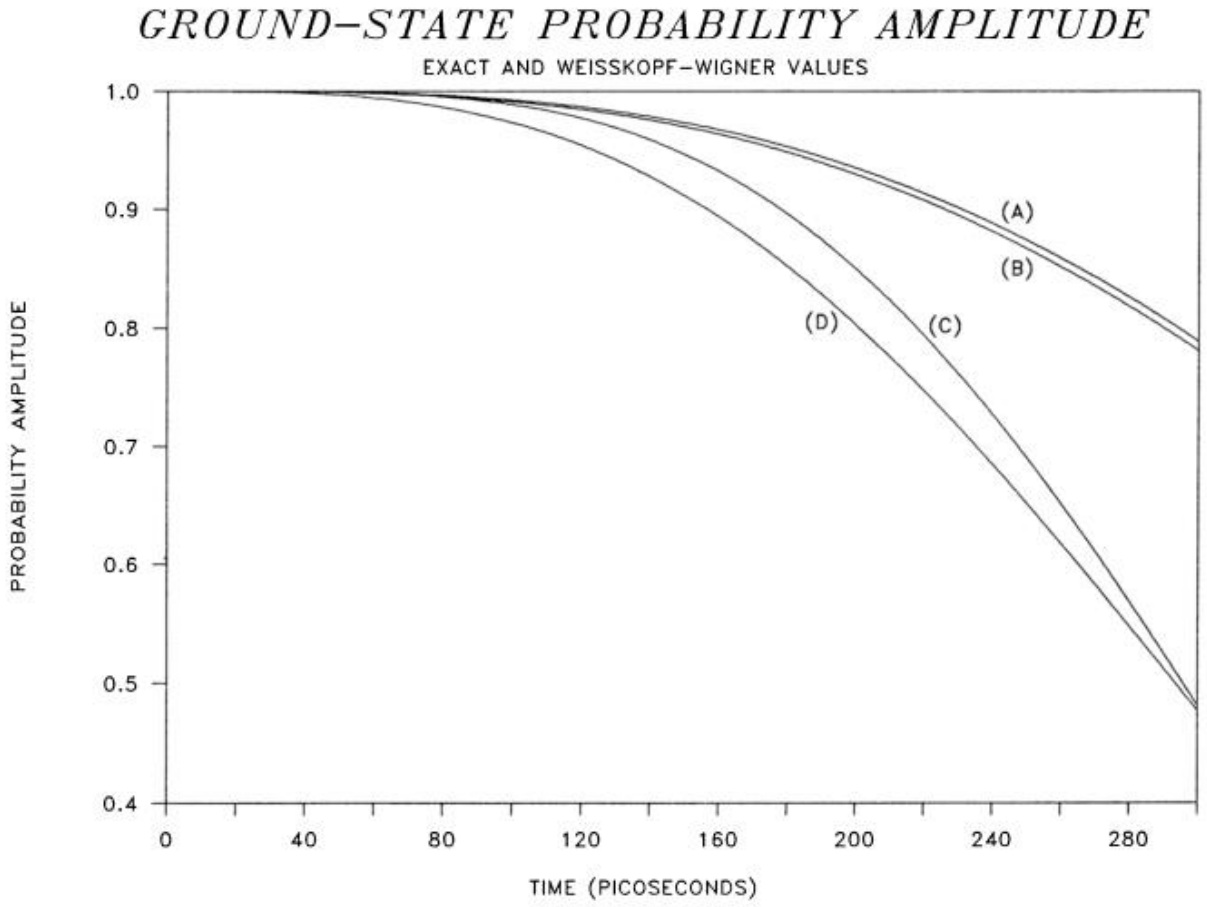

FIGURE 5.8

Comparison of exact and Weisskopf-Wigner solutions as in figure (5.7), but with the turn-on time of the $E(t)$ increased from τ=33 psec. to τ=300 psec.

where φ is some phase due to the non-zero value of τ. For our example, ε_∞ has the value $0.05\,\mathrm{cm.}^{-1}$ so that the period of oscillation should be

$$\frac{1}{0.05\,\mathrm{cm.}^{-1}c} = 667\,\mathrm{picoseconds}.$$

In figure (5.9) we see some numerical results to go along with these ideas. Here, we have gone back to the shorter turn-on time for the field, namely $\tau = 33$ picoseconds, but have computed the ground-state probability amplitude for a much longer time interval. Several different band-widths σ are depicted. For the widest band shown, $\sigma = 0.1\,\mathrm{cm.}^{-1}$, $a(t)$ behaves much like an exponential decay, but with tiny oscillations. However, for the narrowest band shown, $\sigma = 0.01\,\mathrm{cm.}^{-1}$, $a(t)$ exhibits almost a pure oscillation (over the time interval shown). By inspection, the period of oscillation is indeed a little over 650 picoseconds. Of course, if the integrations were carried out over a much longer time interval (as is perfectly feasible with this method), we would eventually see some decay even for the narrowest band.

A final interesting procedure might be to attempt approximating the uniform band using the rational-band techniques of §5.4. How would one go about doing this in practice? We left the discussion of rational approximation (in §5.5) at a very theoretical point. Let us therefore briefly consider the practical details involved in rationally approximating a general continuum, and come back to the specific case of the uniform band in a moment. There are a number of possibilities, including selection of an optimum rational approximation *via* a least-squares fit on a computer. While this may produce a very good result, let us try to find a less mechanical approach.

One conceptually simple approach is as follows: For wide bands, and for narrow bands as well, we expect the approximation to be good if $\mu(\Delta)^2$ is matched well in the neighborhood of $\Delta = 0$. (See Chapter VIII, however.) Moreover, we know that power series can be used easily to approximate smooth functions in the neighborhood of a point. Therefore, let us use the numerator of the rational function to expand $\mu(\Delta)^2$ in a Taylor series (Ref. 2) in the neighborhood of $\Delta = 0$. Unfortunately, any polynomial expansion must increase without bound as $\Delta \to \infty$. Therefore, let us use the denominator of the rational function to create a *window* function that is unity in the neighborhood of $\Delta = 0$, but goes rapidly to zero near $s \pm \sigma$. Thus, we might use an approximation like

$$\mu(\Delta)^2 = \frac{p(\Delta)}{q(\Delta)} \approx \frac{\mu(0)^2 + \Delta \frac{d}{d\Delta}\,\mu(\Delta)^2|_{\Delta=0} + \frac{1}{2}\frac{d^2}{d\Delta^2}\,\mu(\Delta)^2|_{\Delta=0}}{1 + \left(\frac{\Delta - s}{\sigma}\right)^{2\mathrm{n}}}, \tag{5.62}$$

where n is some fair-sized integer (like 5 or 10). In order to find the effective Hamiltonian (5.41), we need to calculate $\chi(t)$ using eq. (5.11), and to put the resulting expression into the form of an expansion as in eq. (5.40). As mentioned in §5.4, this is always possible so long as the roots of the denominator $q(\Delta)$, in this case

$$\Delta_k = s + \sigma\,\exp\left(\frac{i\,k\,\pi}{2\,\mathrm{n}}\right),\ k = 1, 3, 5, ..., 4\mathrm{n} - 1, \tag{5.63}$$

are distinct. $\chi(t)$ is, in practice, computed by an adaptation of the Heaviside expansion theorem. The idea is to treat the definite integral from $-\infty$ to ∞ as a complex contour

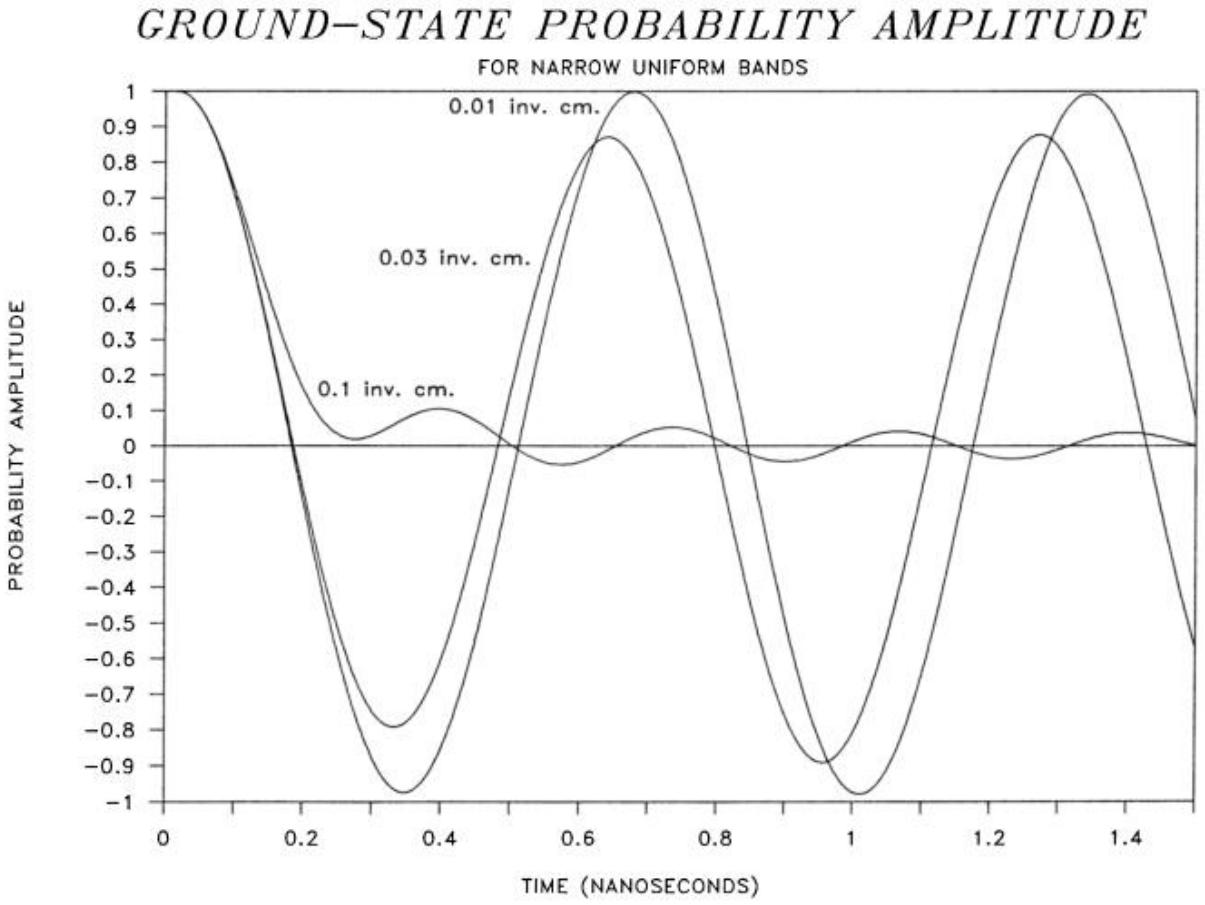

FIGURE 5.9

Ground-state probability amplitude of the $(1, \text{UNIFORM BAND})$ system for various narrow bandwidths and with $s = 0\,\text{cm.}^{-1}$ and with $\gamma E(t)$ ramping linearly from $0\,\text{cm.}^{-1}$ at $t = 0\,\text{psec.}$ to $0.05\,\text{cm.}^{-1}$ at $t = \tau = 33\,\text{psec.}$ The narrower the band, the more closely the system approximates a two-level system.

integral around the lower-half complex-Δ plane; this reduces the integral to a series of residues around the roots Δ_k in the lower half plane:

$$\chi(t) = \sum_{k=1}^{\mathrm{n}} -2\,\pi\,i\,\frac{p\left(\Delta_{2\mathrm{n}+2k-1}\right)}{q'\left(\Delta_{2\mathrm{n}+2k-1}\right)}\,\exp\left(-i\,\Delta_{2\mathrm{n}+2k-1}t\right), \tag{5.64}$$

where the prime on $q(\Delta)$ represents a derivative with respect to Δ. In the case of the rational function given by eq. (5.62), we have

$$q'\left(\Delta_k\right) = -\frac{2\mathrm{n}}{\sigma}\,\exp\left(-\frac{i\,k\,\pi}{2\mathrm{n}}\right). \tag{5.65}$$

The effective Hamiltonian, which will be that of a (1,n) system, is given by eq. (5.41), which reduces to just

$$H_{\text{eff}} = \begin{bmatrix} 0 & E(t)\gamma_1 & E(t)\gamma_2 & \cdots & E(t)\gamma_{\mathrm{n}} \\ E(t)\gamma_1 & \Delta_{2\mathrm{n}+1} & 0 & \cdots & 0 \\ E(t)\gamma_2 & 0 & \Delta_{2\mathrm{n}+3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ E(t)\gamma_{\mathrm{n}} & 0 & 0 & \cdots & \Delta_{4\mathrm{n}-1} \end{bmatrix}, \tag{5.66}$$

where

$$\gamma_k = \sqrt{-2\,\pi\,i\,\frac{p\left(\Delta_{2\mathrm{n}+2k-1}\right)}{q'\left(\Delta_{2\mathrm{n}+2k-1}\right)}}. \tag{5.67}$$

Actually, we have used a symmetrized form of eq. (5.41) which, as discussed in §5.4, is perfectly allowable. This is a good practical measure because it makes the elements of the effective state-vector more comparable in size and makes some numerical differential-equation solving computer programs more effective.

Of course, this effective Hamiltonian doesn't correspond in any reasonable way with the purely Hermitian (16-level) effective Hamiltonian we used so extensively earlier in this section, but it is interesting to compare them anyway. Consider just the diagonal elements of H_{eff}. Recall that the earlier effective Hamiltonian [Figure (5.3)] had discretized levels packed fairly densely near the edges of the band (near $\Delta = s \pm \sigma$), but only sparsely near the center of the band (near $\Delta = s$). Here we have exactly the same thing, but with each level representing a Lorentzian continuum (because of the imaginary part of the "detuning") rather than a discrete level. These Lorentzian continua are wider near the center of the band, and narrower near the edges. Thus, in some sense, the present approximation is like the former, but with the spaces between the levels filled in. Consequently, we would not expect any recurrences of population in this model.

At any rate, in Figure (5.10) we have used eqs. (5.66) and (5.67) to solve the $(1, \text{UNIFORM BAND})$ system we have used so often earlier in the chapter. As in Figure (5.5), we have plotted the error in the ground-state amplitude for this kind of approximation, for various values of n. What we find is that although the convergence to the true solution is much slower than for our purely Hermitian discretization, the approximate solution is qualitatively correct even for very low values of n (such as n=1). In fact, the error curve

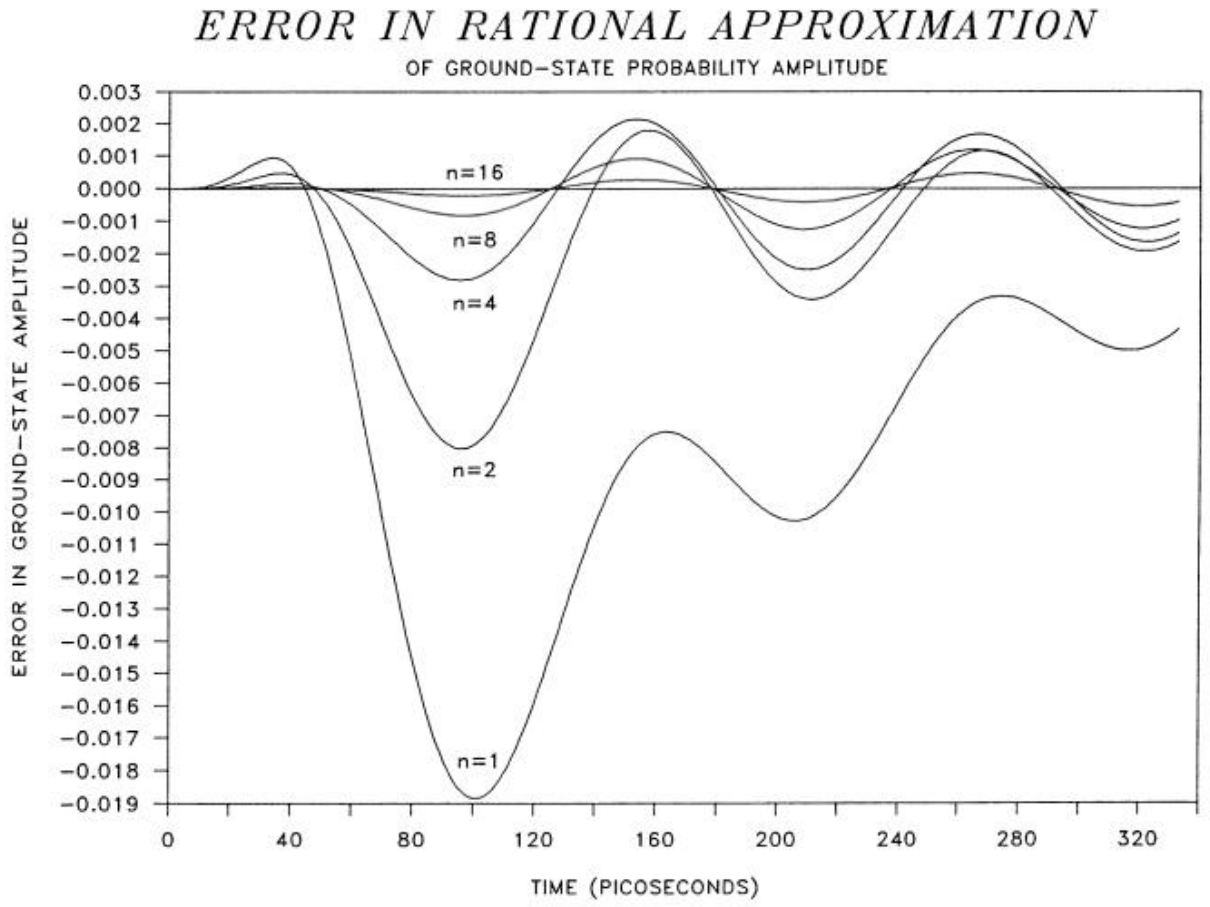

FIGURE 5.10

Error in the ground-state probability amplitude for rational approximations of various degree in the $(1, \text{UNIFORM BAND})$ system. The system has the parameters used before, namely $s = 0$, $\sigma = 0.3\,\text{cm.}^{-1}$, $\varepsilon_\infty = 0.05\,\text{cm.}^{-1}$, and $\tau = 33\,\text{psec.}$ The error converges nicely (but not quickly, by our standards) to zero, but even the n=1 approximation is qualitatively accurate at all times.

for n=1 is reminiscent of the Weisskopf-Wigner error curve in Fig. (5.6), but is slightly smaller in magnitude.

In Chapter VIII, we will see that there are circumstances (for example, in this particular model system if E were to become large) in which $\mu(\Delta)^2$ would need to be accurately approximated in the neighborhoods of points other than $\Delta = 0$. Eqs. (5.62-5.67) extend quite naturally to this case as well.

5.9. (CONTINUUM, CONTINUUM) Population Trapping

As a final illustration, let us continue the discussion of (CONTINUUM, CONTINUUM) population-trapping begun in §4.6.2. In §4.6.2 we discussed, among other things, the behavior of a (CONTINUUM, CONTINUUM) system influenced by a suddenly switched-on interaction (which remained constant thereafter). For broad continua, we found that for either very *weak* or very *strong* interactions, the population remained in the continuum initially containing it. This remarkable result holds whatever the initial conditions (so long as the population is initially contained in just one of the continua). For continua narrower in energy than the interaction energy, this no longer holds.

We can now extend the discussion to the case of a time-varying interaction (*i.e.*, a more slowly switched-on interaction). Specifically, we want to answer the following question: Is it possible by some variation of the interaction strength (such as a change in the externally applied electric field) to transfer population out of the continuum?

For simplicity, let us retain the trivial approximation given by eq. (4.28), which implies that the system has a driver-rank of $\mathrm{M} = 2$, like the$(1, \mathrm{BAND})$ system.

Recall the steps involved: First, we find (by inspection) a decomposition of the dipole operator μ that allows us to define the M-vector $\phi(t)$, which is computed according to an integral equation. If the integral equation cannot be solved explicitly, then it is approximated. Then we generate the full state-vector $\psi(t)$ from a formula involving $\phi(t)$. Although we did not explicitly state the $\mu = DF$ decomposition we used in §4.6.2, a suitable decomposition is

$$D = \begin{bmatrix} \vdots & \vdots \\ 0(\Delta) & V_0(\Delta) \\ \vdots & \vdots \\ \\ \vdots & \vdots \\ V_1(\Delta) & 0(\Delta) \\ \vdots & \vdots \end{bmatrix}, \; F = \begin{bmatrix} \cdots & V_0(\Delta') & \cdots & \cdots & 0(\Delta') & \cdots \\ \cdots & 0(\Delta') & \cdots & \cdots & V_1(\Delta') & \cdots \end{bmatrix}. \tag{5.68}$$

[Note that the V_n functions no longer contain a contribution from $E(t)$, which must be explicitly included in the Hamiltonian.] Because of this, the $X(t)$ matrix [eq. (5.6)] is just

$$X(t) = \begin{bmatrix} 0 & \chi_0(t) \\ \chi_1(t) & 0 \end{bmatrix}, \tag{5.69}$$

where

$$\chi_n(t) = \int V_n(\Delta)^2 e^{-i\Delta t} d\Delta. \tag{5.70}$$

Now, if the population is initially distributed (at time $t = 0$) in continuum 0 according to eq. (4.33), then the integral equations [eq. (5.5)] for the two components $\phi_0(t)$ and $\phi_1(t)$ of $\phi(t)$ are just

$$\left.\begin{aligned} \phi_0(t) &= \widetilde{\alpha}(t) - i\int_0^t E(t')\,\chi_0(t-t')\,\phi_1(t')\,dt' \\ \phi_1(t) &= -i\int_0^t E(t')\,\chi_1(t-t')\,\phi_0(t')\,dt' \end{aligned}\right\}, \tag{5.71}$$

where we put

$$\widetilde{\alpha}(t) = \int_{-\infty}^{\infty} e^{-i\Delta t} V_0(\Delta)\,\alpha(\Delta)\,d\Delta. \tag{5.72}$$

[In spite of the notation, of course, this quantity is not precisely the Fourier transform of $\alpha(\Delta)$.]

Not knowing how to solve eqs. (5.71) in the case of general χ_n, we are forced to approximate the solution. Let us apply the Markov approximation. As discussed in §5.3, loosely speaking we expect the $\chi_n(t)$ functions to decay to zero in a time inversely proportional to the "width" of the continua in frequency space, if the probability amplitudes are initially in phase. If $E(t)$ and $\phi(t)$ vary slowly relative to this, then by the mean-value theorem of calculus eqs. (5.71) reduce to

$$\phi_0(t) \approx \widetilde{\alpha}(t) - i\,\overline{\chi}_0 E(t)\,\phi_1(t)$$

$$\phi_1(t) \approx -i\,\overline{\chi}_1 E(t)\,\phi_0(t),$$

where as in eq. (5.21), the constants $\overline{\chi}_n$ are defined by $\overline{\chi}_n = \int_0^\infty \chi_n(t)\,dt$, which (we have seen) can be easily evaluated. Thus,

$$\left.\begin{aligned} \phi_0(t) &\approx \frac{\widetilde{\alpha}(t)}{1 + E(t)^2\,\overline{\chi}_0\,\overline{\chi}_1} \\ \phi_1(t) &\approx \frac{-i\,\overline{\chi}_1\,E(t)\,\widetilde{\alpha}(t)}{1 + E(t)^2\,\overline{\chi}_0\,\overline{\chi}_1} \end{aligned}\right\}. \tag{5.73}$$

From these formulae, it is clear that $\phi(t)$ varies either on the same time scale as $E(t)$, or else on a time-scale corresponding to the inverse of the width (in frequency space) of the initial probability distribution. For the sake of discussion, let the width of the initial probability distribution be σ, and let the widths of the two continua be σ_0 and σ_1. The validity conditions for our approximation are therefore

$$\sigma, \frac{\dot{E}}{E} \ll \sigma_0, \sigma_1\,.$$

These conditions are satisfied, for example, if we are dealing with featureless continua of infinite width (with $\sigma_0 \to \infty$ and $\sigma_1 \to \infty$). At any rate, it is clear that the generalized Weisskopf-Wigner approximation applies only to broad continua.

Eqs. (5.73) need no further solution before substitution in eq. (5.3) to find the full state-vector. In the notation of §4.6.2 we find the probability amplitudes

$$C_0(\Delta, t) \approx e^{-i\Delta t}\left(\alpha(\Delta) - \overline{\chi}_1 V_0(\Delta)\int_0^t \frac{\widetilde{\alpha}(t')E(t')^2}{1+E(t')^2\overline{\chi}_0\overline{\chi}_1}\, e^{i\Delta t'}dt'\right) \tag{5.74}$$

$$C_1(\Delta, t) \approx -i\, e^{-i\Delta t} V_1(\Delta)\int_0^t \frac{\widetilde{\alpha}(t')E(t')}{1+E(t')^2\overline{\chi}_0\overline{\chi}_1}\, e^{i\Delta t'}dt'. \tag{5.75}$$

It is clear from these equations that the populations reach a steady-state distribution on a time scale $\leq \sigma^{-1}$, regardless of the behavior of $E(t)$. This follows from the fact that $\widetilde{\alpha}(t) \to 0$ on this time scale, while the remaining factors in the integrands above cannot grow without bound even if $E(t) \to \infty$.

Interestingly, eqs. (5.74) and (5.75) are exact for the featureless continua used as examples in §4.6.2 (regardless of whether the Lorentzian initial conditions chosen there are used). In this case, the $\chi_n(t)$ functions evaluate to $2\pi\,\delta(t)$, giving $\overline{\chi}_n = \pi$ (since, roughly speaking, only half of the delta function is integrated).

Another point which is clear from eqs. (5.74) and (5.75) is that the trapping of population in continuum 0 is basically due to the rapid dephasing of the probability amplitudes. Once they become dephased, no possible variation of $E(t)$ can remove population from the continuum. Thus, the picture of the continuum as a population-absorber is somewhat in error. A better picture is to think of the broad continuum as a roach-motel for population: it checks in but it doesn't check out, except during a tiny time-window in which the probability amplitudes are nearly in phase. From this standpoint, population-trapping in broad continuum-continuum transitions is hardly surprising; in fact, it is more remarkable that we have found any conditions at all in which population can be removed from the continuum! Of course, other physical processes such as spontaneous emission or collisional de-excitation can remove population from the continuum, even if the semi-classical process we are considering cannot.

What is the steady-state population of band 1, in the case of featureless continua (for which the results above are exact)? Simple manipulations of eq. (5.75) show that

$$\text{Population of band } 1 \to 2\pi\int_0^\infty \frac{E(t)^2}{\left(1+\pi^2E(t)^2\right)^2}\,\left|\widetilde{\alpha}(t)\right|^2 dt\,, \tag{5.76}$$

as $t \to \infty$. This is consistent with eq. (4.43) (with the identification $E \to \nu$) for Lorentzian initial conditions and a constant field. Recall that $E(t)$ is not the electric field as such. Since it has absorbed part of the dipole operator, in our system of units it is a frequency density (*i.e.*, a frequency per unit frequency), and hence is a dimensionless quantity. Clearly, this steady-state population must be bounded to be less than or equal to

$$2\pi\,\max\left\{\frac{E(t)^2}{\left(1+\pi^2E(t)^2\right)^2}\right\}\int_0^\infty \left|\widetilde{\alpha}(t)\right|^2 dt.$$

Since the integral is itself $\leq 2\pi$, we see that eq. (4.43) [obtained on the assumption of Lorentzian initial conditions and $E(t) \equiv \text{constant}$] still bounds the population transfer from continuum 0 to continuum 1. In fact, we see that the population is more strongly trapped in continuum 0 than our calculations implied in Chapter IV. Thus, we have answered the question posed at the beginning of the section: No conceivable variation of the very strong electric field can transfer population out of the broad continuum. Moreover, even a lower-strength interaction (at the critical value $\nu = \frac{1}{\pi}$) can be ineffective, depending on the initial conditions.

CHAPTER VI
BAND-DIAGONALIZATION OF THE HAMILTONIAN

6.1. Definition of Band-Diagonalization

If one is interested in computing eigenvalues, it is normal to try to diagonalize the Hamiltonian operator matrix. That is, given the matrix elements of the Hamiltonian in some arbitrary basis, one tries to introduce a similarity transformation in order to effect a change of basis to one in which the Hamiltonian happens to be diagonal. These diagonal matrix elements are then the eigenvalues.[1]

As it happens, we are interested in a *time-dependent* $H(t)$, so we are not that interested in finding the eigenvalues *per se* (except for our previous work in Chapter IV). However, it would still be interesting to diagonalize the Hamiltonian, since this would result in the normally coupled Schrödinger's equations becoming uncoupled. Unfortunately, this is not generally feasible if $H(t)$ varies in time since the similarity transformation to the diagonal-H basis then also varies in time and is difficult to incorporate into Schrödinger's equation. It may nevertheless be possible to find some time-independent similarity transformation which, while not producing a strictly diagonal Hamiltonian, could still produce useful simplifications.

Following the method of Lanczos, Haydock[2] has given a construction producing a similarity transformation which can tridiagonalize an arbitrary Hamiltonian. That is, in the resulting basis the Hamiltonian has non-zero matrix elements H_{nm} only for $n = m$ or $n = m \pm 1$. The resulting Hamiltonian is thus that of a (1,1,1,...) system, sometimes known as the *ladder* system. (See review in Ch. II.) This similarity transformation, moreover, has the advantage of being purely constructive, unlike most diagonalization methods. As may be expected, Haydock's similarity transformation is generally time-dependent.

Remarkably, the similarity transformation is not *always* time-dependent. There are instances in which the tridiagonalization algorithm produces a non-time-dependent sim-

[1] G. Forsythe, M. Malcolm, and C. Moler, *Computer Methods for Mathematical Computations* (Prentice-Hall, Englewood Cliffs, New Jersey, 1977).

[2] R. Haydock in *Solid State Physics*, ed. by E. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1980), Vol. 35, p. 215; R. Haydock, *Computer Physics Communications* **20**, 11 (1980).

ilarity transformation.[3] For example, the resulting similarity transformation is time-independent for a $(1, \mathsf{BAND})$ system. That is, a $(1, \mathsf{BAND})$ system can be exactly converted into a ladder system, even if *E(t)* varies in time. We will show how to do this in §6.3.

Since most low-driver-rank systems cannot be time-independently tridiagonalized, we must lower our sights still farther. We cannot hope either to be able to diagonalize or tridiagonalize a general (low driver-rank) system. However, if instead of tridiagonalizing the Hamiltonian we merely try to *band-diagonalize* it, we find that we are then able to proceed. A band-diagonal matrix is, of course, one with non-zero matrix elements H_{nm} only for $|n - m| < \mathrm{k}$, where k is some integer expressing the "width" of the band—that is, the number of distinct non-zero diagonals and co-diagonals.[4] In order to avoid confusing this use of the word "band" with our previous use ("bands of energy levels"), we will attempt to avoid the term "band-diagonal" as much as possible by explicitly referring to the Hamiltonian as tridiagonal, pentadiagonal, heptadiagonal, ..., or even $(2\mathrm{k} + 1)$-diagonal. A $(2\mathrm{k} + 1)$-diagonal matrix has a non-zero diagonal, k co-diagonals above the main diagonal, and k co-diagonals below the main diagonal.

The basic result to be demonstrated in this chapter is this: For a system of driver-rank M, there is a *time-independent* similarity transformation making the Hamiltonian matrix at most $(2\mathrm{M} + 1)$-diagonal. Actually, things will turn out to be a little better than this. It can happen that H is actually $(2\mathrm{M} - 1)$-diagonal, or even that the outermost co-diagonals are zero for all but a finite number of elements, effectively reducing M further. For example, in a $(1, \mathsf{BAND})$ system (with $\mathrm{M} = 2$) we actually get a tridiagonal Hamiltonian rather than a pentadiagonal one. Why we actually get a tridiagonal Hamiltonian will be clear from the derivation below.

One important consequence of this result will be that it completely solves the discretization problem—namely, the problem of producing an equivalent discrete system, given a system with continuous bands of energy levels. While the methods presented in earlier chapters accomplished this also, they did it in an indirect (and sometimes approximate) way. Here, the discretized systems are directly related to the continuous ones by similarity transformations. A system with a band-diagonal Hamiltonian must, of course, be entirely discrete (or else the term "band-diagonal" is meaningless), and this discreteness is a result of our construction rather than a condition for it. Although the discretized Hamiltonian is fully Hermitian, the structure of the discretized system is very different from the structure of the system in the conventional basis. If the system contains continuous bands of energy levels in the conventional basis, for example, those bands (even in discretized form) no longer appear in the discretized (band-diagonal) system.[5] Compare this to the methods of §5.5 and §5.6, in which the discretization process replaces a continuous band of levels with a discrete (though sometimes non-Hermitian) band of levels.

---

[3] R. S. Burkey and C. D. Cantrell, *J. Opt. Soc. Am. B* **1**, 169 (1984); I. Schek and R. Wyatt, *J. Chem. Phys.* **89**, 4924 (1988).

[4] The Scientific Subroutine Package from IBM contains a number of programs for manipulating band-diagonal matrices.

[5] Whether or not it is funny, the pun here (that the band-diagonal Hamiltonian converts a "band" to a "diagonal") is unavoidable.

6.2. Constructing the Band-diagonal Hamiltonian

Unlike the derivations in Chapters IV and V, our proof of $(2\mathrm{M}+1)$-diagonalization is algebraically somewhat formal.[6] Though taking the form of a construction, it is not truly computational in nature. We will postpone introduction of *practical* methods for taking advantage of the results derived here until Chapters VII and VIII. We start from a definition of the Hamiltonian more general than those in Chapters IV and V. In fact, we begin with eq. (3.2) rather than eq. (3.3):

$$H = H_0 + H'(t). \tag{6.1}$$

Up to now, we have mostly been content with the simple assertion that the driving term of the Hamiltonian is of low rank. Now we must be more precise, since if $H'(t)$ is time-varying then it may have different ranks at different times. (Recall §5.2, for example.) This added precision comes about as follows: Let us define a hitherto unmentioned vector spaces $\mathcal{U}$, $\mathcal{V}$ (not to be confused with the "interaction strength" of §4.6), and $\mathcal{W}$ as follows.

First, let

$$\mathcal{V}_0 = \{H'(t)\psi \mid t = \text{any time},\ \psi = \text{any vector}\}\,. \tag{6.2}$$

In essence, $\mathcal{V}_0$ is the space of all vectors which can be produced by the action of $H'(t)$ under any circumstances. We will also find it convenient later to have the initial vector ψ_0 in this space, so let us simply add it in (closing up the resulting space with linear closure):

$$\mathcal{V} = \langle \mathcal{V}_0, \psi_0 \rangle\,. \tag{6.3}$$

It is also advisable to add into $\mathcal{V}$ any additional vectors we might want to explicitly use later. As far as the $(1, \mathsf{BAND})$ system is concerned, ψ_0 would already have been in $\mathcal{V}_0$, so $\mathcal{V} = \mathcal{V}_0$. For a system with a discrete ground-state this is generally the situation, so $\mathcal{V}$ seldom differs from $\mathcal{V}_0$.

Instead of our normal glib definition $\mathrm{M} = \mathrm{rank}\,(H'(t))$, we let

$$\mathrm{M} = \dim \mathcal{V}. \tag{6.4}$$

This definition is consistent with our earlier use, since if $H'(t) = E(t)\mu$ [and if $\psi_0 \in \mathcal{V}_0$] then M is just $\mathrm{rank}(\mu)$. Moreover, this definition is consistent with §5.2. As usual, we require M to be a small integer.

Next, we want to define a vector space $\mathcal{W} \subseteq \mathcal{V}$. We do this as follows: Let $\mathcal{W}$ be the maximal subspace of $\mathcal{V}$ such that

$$H_0\mathcal{W} \subseteq \mathcal{V}. \tag{6.5}$$

No good interpretation of $\mathcal{W}$ can be given at this point in a few words. However, if $H_0\psi_0 = 0$ [*i.e.*, ψ_0 is the ground state, as we have normally assumed], then $\psi_0 \in \mathcal{W}$. In analogy to eq. (6.4), define

[6] I. Herstein, *Current Topics in Algebra* (Xerox College Publishing, Lexington, Mass., 1975).

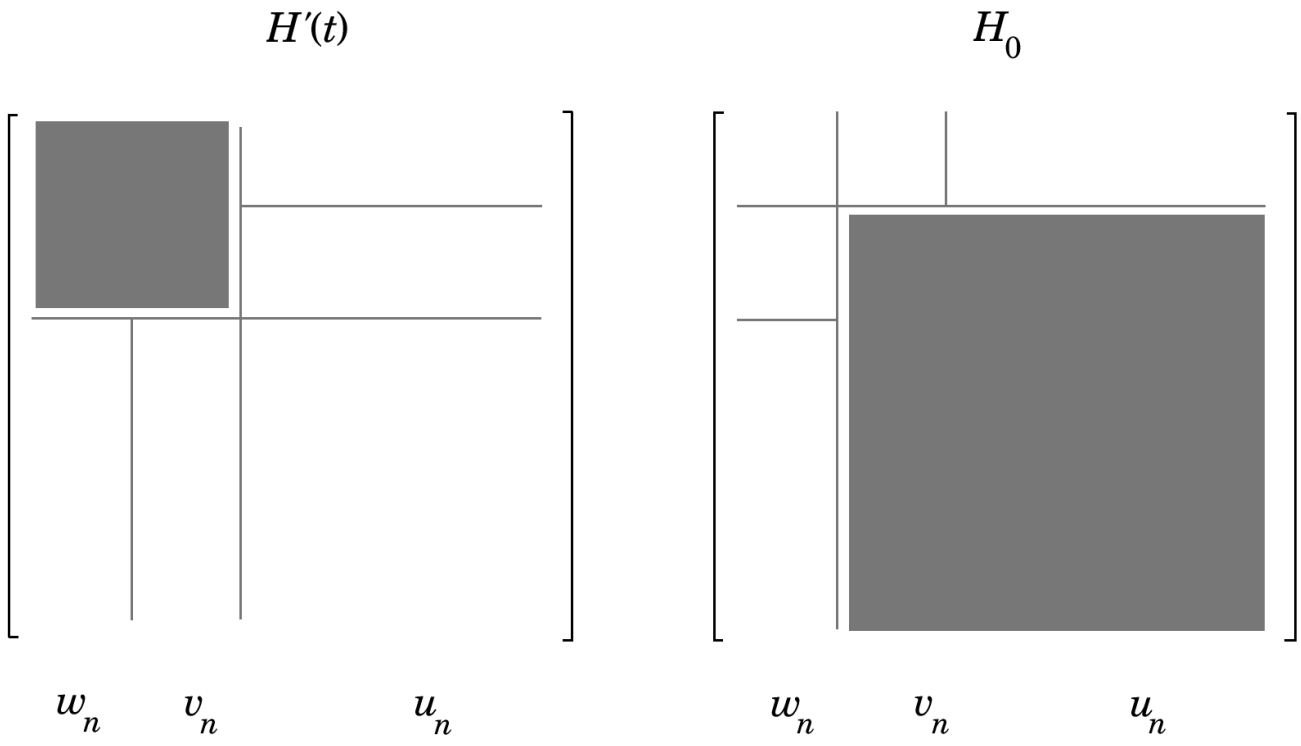

FIGURE 6.1

The forms of the Hamiltonian matrices as implied by eqs. (6.8-6.12). Then non-zero block in $H'(t)$ is $\mathrm{M} \times \mathrm{M}$, while that in H_0 is infinite, but discrete.

$$\mathrm{L} = \dim \mathcal{W}. \tag{6.6}$$

In terms of the quantities defined just now, we can tighten up our somewhat loose formulation that $H(t)$ is "at most" (2M+1)-diagonal. In fact, $H'(t)$ will have only an $\mathrm{M} \times \mathrm{M}$ non-zero block and H_0 will be $(2\mathrm{M}' + 1)$-diagonal, where $\mathrm{M}' = \mathrm{M} - \mathrm{L}$. When we eventually look at the $(1, \mathsf{BAND})$ system in light of the construction we are now defining, we will have $\mathrm{M} = 2$ and $\mathrm{L} = 1$, producing a tridiagonal Hamiltonian.

Finally, we want to define a vector space $\mathcal{U}$ with $\mathcal{V} \subseteq \mathcal{U}$:

$$\mathcal{U} = \mathcal{V} + H_0\mathcal{V} + H_0^2\mathcal{V} + \dots . \tag{6.7}$$

Upon reflection it is easy to see that $\mathcal{U}$ contains every vector which could be generated as an intermediate step in any numerical solution of Schrödingers' equation (3.2). Thus, the state vector ψ (or, at least, any numerical approximation thereof) is certainly in $\mathcal{U}$. Since the dimension of $\mathcal{U}$ is at most countably infinite, a discrete basis can be chosen for it. This is the basis we will construct.

Since $\mathcal{W} \subseteq \mathcal{V} \subseteq \mathcal{U}$, let us choose an orthonormal basis for $\mathcal{U}$ as follows:

$$w_1,\ \dots,\ w_{\mathrm{L}}, v_{\mathrm{L}+1},\ \dots,\ v_{\mathrm{M}},\ u_{\mathrm{M}+1},\ u_{\mathrm{M}+2},\ \dots\ ,$$

where $w_n \in \mathcal{W}$, $v_n \in \mathcal{V} - \mathcal{W}$, $v_n \in \mathcal{U} - \mathcal{V}$. The meanings of the $\mathcal{U}$, $\mathcal{V}$, and $\mathcal{W}$ spaces can best be understood in terms of matrix elements of H_0 and $H'(t)$. Simple manipulations show that

$$w_n^\dagger \, H_0 \, u_m = 0. \tag{6.8}$$

$$v_n^\dagger \, H_0 \, v_m = 0. \tag{6.9}$$

$$u_n^\dagger H' \, u_m = 0. \tag{6.10}$$

$$u_n^\dagger \, H' \, v_m = 0. \tag{6.11}$$

$$u_n^\dagger \, H' \, w_m = 0. \tag{6.12}$$

Of course, the complex conjugates of these equations also hold, doubling the number of selection rules. In short, eqs. (6.8-6.12) imply that $H'(t)$ has only an $\mathrm{M} \times \mathrm{M}$ non-zero block of matrix elements in the upper left-hand corner of the matrix, while eqs. (6.8-6.9) imply that H_0 has several blocks of all-zero elements. This is depicted in Figure (6.1).

If $\psi_0 \in \mathcal{W}$, we can assume without loss of generality that $w_1 = \psi_0$. Other than this, the basis vectors w_n and v_n are already in a form to be used as-is; only the vectors u_n need some manipulation to produce the desired band-diagonal form. As a first step in the construction, let's define

$$u_n = \begin{cases} w_n & , \, n = 1, ..., \mathrm{L} \\ v_n & , \, n = \mathrm{L}+1, ..., \mathrm{M}. \end{cases}$$

The construction algorithm is very simple:

> For $n = \mathrm{M}+1, \mathrm{M}+2, ...$, let u_n be the Gram-Schmidt orthonormalization of the vector $H_0 u_{n-\mathrm{M}+\mathrm{L}}$ with respect to $u_{\mathrm{L}+1}$, ..., u_{n-1}.

It is clear that this algorithm works,[7] if H_0 and $H'(t)$ are bounded operators on U. (If the operators are not bounded, the Gram-Schmidt process can fail, since some of the vectors so produced may not be normalizable.) Consequently, $\mathcal{U}$ must be a Hilbert Space,[8] a hardly surprising conclusion. The first $\mathrm{M} - \mathrm{L}$ steps produce the basis vectors for $H_0\mathcal{V}$, the second $\mathrm{M} - \mathrm{L}$ steps produce the basis vectors for $H_0^2\mathcal{V}$, *etc*. The resulting vectors truly form an orthonormal set. None of the steps in the construction involved any time-varying quantities, so the new basis vectors (and the similarity transformation to the new basis) are time-independent.

Although the $H'(t)$ matrix reduces to an $\mathrm{M} \times \mathrm{M}$ block [thus ensuring that H is $(2\mathrm{M}-1)$-diagonal], the H_0 matrix becomes $(2\mathrm{M}'+1)$-diagonal, where $\mathrm{M}' = \mathrm{M} - \mathrm{L}$. The latter fact

[7] *Ibid.*

[8] J. L. B. Cooper in *Handbook of Physics*, second edition, ed. by E. Condon and H. Odishaw (McGraw-Hill, New York, 1967), Ch. 6.

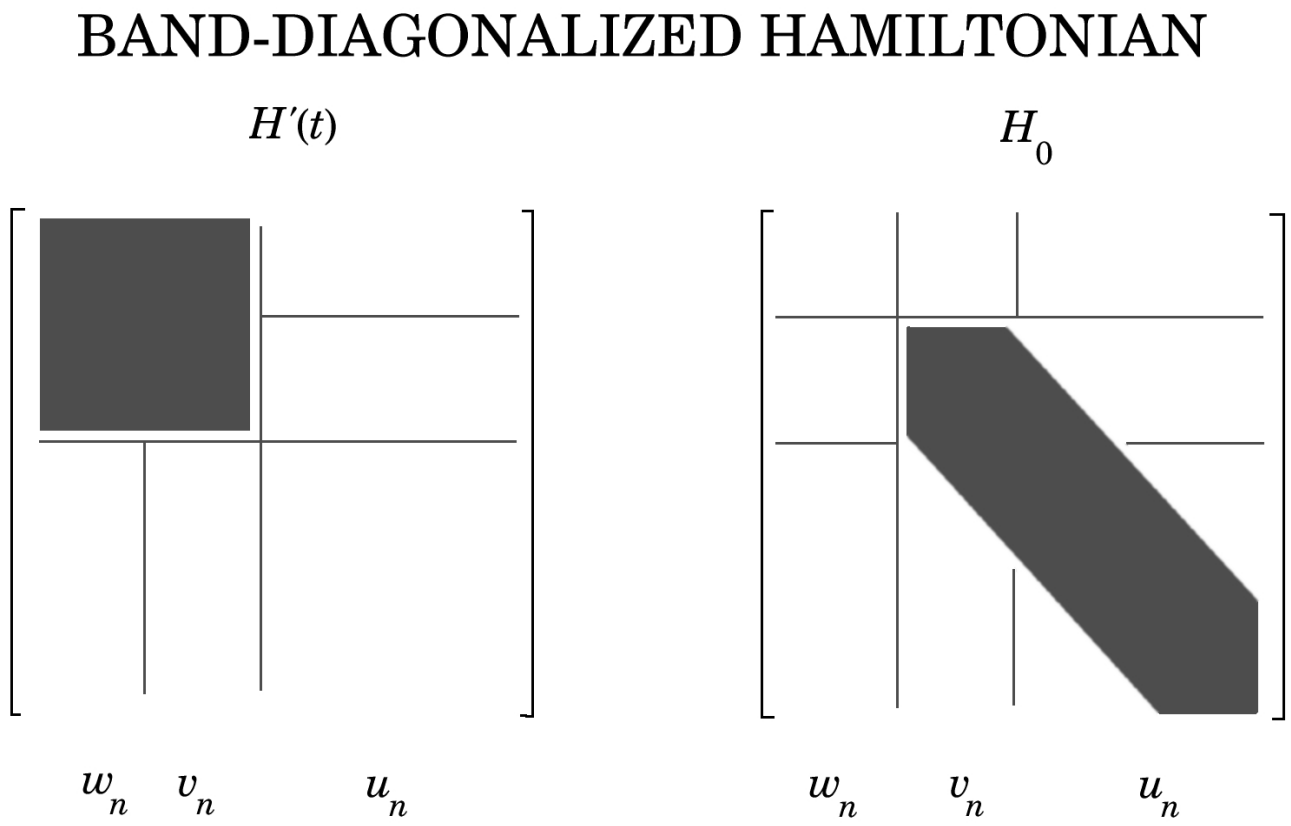

FIGURE 6.2

The fully band-diagonalized Hamiltonian for a quantum system of low driver-rank. The Hamiltonian is effectively $(2\mathrm{M}' + 1)$-diagonal, although $H'(t)$ has a non-zero block which is $\mathrm{M} \times \mathrm{M}$ (where $\mathrm{M} \geq \mathrm{M}'$).

arises from the fact that, by construction, $H_0 u_{n-\mathrm{M}+\mathrm{L}}$ is orthogonal to u_{n+1}, u_{n+2}, ..., and from the fact that $H(t)$ is Hermitian. As mentioned earlier, typically $\psi_0 \in \mathcal{W}$, so $\mathrm{L} > 1$. Thus, in this case, $H(t)$ is at most $(2\mathrm{M}-1)$-diagonal. Let's summarize this as follows:

> There is a *time-independent* similarity transformation for which $H'(t)$ has only an $\mathrm{M} \times \mathrm{M}$ non-zero block and H_0 is $(2\mathrm{M}'+1)$-diagonal (where $\mathrm{M}' = \mathrm{M} - \mathrm{L}$).

This is depicted in Figure (6.2).

6.3. The $(1, \mathsf{CONTINUUM})$ System

The Hamiltonian of a $(1, \mathsf{BAND})$ system [given by eq. (3.11)] can be tridiagonalized by the construction outlined in §6.2. It is amusing to actually find the tridiagonalizing basis and to compute the tridiagonal matrix elements. Rather than carrying out the construction *per se*, we will give the results in a more meaningful way in terms of analytical formulae.

Now, as pointed out above, we require $H'(t) = E(t)\mu$ and H_0 to be bounded operators on the space U, or else the construction algorithm is not guaranteed to work. From our standpoint, this is merely a requirement that

$$\int \mu(\Delta)^2 \Delta^{2n} d\Delta < \infty \tag{6.13}$$

for all non-negative integers n. In turn, this merely means that $\mu(\Delta)$ goes to zero (as $|\Delta| \to \infty$) faster than Δ^{-n}, for any n. This is, of course, the narrow-wing condition introduced in §5.6. Therefore, let us consider narrow-winged continua. [Note, by the way, that the following comments apply to discrete systems as well as continuous ones, but that we are limiting ourselves to continuous systems simply because the concepts to be used will prove more familiar than in the corresponding discrete case.[9]]

Because (as we discussed briefly in §5.6) $\mu(\Delta)^2$ is a non-negative function and satisfies the condition represented by eq. (6.13), once properly normalized it can serve as a weight function for defining a family of orthogonal polynomials.[10] Let us introduce a such a normalized weight function:

$$w(\Delta) = \frac{\mu(\Delta)^2}{\gamma^2}. \tag{6.14}$$

[γ^2 is defined by eq. (3.12).] $w(\Delta)$ is non-negative and integrates to unity. We will define a family of orthogonal polynomials $p_n(\Delta)$ by the conditions

[9] U. Hochstrasser in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), §22.17.

[10] R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1962).

$$\left.\begin{array}{rcl} p_0(\Delta) & \equiv & 1 \\ \partial\, p_n(\Delta) & = & n \\ \displaystyle\int w(\Delta)\, p_n(\Delta)\, p_m(\Delta)\, d\Delta & = & \delta_{nm} \end{array}\right\}. \tag{6.15}$$

(∂ is, of course, the *degree* operator.) Only the following result from orthogonal polynomial theory will be needed. All families of orthogonal polynomials satisfy a recurrence relation[11] of the form

$$p_{n+1}(\Delta) = (a_n + b_n\,\Delta)\; p_n(\Delta) - c_n\, p_{n-1}(\Delta), \tag{6.16}$$

and we will assume that such a relationship (and the constants a_n and b_n) is known here.

Rather than construct the tridiagonal basis vectors according to the prescription of §6.2, we will simply write them down and then verify that the Hamiltonian is tridiagonal. In the notation of §6.2, we define

$$u_n = \begin{cases} \left[\begin{array}{c} 1 \\ 0(\Delta) \end{array}\right] & , \; n = 1 \\ \\ \left[\begin{array}{c} 0 \\ \frac{\mu(\Delta)}{\gamma}\, p_{n-2}(\Delta) \end{array}\right] & , \; n = 2, 3, 4, \ldots . \end{cases} \tag{6.17}$$

Of course, by definition $w_1 = u_1$ and $v_2 = u_2$. Computing the matrix elements of $H(t)$ [defined by eq. (3.11)] in this basis is simplicity itself. Employing eq. (6.16), simple integration gives

$$u_1^\dagger\, H(t)\, u_2 = \gamma\, E(t), \tag{6.18}$$

$$u_n^\dagger\, H(t)\, u_n = -\frac{a_{n-2}}{b_{n-2}}, \;\; n \geq 2, \tag{6.19}$$

$$u_n^\dagger\, H(t)\, u_{n+1} = \frac{1}{b_{n-2}}, \;\; n \geq 2. \tag{6.20}$$

Aside from the transposed matrix elements, all other matrix elements are zero. Clearly, the Hamiltonian is tridiagonal, and the matrix elements can in principle be calculated from orthogonal polynomial theory. In this new basis, we have a ladder system:

[11] See two preceding references.

$$H(t) = \begin{bmatrix} 0 & \gamma E(t) & & & & \\ \gamma E(t) & -\frac{a_0}{b_0} & \frac{1}{b_0} & & & \\ & \frac{1}{b_0} & -\frac{a_1}{b_1} & \frac{1}{b_1} & & \\ & & \frac{1}{b_1} & -\frac{a_2}{b_2} & \frac{1}{b_2} & \\ & & & \frac{1}{b_2} & -\frac{a_3}{b_3} & \\ & & & & & \ddots \end{bmatrix}. \tag{6.21}$$

For various shapes $\mu(\Delta)^2$ the values of these coefficients can simply be looked up,[12] though they generally need correction for normalization standards and integration ranges differing from ours. Alternatively, Schek and Wyatt (Ref. 3) have shown that the first several matrix elements can be computed from a knowledge of the moments of the distribution $\mu(\Delta)^2$. (We will show in §8.5 that only the first few coefficients are important at high field-strengths.) Though we won't carry out either exercise here, there are certain general points of interest about these coefficients.

First, for bandshapes $\mu(\Delta)^2$ symmetric around the point $\Delta = s$, we find that

$$-\frac{a_n}{b_n} = s \tag{6.22}$$

from the general formula

$$-\frac{a_n}{b_n} = \int_{\Delta_{\min}}^{\Delta_{\max}} w(\Delta)\, \Delta\, p_n(\Delta)^2\, d\Delta. \tag{6.23}$$

From this formula we can also easily demonstrate in the non-symmetric case that $\Delta_{\min} < -\frac{a_n}{b_n} < \Delta_{\max}$. Second, from the similar formula

$$\frac{1}{b_n} = \int_{\Delta_{\min}}^{\Delta_{\max}} w(\Delta)\, (\Delta - s)\, p_n(\Delta)\, p_{n+1}(\Delta)\, d\Delta. \tag{6.24}$$

along with the Minkowski inequality,[13] we can show that

$$\left|\frac{1}{b_n}\right| \leq \max\left\{|\Delta_{\min} - s|\,, |\Delta_{\max} - s|\right\}. \tag{6.25}$$

Of course, the right-hand side here is simply σ when $\Delta_{\min}$ and $\Delta_{\max}$ are finite, and is ∞ when they are not. It will turn out in Chapter VIII that we are as interested in the behavior of these coefficients as $n \to \infty$ as in their exact values. For all of the well-known sets of orthogonal polynomials (Legendre, Chebychev, Hermite, Laguerre, Gegenbauer, *etc.*) we can make some specific statements. Namely, for those polynomials defined on an infinite range (Hermite, Laguerre), we find that

[12] *Ibid.*

[13] E. Hewitt and K. Stromberg, *Real and Abstract Analysis* (Springer-Verlag, New York, 1975).

$$\frac{1}{b_n} \to \infty,\ n \to \infty,$$

while for those defined only on a finite range ($\Delta_{\min} = s - \sigma$, $\Delta_{\max} = s + \sigma$), we find that

$$\frac{1}{b_n} \to \frac{\sigma}{2},\ n \to \infty. \tag{6.26}$$

The former point follows from inspection of the recurrence coefficients for Hermite and Generalized Laguerre polynomials, while the latter point follows from inspection of the recurrence coefficients for Jacobi polynomials. (All of the well-known finite-range orthogonal polynomials are special cases of the Jacobi polynomials. See Ref. 9.) These facts may hold more generally, but I know of no such proof. Eq. (6.26) will prove to be of some interest in Chapters VII and VIII.

There is also an interesting relationship between the theory presented above and the narrow-winged discretization theory presented in §5.6. The Hamiltonian (6.21) is discrete, but infinite. [It would be finite if we had started with a $(1, \mathrm{N})$ system rather than a $(1, \mathsf{CONTINUUM})$ system.] To do actual calculations, on actual finite computers, one must truncate the discrete ladder after only a finite number of levels. Suppose that this has been done, and that the truncated system has only $\mathrm{N}+1$ levels. Now, the argument given in §6.2, which showed that a $(1, \mathrm{N})$ system can be converted to an $(\mathrm{N}+1)$-level ladder system by similarity transformation, can be reversed to show that an $(\mathrm{N}+1)$-level ladder system can be converted to a $(1, \mathrm{N})$ system. What $(1, \mathrm{N})$ system corresponds to the truncated ladder?

To convert the truncated ladder back to a $(1, \mathrm{N})$ system, all we need to do is find a similarity transformation on the upper N levels which diagonalizes the upper $\mathrm{N} \times \mathrm{N}$ block of the truncated discretized Hamiltonian. Suppose that such a similarity transformation may be accomplished by the $\mathrm{N} \times \mathrm{N}$ matrix S. Then, the $(1, \mathrm{N})$ system, which we will call the *discretized* $(1, \mathrm{N})$ system, will simply have a Hamiltonian of

$$\underline{\text{Truncated Ladder}}$$
$$\begin{bmatrix} 0 & \gamma E(t) & 0 & \cdots & 0 \\ \gamma E(t) & -\frac{a_0}{b_0} & \frac{1}{b_0} & \cdots & 0 \\ 0 & \frac{1}{b_0} & -\frac{a_1}{b_1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -\frac{a_{\mathrm{N}-1}}{b_{\mathrm{N}-1}} \end{bmatrix} \to \underline{\text{Discretized } (1, \mathrm{N})}$$
$$\begin{bmatrix} 0 & \gamma E(t) S_{11} & \cdots & \gamma E(t) S_{1\mathrm{N}} \\ \gamma E(t) S_{11} & \Delta_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \gamma E(t) S_{\mathrm{N}1} & 0 & \cdots & \Delta_{\mathrm{N}} \end{bmatrix},$$

where the Δ_n are the eigenvalues of the upper $\mathrm{N} \times \mathrm{N}$ submatrix. It has been shown by a number of authors that the eigenvalues of such a matrix are in fact the roots of the N-th orthogonal polynomial with recurrence relation (6.16).[14] Thus,

$$p_{\mathrm{N}}(\Delta_n) = 0\,,\ n = 1, 2, ..., \mathrm{N}. \tag{6.27}$$

[14] J. Eberly, B. Shore, Z. Bialynicka-Birula, and I. Bialynicki-Birula, *Phys. Rev. A* **16**, 2038; Z. Bialynicka-Birula, I. Bialynicki-Birula, J. Eberly, and B. Shore, *Phys. Rev. A* **16**, 2048; C. D. Cantrell, V. S. Letokhov, and A. A. Makarov, in *Coherent Nonlinear Optics: Recent Advances*, ed. by M. S. Feld and V. S. Letokhov (Springer-Verlag, Berlin, 1980), Chap. 5.

It can also be seen rather straightforwardly from eq. (6.16) that the (unnormalized) eigenvectors of the $\mathrm{N} \times \mathrm{N}$ submatrix are

$$\begin{bmatrix} p_0(\Delta_n) \\ \vdots \\ p_{\mathrm{N}-1}(\Delta_n) \end{bmatrix}, \quad n = 1, 2, ..., \mathrm{N}.$$

(This demonstrates, incidentally, that these vectors are orthogonal for distinct n.) Consequently,

$$S_{1n} = \frac{1}{\sqrt{\sum_{m=0}^{\mathrm{N}-1} p_m(\Delta_n)^2}}. \tag{6.28}$$

Now recall §5.6. There, we explicitly derived a discretized Hamiltonian for the $(\underline{\mathrm{N}}, \mathsf{CONTINUUM})$ system. The discretized system was actually an $(\underline{\mathrm{N}}, \mathrm{Q})$ system where Q, like N, is an integer. To compare these results, we need to make the identifications $\mathrm{N} \to 1$ and $\mathrm{Q} \to \mathrm{N}$ in eq. (5.52a-5.52b), and to note that the function $\rho_1(\Delta)$ used in §5.6 is identically unity here. Having done so, we can determine by inspection that the discretized Hamiltonian in eq. (5.52a-5.52b) is identical to the discretized $(1, \mathrm{N})$ Hamiltonian derived above. What is interesting is that, though both are Hamiltonians for a $(1, \mathsf{NARROW\ WING\ CONTINUUM})$ system which has been approximated as a $(1, \mathrm{N})$ system, the rationales behind these these two approximations are entirely different.

On the one hand, in §5.6 we proceeded by determining the integral form of Schrödinger's equation, constructing an optimum integration formula approximating the kernel $K(t)$, and using the resulting weight coefficients and sample points to construct a discretized $(1, \mathrm{N})$ system. On the other hand, in the present section we exactly tridiagonalized the Hamiltonian (thus creating a ladder system) by means of a similarity transformation, then truncated the ladder after a certain number of levels, and performed another similarity transformation to get a $(1, \mathrm{N})$ system. However, our argument shows that these two methods produce precisely the same discretized system.

This is not only remarkable, but quite useful since we can now analyze the discretized system in two entirely different ways—namely, using integral equations and using ladder systems. For example, we have already seen in §5.6 (by means of the integral equation) that the discretized system is accurate up to the recurrence time $t = \tau_{\mathrm{R}} = \frac{2\pi}{\omega}$, where ω is the widest level spacing $\Delta_{n+1} - \Delta_n$ in the discretized system. This point will gain new significance when we analyze the dynamics of the ladder form of the discretized system in Chapter VIII.

As a numerical example of this, we can solve the $(1, \mathsf{UNIFORM\ BAND})$ system solved previously in §5.8. The result of this calculation is depicted in figure (6.3). As expected, there is no visual discrepancy from figure (5.4).

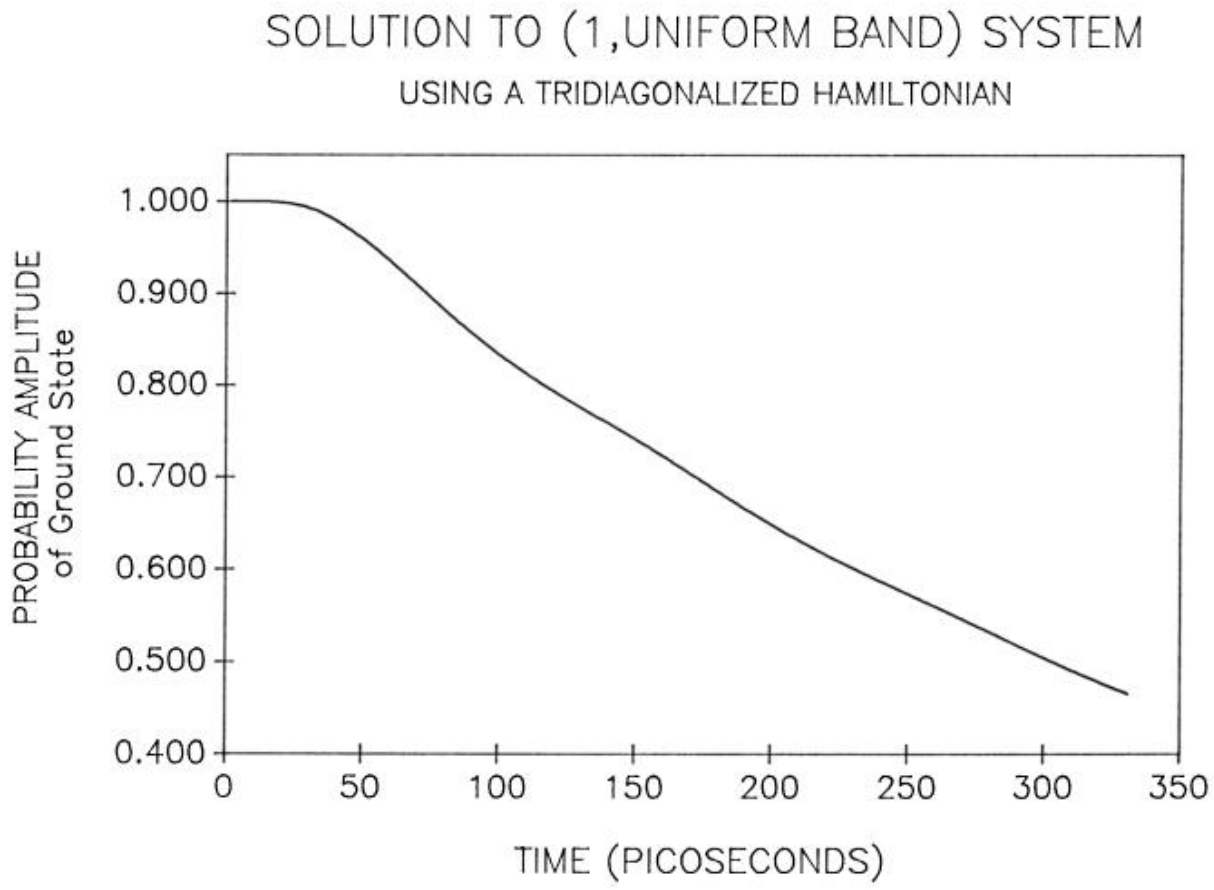

FIGURE 6.3

Ground-state probability amplitude of the $(1, \text{UNIFORM BAND})$ system as calculated from the tridiagonal Hamiltonian. Here, $s = 0$, $\sigma = 0.3\,\text{cm.}^{-1}$, with $\gamma E(t)$ ramping linearly from 0 to $0.05\,\text{cm.}^{-1}$ at $t = 33\,\text{psec}$. Since these are the same parameters leading up to figure (5.4), the result should be identical (except for roundoff error) to figure (5.4).

6.4. Continuum-Continuum Population Trapping and Time-Varying Interactions

As we will see in Chapter VII, in which more practical methods are introduced, the results we have presented so far in this chapter have certain limitations when applied to nontrivial problems. Thus, the technique for band-diagonalizing the Hamiltonian of §6.2 is better interpreted as an existence theorem than as a construction technique. Similarly, the $(1, \mathsf{CONTINUUM})$ method of §6.3 cannot be used easily without knowledge of the orthogonal polynomials with respect to the weight-function $\mu(\Delta)^2$, and these are known for only a limited variety of functions.

Nevertheless, it would be interesting to see an application of the band-diagonalization technique. To this end, let us continue the discussion of continuum-continuum population-trapping begun in §4.6.2 and §5.8. In those sections we discussed, among other things, the behavior of a $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ system influenced by a suddenly switched-on interaction (which remained constant thereafter). In §4.6.2, we found that if the continua were *broad* (the prototype being the infinite featureless continuum) then for either very *weak* or very *strong* interactions, the population remained in the continuum initially containing it. This remarkable result holds whatever the initial conditions (so long as the population is initially contained in just one of the continua). For continua narrower in energy than the interaction energy (prototype, Lorentzian continuum), this result no longer holds. In §5.8, we extended the discussion to the case of a time-varying interaction (*i.e.*, a more-slowly-switched-on interaction). We found that population was even more completely trapped than supposed. However, the discussion there was based on the generalized Weisskopf-Wigner approximation, which applied *only* to very broad bands.

Neither of the prototype continua used so far (the infinite featureless continuum and the Lorentzian continuum) is what we have called *narrow* (or "limited") continua. They do not die away quickly enough as $|\Delta| \to \infty$ to allow the definition of orthogonal polynomials. Let us therefore consider the case of two coupled narrow continua. We already have reason to suspect, and will see explicitly in Chapter VIII, that the band-diagonalization technique is particularly applicable to this case. For simplicity, however, for the moment let's just stick to the simplest possible case and retain the trivial approximation given by eq. (4.28). That is, we will assume that the system has a driver-rank of $\mathrm{M} = 2$, like the $(1, \mathsf{BAND})$ system.

Though we could carry out the construction process envisaged in§6.2 in order to band-diagonalize the Hamiltonian, let us follow §6.3 instead and try to guess the band-diagonal basis-functions. Instead of introducing a single set of orthogonal polynomials, suppose we introduce *two* sets of orthogonal polynomials $p_n^{(0)}(\Delta)$ and $p_n^{(1)}(\Delta)$, respectively based on the weight functions $w^{(0)}(\Delta)$ and $w^{(1)}(\Delta)$, where

$$w^{(k)}(\Delta) = \frac{V_k(\Delta)^2}{\left(\gamma^{(k)}\right)^2} \ , \ k = 0, 1, \tag{6.29}$$

and

$$\gamma^{(k)} = \sqrt{\int V_k(\Delta')^2 \, d\Delta'} \ , \ k = 0, 1. \tag{6.30}$$

Thus,

$$\int w^{(k)}(\Delta) \, p_n^{(k)}(\Delta) \, p_m^{(k)}(\Delta) \, d\Delta = \delta_{nm} \ , \ k = 0, 1. \tag{6.31}$$

In place of eq. (6.16), we have

$$p_{n+1}^{(k)}(\Delta) = \left(a_n^{(k)} + \Delta \, b_n^{(k)}\right) \, p_n^{(k)}(\Delta) - c_n^{(k)} \, p_{n-1}^{(k)}(\Delta) \ , \ k = 0, 1. \tag{6.32}$$

We define basis vectors u_n for $n = \pm 1, \pm 2, ...$, omitting $n = 0$, by

$$u_{-n} = \begin{bmatrix} \frac{V_0(\Delta)}{\gamma^{(0)}} p_{n-1}^{(0)}(\Delta) \\ 0(\Delta) \end{bmatrix} \ , \ \ u_n = \begin{bmatrix} 0(\Delta) \\ \frac{V_1(\Delta)}{\gamma^{(1)}} p_{n-1}^{(1)}(\Delta) \end{bmatrix} . \tag{6.33}$$

Computing the matrix elements of the Hamiltonian is now straightforward, and gives

$$H = \begin{bmatrix} \ddots & \ddots & & & & & \\ \ddots & -\frac{a_1^{(0)}}{b_1^{(0)}} & \frac{1}{b_0^{(0)}} & & & & \\ & \frac{1}{b_0^{(0)}} & -\frac{a_0^{(0)}}{b_0^{(0)}} & \gamma E(t) & & & \\ & & \gamma E(t) & -\frac{a_0^{(1)}}{b_0^{(1)}} & \frac{1}{b_0^{(1)}} & & \\ & & & \frac{1}{b_0^{(1)}} & -\frac{a_1^{(1)}}{b_1^{(1)}} & \ddots & \\ & & & & \ddots & \ddots & \end{bmatrix} . \tag{6.34}$$

where

$$\gamma = \gamma^{(0)} \gamma^{(1)}. \tag{6.35}$$

Finding the initial conditions in this basis requires a little more work than in the $(1, \mathsf{CONTINUUM})$ system, especially since we have ignored the injunction of §6.2 to choose the initial state as one of our basis states. (Had we done so, the states u_{-n} and their associated matrix elements—but not u_n—would have been more complicated.) If we denote the probability amplitude of state u_n by $a_n(t)$, then simple expansion of $\alpha(\Delta)$ in terms of the orthogonal polynomials $p_n^{(0)}(\Delta)$ gives

$$a_{-n}(0) = \int \sqrt{w^{(0)}(\Delta)} \, \alpha(\Delta) \, p_n^{(0)}(\Delta) \, d\Delta. \tag{6.36}$$

Of course, $a_n(0) = 0$ for $n > 0$.

For the sake of argument, let's just suppose that $a_{-1}(0) = 1$, and that $a_n(0) = 0$ for $n \neq -1$. That is, let's assume that the population is originally distributed in continuum 0 according to

$$C_0(\Delta, 0) = p_0^{(0)}(\Delta).$$

What should we qualitatively expect the subsequent behavior of the populations to be, from eq. (6.34)?

If the electric field $E(t)$ were constant, there would be three regimes of interest. For γE small, ladders 0 and 1 will be nearly decoupled, and the population will simply spread in time throughout the levels of ladder 0. ("Ladder 0" consists of a_{-1}, a_{-2}, ..., while "ladder 1" consists of a_1, a_2, ...) This represents simple dephasing of the probability amplitudes in continuum 0.

For $\gamma E \approx 1/b_1^{(0)}$, on the other hand, there is no particular reason why the population initially in a_{-1} should not move as easily to $a_1$as to a_{-2}. Thus, it would be reasonable to suppose that the population might spread out equally into the two bands (supposing that widths and detunings of the two bands were comparable).

Finally, for $\gamma E \gg 1/b_1^{(0)}$, we might expect a_{-1} and a_1 together to behave much like a rapidly oscillating two-level system, with population eventually leaking out into the other states. Thus, we might suppose that the population would eventually distribute itself evenly between the two continua (ladders). This is, of course, what we found in the case of the Lorentzian continuum.

To find out whether these guesses are accurate, we need to become more specific and either perform some numerical calculations or else to solve the system analytically using eq. (6.34). We will take the latter approach, but defer it to Chapter VIII where it will be more convenient. We will find that our guesses are *not* entirely accurate.

CHAPTER VII
APPROXIMATE BAND-DIAGONALIZATION

7.1. Introduction

In Chapters VII and VIII, unless it is explicitly stated otherwise, whenever we speak of a "continuum" or a "continuous band of levels", we will always mean a *strictly limited continuum*. A strictly limited continuum is the most extreme case of a narrow-winged continuum (defined in §5.5). For a limited continuum, the operator μ has non-zero matrix elements only the range $|\Delta - s| < \sigma$. (Recall that $\Delta = s$ is the center of the continuous band, and σ is the band's width.) In many respects, however, what we say will be relevant to the unlimited continuum ($-\infty < \Delta < \infty$) as well; we will indicate this as we go.

Now, in Chapter VI we learned that the Hamiltonian of a system of driver-rank M can be $(2\mathrm{M}+1)$-diagonalized. That is, there is a similarity transformation (independent of time) which converts the system to a generalized ladder system. In a normal ladder system, only adjacent levels are connected by transitions, but in this ladder-like system, each level is connected to the M levels above, and the M levels below. It will become apparent below, and in Chapter VIII, that it is somewhat easier to understand the dynamics of a ladder-like system than it is to understand the dynamics of a system with continuous bands of levels. For this reason, it is an advantage to deal with the ladder-like system, as opposed to a system with bands.

Unfortunately, problems arise when we actually try to apply the construction outlined in §6.2. The problem is that the construction is mainly applicable (though not entirely without difficulty) to computer-implemented calculations on a discrete Hamiltonian given numerically. The construction is more difficult to adapt to analytic or numerical production of an infinite sequence of basis vectors and matrix elements from an analytically known continuous Hamiltonian. (Two possible approaches for direct application include the method of Schek and Wyatt[1] for using the moments of $\mu(\Delta)^2$ to compute the matrix elements of the Hamiltonian, or to use computer-algebra systems[2] for this purpose.) This difficulty is why the tridiagonal Hamiltonian for the $(1, \mathsf{CONTINUUM})$ system was derived separately in §6.3, rather than through application of the band-diagonalizing construc-

[1] I. Schek and R. Wyatt, *J. Chem. Phys.* **89**, 4924 (1988).

[2] For example, some of the algebra in this paper was aided by the muMath program from Microsoft Consumer Products. It runs on the IBM PC family computers.

tion. Consequently, §6.2 is best regarded mathematically as an existence proof, even though it superficially takes the form of a construction.

However, since we know that a band-diagonal form of the Hamiltonian exists, it behooves us to look for a different way of carrying out the band-diagonalization process.

This is our task in the present chapter and in Chapter VIII. We will not discover any good way to find the actual $(2\mathrm{M}+1)$-diagonal Hamiltonian of Chapter VI, but will instead discover approximations that conveniently allow us to find a Hamiltonian that is effectively $(2\mathrm{M}+1)$-diagonal (with only a finite number of additional non-zero matrix elements). What we will do is to find a similarity transformation to a basis in which the Hamiltonian has a "large" band-diagonal portion and "small" matrix elements elsewhere. Indeed, the Hamiltonian matrix elements will become progressively smaller as they get farther from the diagonal. This method, in conjunction with the methods presented in Chapter VIII, can provide a remarkable degree of (global) accuracy using only a small number of discrete levels in place of continua.

Before beginning, one final comment is in order: To a certain extent, the approximating technique we will develop *creates* a low driver-rank in the system under consideration, and does not require a low driver-rank as such. In this regard, for systems with continuous bands of levels the approximate technique is superior to the exact techniques developed so far. The reason we are able to get away with this if the system contains continuous bands (and not if it is purely discrete) is that the set of finite-rank matrices is dense within the set of continuous matrices.[3] Thus, for any continuous matrix (by this we mean not merely a matrix expressed in our "continuous matrix" notation but one which, in addition, has matrix elements expressed by functions which are mathematically continuous), we can find an approximating low-rank matrix, accurate to any desired degree. For discrete matrices, in contrast, there may not be any singular matrix representing a close approximation. Although we will not do so (except briefly in §8.3), the approximations introduced below can actually be used with the methods of Chapters IV and V to somewhat extend their range of application.

7.2. Polynomial Approximations and the $(1, \mathrm{CONTINUUM})$ System

In this section, we will introduce the major idea behind our approximating technique, and apply it to the $(1, \mathrm{CONTINUUM})$ system. In so doing, we will gain enough understanding of the technique to apply it to successively more general systems (in §7.3-5), until we eventually understand how to apply it to the most general system with continuous bands.

Our idea involves approximating band-shapes (matrix elements of μ) with Chebychev orthogonal polynomials. Therefore, in what follows, let us define

[3] This is really a restatement of the Stone-Weierstrass theorem [see Rudin, *Principles of Mathematical Analysis* (McGraw-Hill, New York)], which states that the set of all polynomials on a compact interval is dense within the space of continuous functions on that interval. In the simplest case applying to us, this means that the set of matrices (in "continuous matrix" notation) $[p(\Delta, \Delta')]$ where the p functions are polynomials (on a given closed, finite interval) is dense in the set of all matrices $[\mu(\Delta, \Delta')]$. μ represents a continuous function.

$$w(\Delta) = \frac{1}{\pi\,\sigma}\left(1 - \frac{(\Delta - s)^2}{\sigma^2}\right)^{-\frac{1}{2}}. \tag{7.1}$$

[See eq. (3.18).] This is the weight-function for Chebychev orthogonal polynomials of the first kind, as adapted to the interval $\Delta \in (s-\sigma, s+\sigma)$ [as opposed to the standard range of $\Delta \in (-1, 1)$].[4] Furthermore, let $p_n(\Delta)$ represent the n-th Chebychev polynomial of the first kind, adapted to the range mentioned above, and normalized. Under these conditions, the orthonormalization condition (6.15) is satisfied.

Now, the Hamiltonian of a $(1, \mathsf{CONTINUUM})$ system is given by eq. (3.11). If we recall that $\mu(\Delta)$ has the normalization given by eq. (3.12), it is natural to attempt to approximate the $(1, \mathsf{CONTINUUM})$ system by another system with Hamiltonian

$$H(t) \approx \begin{bmatrix} 0 & E(t)\,\gamma\,q(\Delta')\,\sqrt{w(\Delta')} \\ E(t)\,\gamma\,q(\Delta)\,\sqrt{w(\Delta)} & \delta(\Delta - \Delta')\,\Delta \end{bmatrix}, \tag{7.2}$$

where $q(\Delta)$ is some polynomial selected to make the fit

$$\mu(\Delta)^2 \approx \gamma^2 q(\Delta)^2 w(\Delta) \tag{7.3}$$

as accurate as possible for a given polynomial degree ∂q. In general, this is quite easy to do, since

$$\mu(\Delta) = \gamma\,\sqrt{w(\Delta)} \sum_{n=0}^{\infty} \alpha_n\, p_n(\Delta), \tag{7.4}$$

where

$$\alpha_n = \frac{1}{\gamma} \int_{s-\sigma}^{s+\sigma} \sqrt{w(\Delta)}\,\mu(\Delta)\,p_n(\Delta)\,d\Delta. \tag{7.5}$$

It is known that truncation of the series in eq. (7.4) to ∂q terms produces a very good polynomial approximation (in a least-squares sense) to eq. (7.3).[5] Eq. (7.5), of course, involves only known quantities, so the coefficients α_n can be regarded as known. In general, series in terms of Chebychev polynomials of the first kind converge faster than any other polynomial series, so we expect the summation in eq. (7.4) to converge rapidly. As we will see, the main advantage of this approximation is that it makes it easier for us to compute the Hamiltonian matrix elements in a systematic way.

Though this approximation will be our final goal, we can begin by introducing a similarity transformation that converts the $(1, \mathsf{CONTINUUM})$ Hamiltonian *exactly* into a discrete Hamiltonian, as follows. As mentioned, we introduce new basis vectors analogously to those in eq. (6.17):

$$u_1 = \begin{bmatrix} 1 \\ 0(\Delta) \end{bmatrix}\ ,\ u_n = \begin{bmatrix} 0 \\ \sqrt{w(\Delta)}\,p_n(\Delta) \end{bmatrix}\ ,\ n = 2, 3, ... \tag{7.6}$$

[4] U. Hochstrasser in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), Ch. 22.

[5] R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1962).

If we calculate the matrix elements of $H(t)$ in this basis [employing eqs. (6.18-6.20) to compute the matrix elements of H_0], and if we look up the constants a_n, b_n, and c_n appearing in eq. (6.16) (see Ref. 4), we find immediately

$$H(t) = \begin{bmatrix} 0 & E(t)\,\gamma\,\alpha_0 & E(t)\,\gamma\,\alpha_1 & E(t)\,\gamma\,\alpha_2 & E(t)\,\gamma\,\alpha_3 & \cdots \\ E(t)\,\gamma\,\alpha_0 & s & \frac{\sigma}{\sqrt{2}} & 0 & 0 & \cdots \\ E(t)\,\gamma\,\alpha_1 & \frac{\sigma}{\sqrt{2}} & s & \frac{\sigma}{2} & 0 & \cdots \\ E(t)\,\gamma\,\alpha_2 & 0 & \frac{\sigma}{2} & s & \frac{\sigma}{2} & \\ E(t)\,\gamma\,\alpha_3 & 0 & 0 & \frac{\sigma}{2} & s & \\ \vdots & \vdots & \vdots & & & \ddots \end{bmatrix}. \tag{7.7}$$

Except for the matrix elements proportional to $E(t)$, this is just a tridiagonal matrix. Also, the α_n decrease rapidly to zero and, in the approximation (7.3), are actually assumed to be zero after a certain point. Thus, except for a finite number of matrix elements, $H(t)$ is essentially tridiagonal.

The convenient fact that $H_{nn} \equiv s$ for $n \geq 2$ and that $H_{n,n+1} = H_{n+1,n} \equiv \frac{\sigma}{2}$ for $n \geq 3$ is a result of choosing $w(\Delta)$ as the weight function for Chebychev polynomials of the first kind. $w(\Delta)$ could have been chosen as the weight function for some other family of orthogonal polynomials, but then the matrix elements would have varied as a function of n. (An exception is the Chebychev polynomials of the second kind.) Moreover, no other choice would have resulted in as quick convergence of eq. (7.4), which causes the α_n to die out quickly.

This choice is not merely convenient: the dynamical implications of eq. (7.7) are profound. We analyze the dynamics in Chapter VIII, but it is convenient to give some hint of them here. Let us, therefore, perform a simple test calculation to help us understand the behavior of a system like that of eq. (7.7).

Incidentally, as a practical matter eq. (7.5) is not necessarily the best method for finding the values of α_n. There are discrete Fourier Transform methods for fitting the values of α_n which are much faster (in computer terms), and not necessarily less accurate. The method used here is CHEBFT from the *Numerical Recipes*[6][7] series of programs.

As a trivial numerical test case, let us choose the $(1, \text{UNIFORM BAND})$ system whose behavior we examined already in §5.7 and §6.3. Recall that the uniform band is defined by eq. (3.13), and that we chose to stimulate the system with a field $E(t)$ that ramped linearly in magnitude from time $t = 0$, but maintained a constant value after time $t = \tau$. In §5.7 our approach was to introduce an effective Hamiltonian in which the continuum was discretized into a band of 16 levels according to the technique developed in §5.5. In §6.3, we used the theoretically equivalent (but practically different) method of exact tridiagonalization. Sixteen discrete levels were used simply because they allowed accurate

[6] W. Press, B. Flannery, S. Teukolsky, and W. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986).

[7] Practical details of using CHEBFT are these: you try to fit a Chebychev series to the function

$$\mu(\Delta)\gamma^{-1}\sqrt{\pi\sigma}\left(1 - \frac{(\Delta - s)^2}{\sigma^2}\right)^{\frac{1}{4}}.$$

At the conclusion of the calculation, the first coefficient returned must be divided by 2, while the remainder must be divided by $\sqrt{2}$, for normalization reasons.

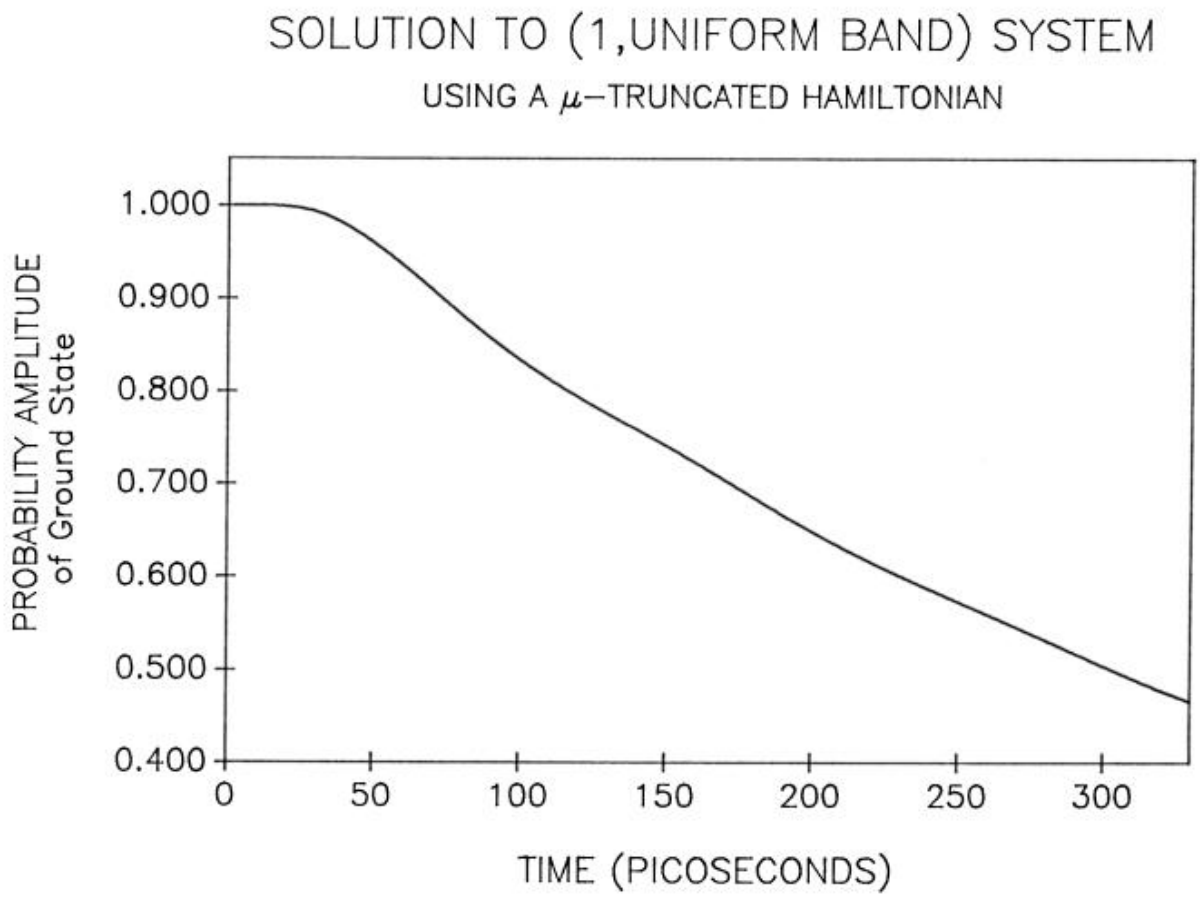

FIGURE 7.1

Ground-state probability amplitude of the $(1, \text{UNIFORM BAND})$ system as computed in the ladder basis.

calculation to six significant figures on the time interval we were interested in, although at the time we were not fully able to explain why. Recall the not entirely unexpected results we obtained [figures (5.4-5.9,6.3)]. For "wide" bands, we found that the Weisskopf-Wigner prediction of exponential decay of the ground-state probability amplitude was a fair approximation, except that the actual appearance of $a(t)$ was more that of a sequence of piecewise linear decays, approximately lying along an exponential curve. For "narrow" bands, we found approximate two-level-system behavior (*i.e.*, sinusoidal oscillation of the ground-state probability amplitude), but with mild damping. For intermediate widths, of course, we found clearly damped sinusoidal behavior. Obviously, we don't want to go through all of these calculations just to see results we already understand. Let us just repeat the type of calculations leading up to fig. (5.4) and the identical (6.3), using our new technique. Again, we retain the lowest 17 levels in our calculations.

Figure (7.1) depicts the result of the ground-state probability amplitude obtained from this calculation. Comparison with fig. (5.4) and fig. (6.3) reveals no visual difference from the results obtained earlier, nor would a more detailed investigation of the actual numbers obtained in the two cases. Incidentally, it is worth noting that (with the method of the rational band), this is the *fourth* accurate solution we have derived for this system.

Now, all figures derived from discretized 17-level systems, but with very different matrix elements and structures. In this calculation, the practical advantages of the effective 17-level Hamiltonian gotten from eq. (7.7) are substantial compared to those from eq. (5.52a-5.52b), even though there are more non-zero matrix elements. What are these advantages? First, there is the fact that in eq. (7.7) only two matrix elements of the Hamiltonian depend on $E(t)$,[8] whereas many of the matrix elements in eq. (5.52a-5.52b) depend on $E(t)$. This means that, using the present method, only the lowest two probability amplitudes need to be known accurately to compute the polarization $< \mu >$ or the *complex polarization* $\mathcal{P}$, whereas all of the probability amplitudes are needed in the previous method.[9] (In solving the coupled Maxwell-Schrödinger equations encountered in propagation problems, the polarization is of primary interest while the probability amplitudes are of little interest in themselves, since it is the polarization which generates the electromagnetic field.) Second, it is easier to compute the matrix elements of the Hamiltonian in the present instance, since they derive from simple integrals like those in eq. (7.5), rather than from knowledge of the roots of the orthogonal polynomials as in eq. (5.51). Third, the Hamiltonian is, in a sense, recursive. That is, given the 17-level discretized Hamiltonian, we are able to construct the 18-level discretized Hamiltonian simply by adjoining another row and column. For the previous method, there was no overlap at all between the $(1, 16)$ and $(1, 17)$ effective Hamiltonians. Of course, we also have the advantage here of being able to write down an exact (albeit infinite) Hamiltonian as in eq. (7.7).

There is a much more important advantage, however. This advantage is seen by looking at results in a different way. Now, in figure (7.1) we simply graphed the ground-state probability amplitude *vs*. time. Instead of doing this, let us look at *all* of the populations in the system at once, by graphing population *vs*. energy level. This is done in figure (7.2) for the model system and stimulation conditions we have been discussing. The population *vs*. level curves are shown at various times. For reasons that will become clear, however, we have added many more discretized levels to the system, and so have done these calculations using a 41-level discretized system.

What do we see in figure (7.2)? We see something remarkable. The appearance of this graph is that of a "wave packet" of population moving at a constant speed from the lower levels of the system to the higher levels. Though it is logical for population to spread throughout the system, the wave-packet phenomenon is something we could hardly have predicted from any simple idea of the ground-state probability amplitude decaying exponentially.

What happens after longer time intervals? Figure (7.3) continues the calculation for longer times. Apparently, the "wave packet" reaches the top of the truncated system, then reflects and moves at a constant speed back to the lower levels. Of course, this truncation

[8] Because in this example, only α_0 is non-zero—RSB, 3/2003.

[9] For example, C. D. Cantrell and W. M. Lee, *J. Chem. Lett.* **93**, 267 (1982).

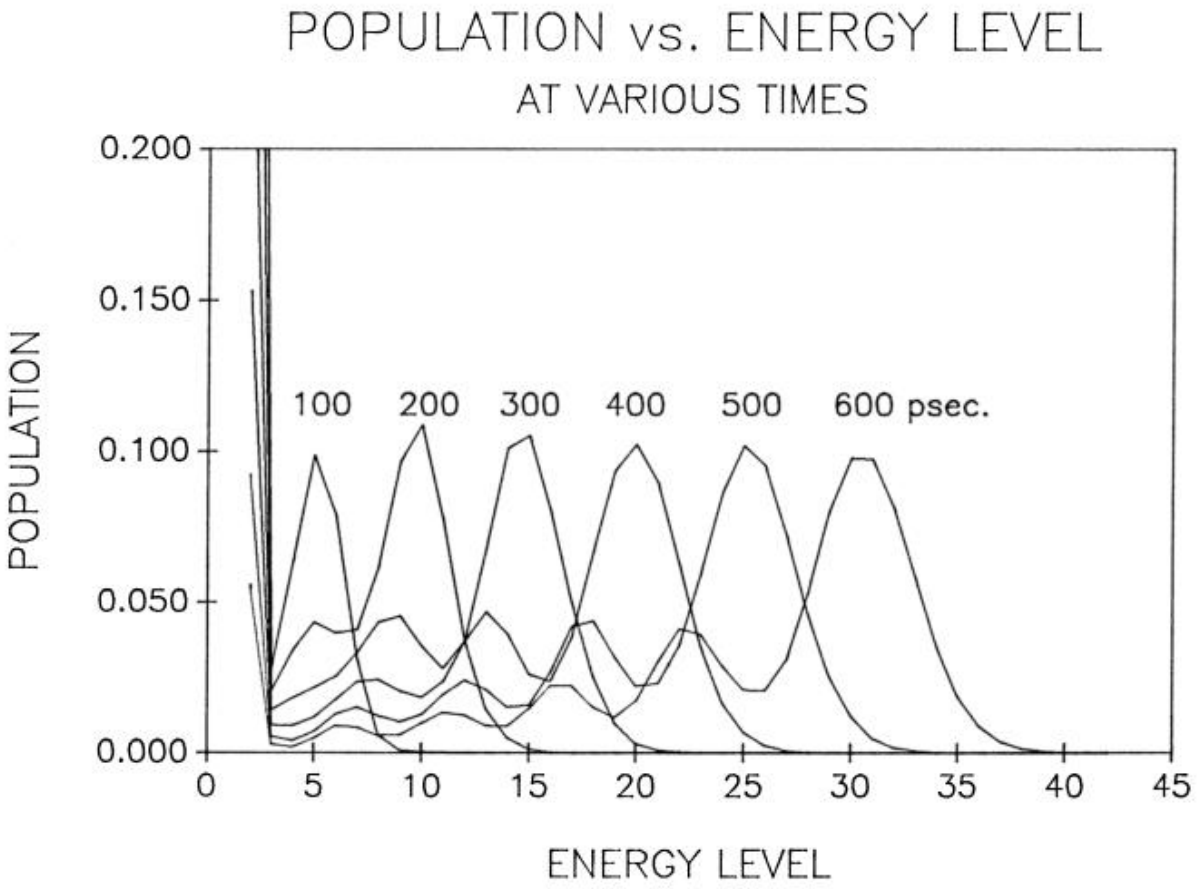

FIGURE 7.2

Populations in the ladder basis of the $(1, \text{UNIFORM BAND})$ system for all ladder levels, at various times.

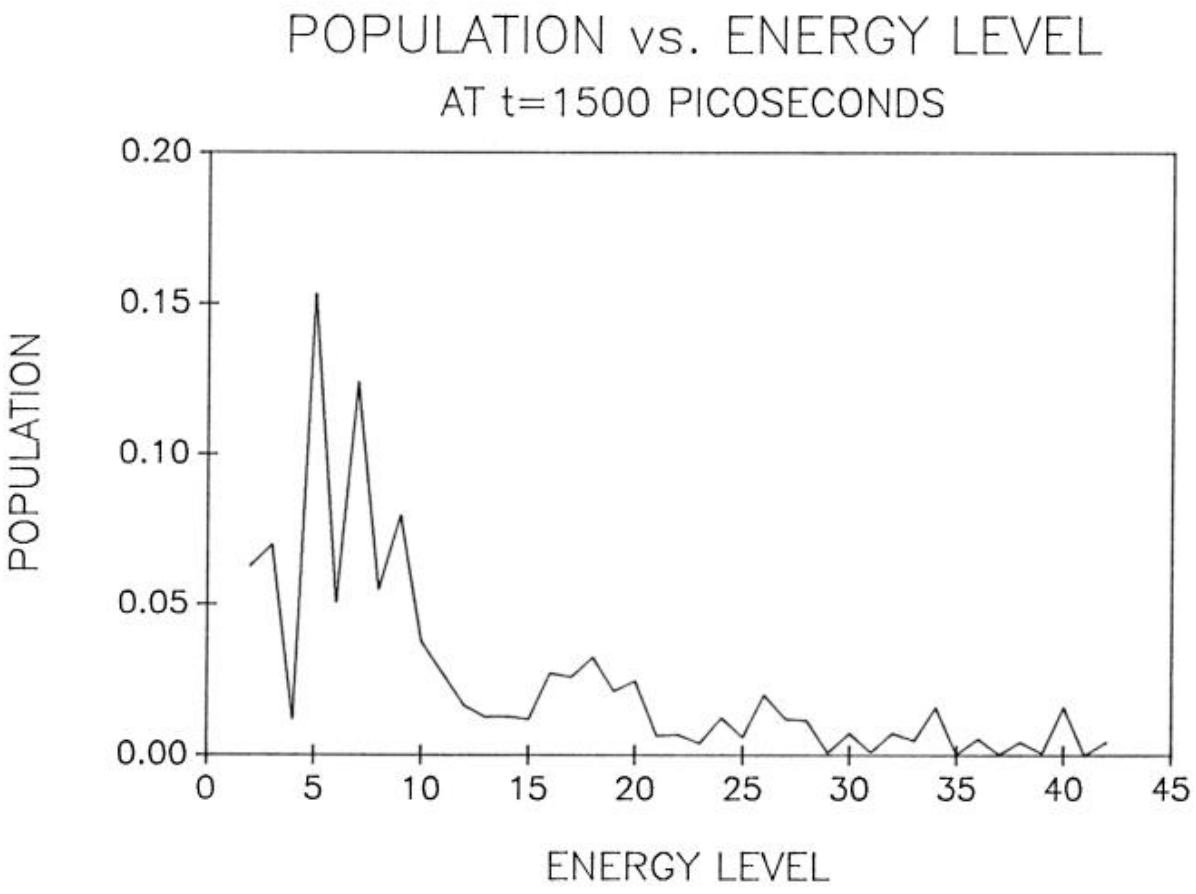

FIGURE 7.3

Continuation of Figure (7.2) for much longer times. The wave-packet of population is now moving downward (to the left).

of the system was introduced solely for the computer calculation, and the totally correct Hamiltonian would have infinitely many levels—and hence no such reflection. Nevertheless, the reflection is interesting, since when the population eventually reaches the ground state it causes something like a recurrence.

In fact, both assertions are correct and will be proved in Chapter VIII. There *is* a wave packet moving at constant speed, and the reflection *does* cause a recurrence. Moreover, we will find that this effect is not limited to the simple $(1, \mathsf{UNIFORM\,BAND})$ system, or even to $(1, \mathsf{BAND})$ systems generally, but can be seen in all strictly limited continua.

Actually, the truncating approximation we made above to convert the infinite-dimensional Hamiltonian (7.7) to a finite-dimensional Hamiltonian was rather crude. In the kind of calculation we have just done, there is the potential for two distinctly different kinds of finitizing approximations on the Hamiltonian (7.7). First, the α_n die quickly to zero (for $n \to \infty$) and hence we could just ignore them after a point. In this, we would be throwing away parts of the dipole operator. For this reason, we will refer to this type of approximation as μ-truncation. Second, since the discretized ladder system has infinitely many levels, we must throw most of the upper levels away during an actual computer calculation. This type of approximation will be called δ-truncation. What we did above, of course, was simply to apply μ-truncation and δ-truncation to the same extent without thinking very much about their relative importance (or even whether truncation makes any sense at all).

Both μ-truncation and δ-truncation are individually adjustable to any desired accuracy. δ-truncation affects the time interval for which the approximation is good. From our sample calculation (and as will be discussed in more detail in Chapter VIII), for initial times we know that there is no population in the upper ladder levels. As long as the wave-packet of population is able to continue moving upwards through the energy levels, the accuracy of the calculation must be excellent. When the wave-packet reflects from the δ-truncation point, the probability amplitudes of the upper levels begin to be inaccurate. Finally, as the wave-packet moves downwards and reaches the ground-state, all of the probability amplitudes become qualitatively wrong. At this point, as we will show later, a recurrence (caused entirely by the discretization and not inherent in the original continuum) has occurred. μ-truncation, on the other hand, clearly affects only the rate at which population is injected from the lower levels into the discretized ladder—*i.e.*, it affects only the shape of the wave-packet. Thus, in a qualitative sense, the calculation is hardly sensitive to μ-truncation at all. The actual effect of the μ-truncation is to bring about the approximation seen in eqs. (7.2) and (7.3), in which the true bandshape is approximated by polynomials. Clearly, the behavior of the system is not going to be very sensitive to tiny changes in the bandshape. We will generally, therefore, be μ-truncating at a much lower energy level than the δ-truncation point. In Chapter VIII this will be seen to have further advantages.

In both cases, it is easy to get a handle on how accurate the calculation really is. For δ-truncation, one need merely make the δ-truncation point at a high enough level that the wave-packet never reflects. (Or, if only the values of the lower levels are of interest, that the reflected wave does not manage to reach the lower levels during the time-scale of the calculation.) The error from this is zero in any practical sense. For the μ-truncation, one

can use Parseval's theorem[10]

$$\sum_{n=0}^{\infty} \alpha_n^2 = 1. \tag{7.8}$$

If the truncated α_n^2 add up to something much less than 1, the μ-truncation is clearly very accurate.

Since δ-truncation error manifests itself almost entirely through reflection and recurrence, it could be substantially eliminated if there were a way to prevent reflection of the population wave-packet. In the present chapter we are powerless to do this, since we have not yet analyzed the dynamics of the discretized ladder. In Chapter VIII, however, we will discover non-Hermitian additions to the Hamiltonian, allowing qualitatively accurate calculations (with no recurrences) at very low δ-truncation points.

7.3. Generalization: $(\mathrm{N}, \textsc{continuum})$ Transitions

Of course, this technique wouldn't be very useful if it applied only to $(1, \textsc{continuum})$ systems. Let us now see how to account for $(\mathrm{N}, \textsc{continuum})$ transitions, as we we did in §5.3-5.5. The Hamiltonian (or Hamiltonian submatrix) governing such transitions is of the form

$$H(t) = \begin{bmatrix} \delta_1 & 0 & \cdots & 0 & E(t)\mu_1(\Delta') \\ 0 & \delta_2 & \cdots & 0 & E(t)\mu_2(\Delta') \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \delta_{\mathrm{N}} & E(t)\mu_{\mathrm{N}}(\Delta') \\ E(t)\mu_1(\Delta) & E(t)\mu_2(\Delta) & \cdots & E(t)\mu_{\mathrm{N}}(\Delta) & \Delta\,\delta(\Delta-\Delta') \end{bmatrix}. \tag{7.9}$$

Let's develop an exact discrete Hamiltonian for this system similar to that of eq. (7.7). As before, our eventual goal (with μ-truncation) will be the introduction of a sequence of polynomials $q_1(\Delta)$, $q_2(\Delta)$, ..., $q_{\mathrm{N}}(\Delta)$ so that

$$\mu_n(\Delta)^2 \approx \gamma^2 q_n(\Delta)^2 w(\Delta). \tag{7.10}$$

This will be accomplished by means of the exact formulae

$$\mu_n(\Delta) = \gamma \sqrt{w(\Delta)} \sum_{m=0}^{\infty} \alpha_{nm} p_m(\Delta), \tag{7.11}$$

where

$$\alpha_{nm} = \frac{1}{\gamma} \int_{s-\sigma}^{s+\sigma} \sqrt{w(\Delta)}\, \mu_n(\Delta)\, p_m(\Delta)\, d\Delta. \tag{7.12}$$

In analogy to eq. (7.6), the new basis vectors will obviously be

[10] J. Todd in *Handbook of Physics*, second edition, ed. by E. Condon and H. Odishaw (McGraw-Hill, New York, 1967), Ch. 3.

$$u_1 = \begin{bmatrix} 1 \\ \vdots \\ 0 \\ 0(\Delta) \end{bmatrix}, \ \ldots, \ u_{\mathrm{N}} = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0(\Delta) \end{bmatrix}, \ u_n = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \sqrt{w(\Delta)}\, p_{n-\mathrm{N}-1}(\Delta) \end{bmatrix} \text{ for } n > \mathrm{N},$$

from which we immediately find the matrix elements

$$H(t) = \begin{bmatrix} \delta_1 & & & E(t)\alpha_{10} & E(t)\alpha_{11} & E(t)\alpha_{12} & E(t)\alpha_{13} & \cdots \\ & \ddots & & \vdots & \vdots & \vdots & \vdots & \\ & & \delta_{\mathrm{N}} & E(t)\alpha_{\mathrm{N}0} & E(t)\alpha_{\mathrm{N}1} & E(t)\alpha_{\mathrm{N}2} & E(t)\alpha_{\mathrm{N}3} & \cdots \\ E(t)\alpha_{10} & \cdots & E(t)\alpha_{\mathrm{N}0} & s & \frac{\sigma}{\sqrt{2}} & & & \\ E(t)\alpha_{11} & \cdots & E(t)\alpha_{\mathrm{N}1} & \frac{\sigma}{\sqrt{2}} & s & \frac{\sigma}{2} & & \\ E(t)\alpha_{12} & \cdots & E(t)\alpha_{\mathrm{N}2} & & \frac{\sigma}{2} & s & \frac{\sigma}{2} & \\ E(t)\alpha_{13} & \cdots & E(t)\alpha_{\mathrm{N}3} & & & \frac{\sigma}{2} & s & \\ \vdots & & \vdots & & & & & \ddots \end{bmatrix}, \tag{7.13}$$

where we have taken the liberty of simply omitting all zero matrix elements. This Hamiltonian is exact. μ-truncation and δ-truncation will work as described in the previous section. With μ-truncation the α_{nm} will be absent after some point (say, $n, m > \mathrm{N}'$), and this will be equivalent to making the approximation (7.10) using polynomials of degree $\mathrm{N}' - \mathrm{N}$.

Visual comparison of the Hamiltonians (7.7) and (7.13), after μ-truncation, makes it clear that there will be no real difference in their time-evolution, at least as far as the dynamics of the Chebychev ladder are concerned. In both cases, the μ-truncated system will be a Chebychev ladder with a finite number of additional low-level matrix elements remaining in an $\mathrm{N}' \times \mathrm{N}'$ block. These low-level matrix elements will cause a population wave-packet of some kind to be injected into the ladder, and this wave-packet will then move up the ladder, eventually to be reflected from the δ-truncation point. However, once this wave-packet has passed the μ-truncation point N', its evolution no longer depends on these low-level matrix elements.

7.4. Generalization: (CONTINUUM, CONTINUUM) Transitions

Next, let's consider the case in which the system has two separate continuous bands, with transitions occurring between the two bands. In this case, the submatrix of the Hamiltonian governing such transitions will be of the form

$$H(t) = \begin{bmatrix} \Delta\, \delta(\Delta - \Delta') & E(t)\, \mu(\Delta, \Delta') \\ E(t)\, \mu(\Delta', \Delta)^\star & \Delta\, \delta(\Delta - \Delta') \end{bmatrix}. \tag{7.14}$$

(Recall that in "continuous matrix" notation, Δ indexes rows and Δ' indexes columns.)

In this case, as in Chapter VI, we must introduce two Chebychev weight functions, $w_1(\Delta)$ (with center s_1 and width σ_1) for the lower band, and $w_2(\Delta)$ (with center s_2 and

width σ_2) for the upper band. ("Upper" and "lower" refer to the positions in the matrices, and not to higher or lower energies.) Similarly, we must have separate sets of orthogonal polynomials $p_n^{(1)}(\Delta)$ and $p_n^{(2)}(\Delta)$ for the two bands.

Obviously, we will eventually be performing μ-truncation by approximating the dipole matrix elements with a polynomial $q(\Delta, \Delta')$ in two variables:

$$\mu(\Delta, \Delta')^2 \approx q(\Delta, \Delta')\, w_1(\Delta)\, w_2(\Delta'). \tag{7.15}$$

[Since no normalization standard has been defined for functions such as $\mu(\Delta, \Delta')$, we no longer introduce a normalizing constant γ into our calculations.] As always, however, we begin by writing down an exact discrete Hamiltonian. In analogy with our previous work, we write

$$\mu(\Delta, \Delta') = \sqrt{w_1(\Delta) w_2(\Delta')} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \alpha_{nm}\, p_n^{(1)}(\Delta)\, p_m^{(2)}(\Delta'). \tag{7.16}$$

Solving for α_{nm} we immediately find

$$\alpha_{nm} = \int_{s_1-\sigma_1}^{s_1+\sigma_1} \int_{s_2-\sigma_2}^{s_2+\sigma_2} \sqrt{w_1(\Delta) w_2(\Delta')}\, \mu(\Delta, \Delta')\, p_n^{(1)}(\Delta)\, p_m^{(2)}(\Delta')\, d\Delta' d\Delta. \tag{7.17}$$

As we have seen previously in Chapter VI, the basis vectors and Hamiltonian have a somewhat more complex appearance than in our previous cases, because there are two infinite ladders in the system—one for the lower continuous band, and one for the upper. Two such tridiagonal ladders can be intermingled by permutation of the order of the basis vectors to form an effectively pentadiagonal Hamiltonian, but we will resist the temptation to do this. (To be honest, the temptation is minimal.) Instead, as in the previous chapter, we'll adopt an indexing scheme for the discretized system in which levels are numbered from $-\infty$ to ∞ (omitting zero). The new basis vectors will be:

$$u_{-n} = \begin{bmatrix} \sqrt{w_1(\Delta)}\, p_{n-1}^{(1)}(\Delta) \\ 0(\Delta) \end{bmatrix}, \; u_n = \begin{bmatrix} 0(\Delta) \\ \sqrt{w_2(\Delta)}\, p_{n-1}^{(2)}(\Delta) \end{bmatrix}, \; n = 1, 2, 3, \ldots.$$

Consequently, the Hamiltonian will be

$$H(t) = \begin{bmatrix}
\ddots & & & & & \vdots & \vdots & \vdots & \vdots & \\
 & s_1 & \frac{\sigma_1}{2} & & & E(t)\alpha_{30} & E(t)\alpha_{31} & E(t)\alpha_{32} & E(t)\alpha_{33} & \cdots \\
 & \frac{\sigma_1}{2} & s_1 & \frac{\sigma_1}{2} & & E(t)\alpha_{20} & E(t)\alpha_{21} & E(t)\alpha_{22} & E(t)\alpha_{23} & \cdots \\
 & & \frac{\sigma_1}{2} & s_1 & \frac{\sigma_1}{\sqrt{2}} & E(t)\alpha_{10} & E(t)\alpha_{11} & E(t)\alpha_{12} & E(t)\alpha_{13} & \cdots \\
 & & & \frac{\sigma_1}{\sqrt{2}} & s_1 & E(t)\alpha_{00} & E(t)\alpha_{01} & E(t)\alpha_{02} & E(t)\alpha_{03} & \cdots \\
\cdots & E(t)\alpha_{30}^\star & E(t)\alpha_{20}^\star & E(t)\alpha_{10}^\star & E(t)\alpha_{00}^\star & s_2 & \frac{\sigma_2}{\sqrt{2}} & & & \\
\cdots & E(t)\alpha_{31}^\star & E(t)\alpha_{21}^\star & E(t)\alpha_{11}^\star & E(t)\alpha_{01}^\star & \frac{\sigma_2}{\sqrt{2}} & s_2 & \frac{\sigma_2}{2} & & \\
\cdots & E(t)\alpha_{32}^\star & E(t)\alpha_{22}^\star & E(t)\alpha_{12}^\star & E(t)\alpha_{02}^\star & & \frac{\sigma_2}{2} & s_2 & \frac{\sigma_2}{2} & \\
\cdots & E(t)\alpha_{33}^\star & E(t)\alpha_{23}^\star & E(t)\alpha_{13}^\star & E(t)\alpha_{03}^\star & & & \frac{\sigma_2}{2} & s_2 & \\
 & \vdots & \vdots & \vdots & \vdots & & & & & \ddots
\end{bmatrix}.$$

As before, we have simply omitted any matrix elements which are zero. Of course, because of μ-truncation, only a finite number of the α_{nm} will be taken to be non-zero, so the Hamiltonian is essentially tridiagonal (or, as mentioned earlier, pentadiagonal if only a semi-infinite sequence of basis vectors is used). In practice, there will always be other matrix elements connecting these bands to other levels of the system. These matrix elements will inject population into one or the other ladder. Once population manages to get into one of the ladders associated with the lower or the upper band, and gets out of range of the non-zero α_{nm} matrix elements, we will observe wave-packets of population moving along the ladders, just as in the $(1, \mathsf{CONTINUUM})$ and $(\mathrm{N}, \mathsf{CONTINUUM})$ cases.

Note that this is the first instance we have seen in which μ-truncation *forces* the discretized dipole operator to have low rank. In §7.2 and §7.3, the systems were initially of low dipole rank before approximation (and, of course, afterwards as well). The matrices governing $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ transitions, on the other hand, are potentially of very high rank, and the fact that the eventual discretized matrix has low dipole rank is entirely a consequence of μ-truncation.

7.5. Generalization: $(\underline{\mathsf{CONTINUUM}})$ Transitions

The final required generalization—and, incidentally, the only case we have not analyzed earlier using other methods—is to allow transitions within a continuum. With this, and with the techniques of §7.3 and §7.4, we will be able to solve for the time evolution of the most general system containing only limited (*i.e.*, finite-width) bands. (This case could probably be handled using rational-function approximations as well, but we will not bother to do so here.)

Suppose, therefore, that we have the Hamiltonian submatrix

$$H(t) = \left[\Delta\,\delta(\Delta - \Delta') + E(t)\,\mu(\Delta, \Delta')\right]. \tag{7.18}$$

Fortunately, as in §7.2 and §7.3 we need only one Chebychev weight function and set of orthogonal polynomials. Clearly, we will perform μ-truncation by approximating $\mu(\Delta, \Delta')^2$

$$\mu(\Delta, \Delta')^2 \approx q(\Delta, \Delta')^2 w(\Delta)\, w(\Delta'), \tag{7.19}$$

where $q(\Delta, \Delta')$ is a polynomial in the two variables Δ and Δ'. This is done by means of the formula

$$\mu(\Delta, \Delta') = \sqrt{w(\Delta) w(\Delta')} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \alpha_{nm}\, p_n(\Delta)\, p_m(\Delta'). \tag{7.20}$$

where

$$\alpha_{nm} = \int_{s_1-\sigma_1}^{s_1+\sigma_1} \int_{s_2-\sigma_2}^{s_2+\sigma_2} \sqrt{w(\Delta) w(\Delta')}\, \mu(\Delta, \Delta')\, p_n(\Delta)\, p_m(\Delta')\, d\Delta'\, d\Delta. \tag{7.21}$$

Not all of these α-coefficients need to be calculated, since $\alpha_{nm} = \alpha^{\star}_{mn}$. As always, the μ-truncation will work by simply ignoring α_{nm} for n and m sufficiently large. As with

(CONTINUUM, CONTINUUM) transitions, this automatically introduces a low dipole rank which was not present in the original Hamiltonian.

Obviously, we should define basis vectors

$$u_n = \left[\sqrt{w(\Delta)}\, p_n(\Delta)\right], \tag{7.22}$$

and the resulting Hamiltonian matrix elements will clearly be

$$H(t) = \begin{bmatrix} s & \frac{\sigma}{\sqrt{2}} & & & \\ \frac{\sigma}{\sqrt{2}} & s & \frac{\sigma}{2} & & \\ & \frac{\sigma}{2} & s & \frac{\sigma}{2} & \\ & & \frac{\sigma}{2} & s & \\ & & & & \ddots \end{bmatrix} + E(t) \begin{bmatrix} \alpha_{00} & \alpha_{01} & \alpha_{02} & \alpha_{03} & \cdots \\ \alpha_{10} & \alpha_{11} & \alpha_{12} & \alpha_{13} & \cdots \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & \alpha_{23} & \cdots \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}.$$

Once again, with μ-truncation, this matrix is effectively tridiagonal (except for a finite number of matrix elements).

7.6. Unlimited Continua

We have confined our discussion above to strictly limited continua, in which there are non-zero matrix elements only on the index interval $\Delta \in (s-\sigma,\, s+\sigma)$. At low energies this is unlikely to be a problem, since only a small part of the continuous band (near resonance) is likely to be excited. Nevertheless, as we will see in Chapter VIII, this is somewhat pesky at high energies since sidebands far from resonance can be excited. Therefore, let us now consider the case of the *unlimited* continuum, in which $\Delta_{\max} \to \infty$ or $\Delta_{\min} \to \infty$. There are actually many possibilities for analyzing this case, and we will point out just a few of them.

The first possibility of analysis is simply to repeat all of the above work with a weight function $w(\Delta)$ other than the Chebychev function. For example, choosing $w(\Delta) = x^{\mathrm{n}} \exp\left(-\frac{\Delta}{\sigma}\right)$ would allow modelling of semi-limited bands, while choosing $w(\Delta) = \exp\left(-\Delta^2/\sigma^2\right)$ would allow modelling of unlimited bands. The appropriate orthogonal polynomials in these cases would be the generalized-Laguerre and the Hermite polynomials (see Ref. 4), respectively. This would retain the effectively tridiagonal discretized Hamiltonian. Relative to the Chebychev polynomials, the Laguerre and Hermite polynomials are somewhat inconvenient for our purposes. For one thing, we could not count on quick convergence of the α_n or α_{nm} to zero. Also, because different families of orthogonal polynomials obey different three-term recurrence formulas [eq. (6.16)], the off-diagonal matrix elements of H_0 would not all have the value $\frac{\sigma}{2}$. This, it will turn out, would completely alter the dynamics of population movement in the discretized ladder, and would invalidate all of the beautiful (and convenient) results to be presented in Chapter VIII. However, a workable system using these weight functions could undoubtedly be worked out.

A second possibility is the *rational band* approximation disscussed in §5.4. This is the idea of approximating the various $\mu(\Delta)$ and $\mu(\Delta, \Delta')$ functions describing the bandshapes by means of rational functions. This would serve the same purpose (for broad-winged

continua, at least) as the approximations described earlier in this chapter, but with somewhat more difficulty, and at the cost of a non-Hermitian discretized Hamiltonian.

A third (very simple) possibility is to think of the unlimited continuum as a sequence of limited continua. Thus, a single continuous bandwith $\Delta \in (-\infty, \infty)$ could simply be treated as a sequence of continuous bands

$$\ldots\,,\ \Delta \in (\Delta_{n-1}, \Delta_n)\,,\ \Delta \in (\Delta_n, \Delta_{n+1})\,,\ \Delta \in (\Delta_{n+1}, \Delta_{n+2})\,,\ \ldots$$

Each of the limited continua can then be treated separately according to the prescriptions given in the preceding sections.

Of course, since there is an infinite sequence of these limited continua, for practical calculation we must simply omit many of them. This is not a problem *if* we understand the distribution of population in the system. For example, consider the $(1, \mathsf{CONTINUUM})$ system. At low energies (Ω small), the population in the continuum is all concentrated near $\Delta = 0$. At high energies, however, the population is lumped into two sidebands near $\Delta = \pm\Omega$. Thus, in the former case we would need to approximate the unlimited continuum with a single limited continuum near $\Delta = 0$, while in the latter we would need two limited continua near $\Delta = \pm\Omega$. This technique has a great advantage, in that it enables us to model closely those parts of the band (or of the transition matrix) which are important to the dynamics, and ignore or only model roughly those parts which are unimportant to the dynamics. For example, a very complex feature in the continuum near resonance could be modelled very closely, while a broad sweep of levels far from resonance could be modelled very crudely. This general idea of chopping up the band is illustrated in figure (7.4).

7.7. Multi-Dimensional Continua

So far, we have limited our discussion to one-dimensional continua—that is, we have dealt only with continua indexed by a single variable Δ. There are, of course, physical continua which are multi-dimensional. For example, the free-particle continuum[11] is at least three-dimensional with basis wavefunctions

$$e^{-i(\mathbf{k}\bullet\mathbf{r}-\omega t)}.$$

Here, the wave-vector k is a 3-vector index to the wave-functions. Consequently, the continuum is 3-dimensional.

Now, there is nothing in the methods of Chapters III-VI which depends on the dimensionality of the continuum at all. Hence, these methods are as directly applicable to the multi-dimensional continuum as to the one-dimensional continuum. In the present chapter, however, the methods presented are all specifically tailored to the one-dimensional case, and need some modification before they are more generally applicable.

There are several available options, of which we will just mention the easiest. For simplicity, let's consider a 2-dimensional continuum indexed by the 2-vector (Δ_1, Δ_2). Now,

[11] L. Landau and E. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)*, third edition (Pergamon, Oxford, 1977).

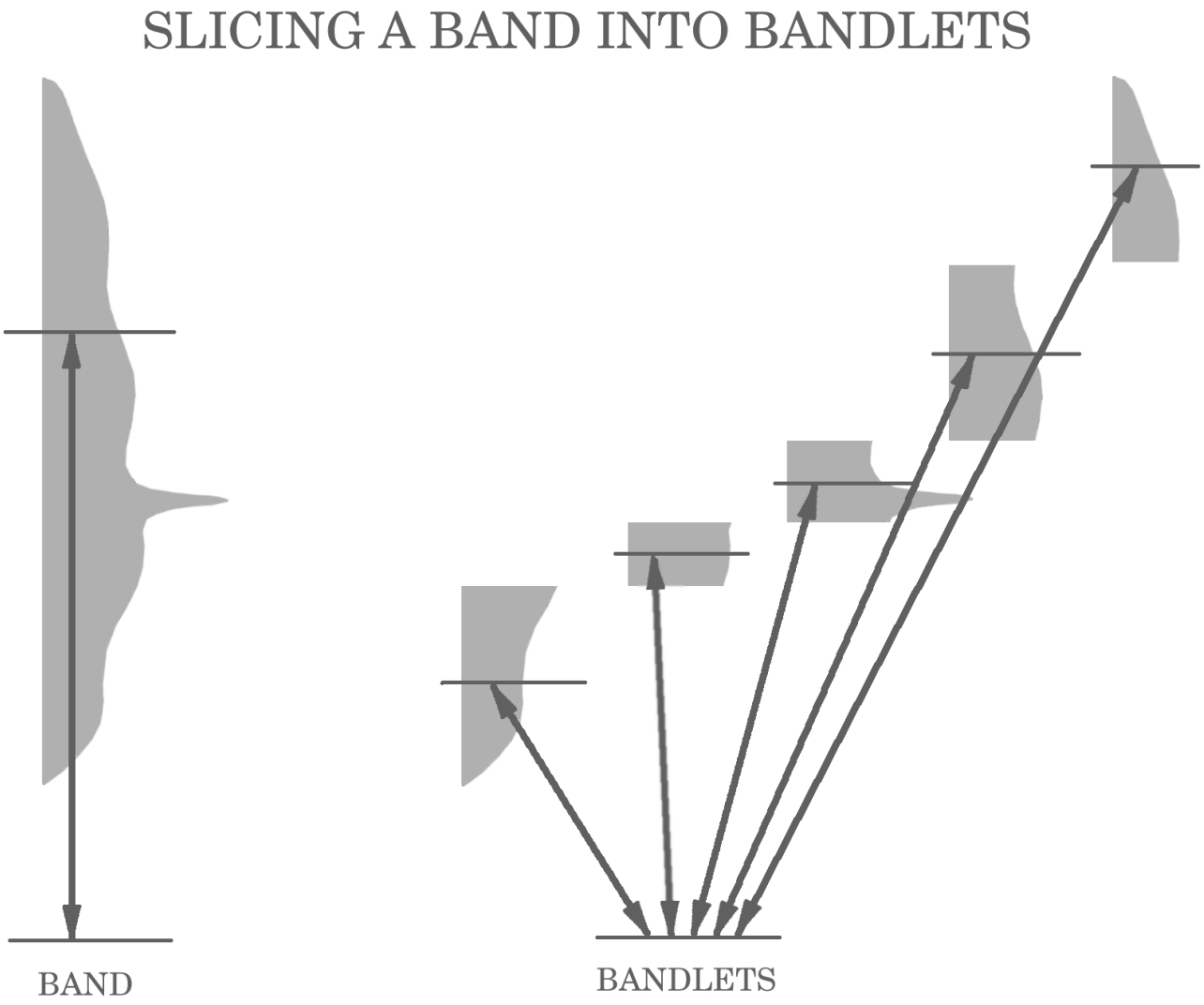

FIGURE 7.4

An unlimited continuum “sliced up” into limited continua.

in all the previous arguments in this chapter, we discretized continuous bands by introducing a Chebychev weight function $w(\Delta)$, Chebychev orthogonal polynomials $p_n(\Delta)$, and modelling the continuous matrix elements in terms of series of orthogonal polynomials. This resulted in $H'(t)$ having only a small number (*i.e.*, a finite number) of large matrix elements, and an infinite number of small matrix elements. H_0, in turn, was tridiagonal. Assuming that the discretized levels were indexed by n, H_0 allowed only transitions from $n \to n \pm 1$.

Fortunately, this scheme is easily generalized. If, in our previous one-dimensional discussions, we replace $w(\Delta)$ by $w(\Delta_1)w(\Delta_2)$ and $p_n(\Delta)$ by $p_n(\Delta_1)p_m(\Delta_2)$, we now have an appropriate way of modelling 2-dimensional continua. Namely, the continuous matrix elements are represented as a series in the functions $p_n(\Delta_1)p_m(\Delta_2)$. Once again, this results in the discretized $H'(t)$ having only finitely many large matrix elements. There is a difference in the discretized form of H_0 from the 1-dimensional case, however. In the 1-dimensional case, we were always able to suppose that the diagonal element of H_0 was used as the indexing quantity Δ. Now we have two indexing quantities Δ_1 and Δ_2. Let us assume that Δ_1 is chosen as the diagonal element of H_0, and Δ_2 is some other parameter selecting among the degenerate states. [For example, in the free-particle case mentioned already, rather than measure **k** in Cartesian components, we could introduce spherical polar coordinates $k \propto \text{Energy}$, $\theta \in (0, \pi)$, and $\varphi \in (0, 2\pi)$. These would be, respectively, Δ_1, Δ_2, and Δ_3.]

Our selection of basis functions $p_n(\Delta_1)p_m(\Delta_2)$ implies that the discretized states will be indexed by the pair (n, m). Computing the matrix elements of H_0, we find that H_0 will allow only the transitions $(n, m) \to (n \pm 1, m)$. This boils down to saying that in the discretized system there is a separate Chebychev ladder (indexed by n) for each $m = 0, 1, 2, ...$ Each Chebychev ladder has identical s and σ parameters. This notion is illustrated in Figure (7.5).

Thus, as in all of the other cases considered so far, the dynamics of the system is basically trivial. Population is injected into one or more Chebychev ladders, and is then carried away at constant speed. Only details like the rate at which population is injected, or the precise shape of the wave-packet of population, are affected by the precise numerical parameters of the system.

In a normal theoretical treatment, of course, multi-dimensional continua are generally forced into a one-dimensional form by simply indexing with the energy, and multiplying the matrix elements by some degeneracy factor. If this is to be done *a priori* the resulting equations contain only one-dimensional continua, and the immediately preceding discussion is moot.

7.8. Summary of the Theoretical Discussion

Because of the range of topics covered so far in this chapter, it would be good to briefly summarize them.

Our main result has been to find a class of approximations (adjustable to any degree of accuracy) which effectively band-diagonalizes the Hamiltonian of any system with strictly limited continuous band of levels. These systems can include as many interact-

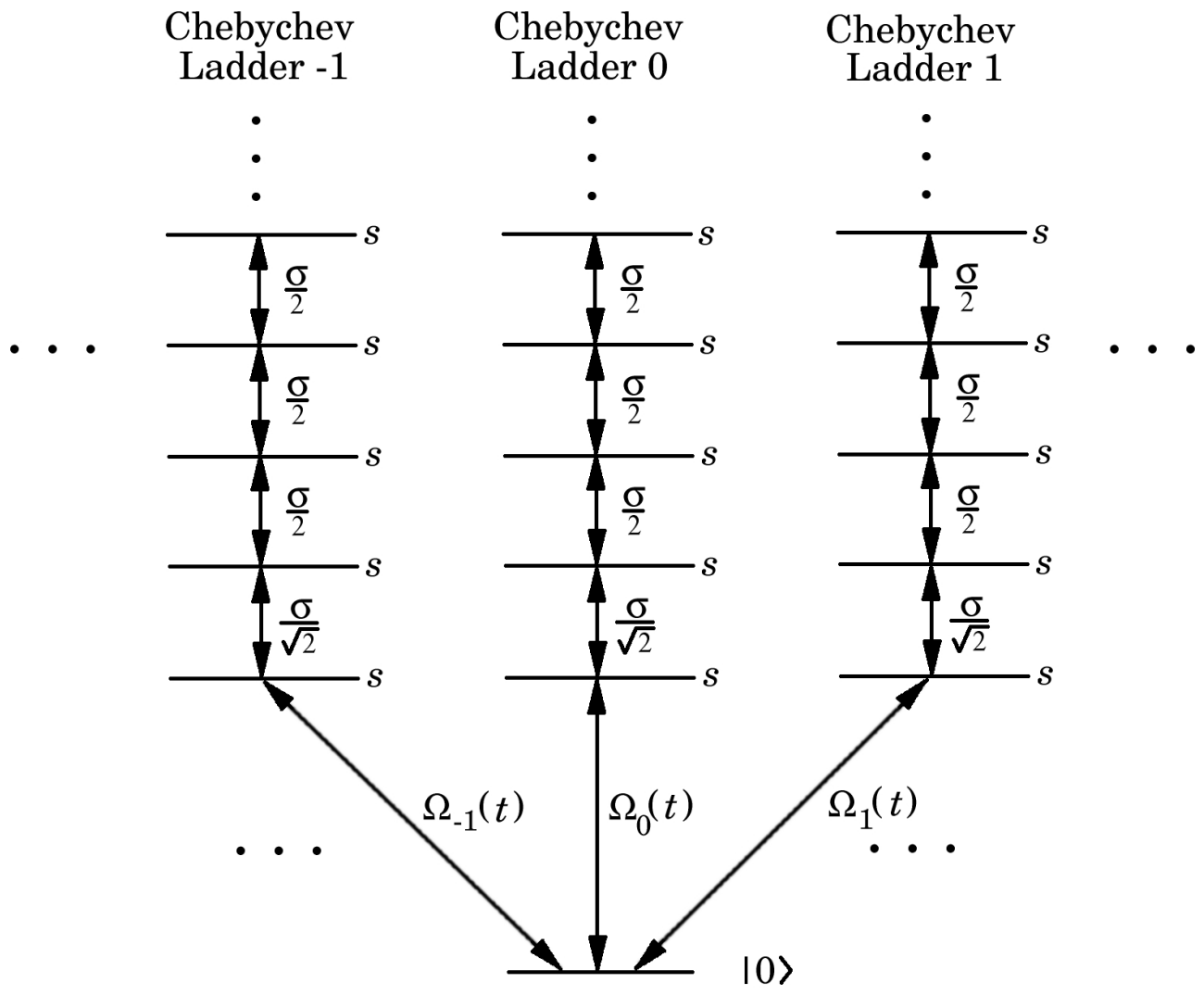

FIGURE 7.5

Representation of a two-dimensional continuum as a sequence of Chebychev ladders.

ing continua and discrete levels as desired, and can have transitions within any of the continua. The approximations require only that the dipole matrix elements representing transitions from or to a continuous band, which are always of the form $\mu(\Delta)$ or $\mu(\Delta, \Delta')$, be mathematically continuous functions.

Our approximations, known as μ-truncation and δ-truncation, were not actually required in order to define the similarity transformations we introduced, but only for subsequent computer calculations. Thus, if μ-truncation and δ-truncation are not used, our resulting Hamiltonians are exact. Though not finite, the exact Hamiltonians are discrete, and completely solve the problem of discretizing a continuous system.

In all cases, we find that a continuous limited band (of half-width σ) becomes effectively an infinite ladder after similarity transformation. It is only "effectively" a ladder, since (after μ-truncation) there are a finite number of additional matrix elements due to transitions between the levels of the band and discrete levels, levels in the same band, or levels in other bands.

In the next chapter, the apparently all-important dynamics of the Chebychev ladder are explored.

CHAPTER VIII
DYNAMICS OF THE CHEBYCHEV LADDER

8.1. Introduction

In Chapters IV-VI, we saw various new analytically exact and approximate methods helping us to find the time-evolution of low driver-rank systems. Although some of these techniques (such as the generalized Weisskopf-Wigner approximations) can potentially be quite useful in investigating realistic systems, they are oriented mainly towards solving the kinds of analytical problems typically posed in the literature.

Chapter VII took a somewhat different path. There, exact techniques were supplemented by a related approximation scheme, applicable to more realistic systems (with continuous bands). This approximation does not require low driver-rank in the given system but, instead, constructs an approximating low driver-rank system.

Chapter VII showed that a continuous band can be (exactly) discretized by similarity transformations. The discretizing similarity transformation is independent of time. No matter what selection rules hold in the continuous system, the discretized system always has the same form. H_0 always becomes tridiagonal. μ always has matrix elements α_{nm} going rapidly to zero as n and m become large. This is true no matter what kind of transitions the continuous system allows. It doesn't matter whether there are $(\mathsf{DISCRETE}, \mathsf{CONTINUUM})$ transitions, $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ transitions, $(\underline{\mathsf{CONTINUUM}})$ transitions, or any combination of these. Basically, each continuous band gives rise to a ladder of levels in the discretized system. Other (mostly negligible) transitions appear among the lower ladder-levels. These ladders have been called Chebychev ladders. They are based on Chebychev orthogonal polynomials.

The discretized system is an exact equivalent of the continuous one. However, there are infinitely many discretized levels. For computation we need to limit the number of energy levels. Two specific "finitizing" approximations have been introduced for this purpose. We have referred to these approximations as μ-truncation and δ-truncation, which may be summarized as follows:

μ-truncation discards all but a finite number of the matrix elements of μ (in the Chebychev ladder basis). Consequently, the discretized system is of low driver-rank. However, μ-truncation does not eliminate any transitions in the conventional basis, but merely alters the bandshapes in a minor way. Thus, μ-truncation is, in a sense, qualitatively

benign.

δ-truncation cuts off the Chebychev ladder after only a finite number of levels. δ-truncation is *quantitatively* unimportant for small times t, but very *qualitatively* important as t increases past a certain point τ_{R}. After $t = \tau_{\mathrm{R}}$, δ-truncation causes population *recurrences* not present in the original continuous system.

Two problems remain to be addressed in this chapter. The first problem involves the dynamics of the Chebychev ladder. In the calculations of earlier chapters, we noticed odd wavelike behavior in the movement of Chebychev populations. It would be nice to know whether this wave-behavior is real or mere appearance. If real, can it be exploited? §8.2 will show us that the wavelike behavior of the Chebychev populations are indeed real.

The second problem is one of computational efficiency. The $t = \tau_{\mathrm{R}}$ limit on the utility of δ-truncation is a big disadvantage. Modifying the discretized system so that it is useful for times greater than τ_{R} will fall to §8.3 and §8.4.

Of course, we will also return for a final look at our favorite problem of continuum-continuum population trapping. We will do this in §8.6, proving more unusual and unexpected results. First, however, we will exhibit an analytically exact solution for the $(1, \mathsf{CHEBYCHEV\ 2ND\ KIND})$ system in §8.5. This solution will also have some novel features.

8.2. The Dispersion Relation for the Chebychev Ladder

In discretizing a continuous system, H_0 is converted to the Hamiltonian for a Chebychev ladder. In the discretized basis, μ has matrix elements that are mostly small. Indeed, after the subsequent approximation of μ-truncation, only a finite number of matrix elements of μ are non-zero.

The time-evolution of such discretized systems seems rather simple from our previous computer work. Numerically, it is found that population forms a wave-packet that moves up the Chebychev ladder, away from the lower levels and the area of μ-induced transitions.[1] Thus, the very presence of the dipole operator μ in the system is only important at small times. At large times, the transitions due to μ are entirely irrelevant to the movement of the Chebychev populations. To understand the dynamics of the Chebychev ladder, the μ operator should consequently be eliminated, and we should look at an idealized system with Hamiltonian

[1] We often state loosely that a wave packet of population is moving "up" or "down" the Chebychev ladder. This should not be confused with moving to lower or higher energies. States high in the Chebychev ladder are not at higher energy than those low on the ladder. In fact, they are all at equal energy. If not, population could not continue to move around if, say, the driving fields were turned off. Instead, position on the Chebychev ladder can be thought of as representing dephasing. For low-lying Chebychev levels, all of the true continuum probability amplitudes are nearly in phase. For the high Chebychev levels, the true continuum probability amplitudes are out of phase. This is why other levels of the system can only inject or remove population from low-lying Chebychev levels.

$$H(t) = \begin{bmatrix} \ddots & & & & & & & \\ & s & \frac{\sigma}{2} & & & & & \\ & \frac{\sigma}{2} & s & \frac{\sigma}{2} & & & & \\ & & \frac{\sigma}{2} & s & \frac{\sigma}{2} & & & \\ & & & \frac{\sigma}{2} & s & \frac{\sigma}{2} & & \\ & & & & \frac{\sigma}{2} & s & & \\ & & & & & & \ddots & \end{bmatrix}.$$

As usual, any matrix elements not shown are zero.

Let us give the Chebychev ladder probability amplitudes the names

$$a_n(t) \ , \quad n = 0, \pm 1, \pm 2, \pm 3, \ldots .$$

Schrödinger's equation [eq. (3.1)] in terms of these probability amplitudes and this Hamiltonian is

$$i \, \frac{d}{dt} \, a_n(t) = \frac{\sigma}{2} \, a_{n-1}(t) + s \, a_n(t) + \frac{\sigma}{2} \, a_{n+1}(t). \tag{8.1}$$

As it happens, this differential-difference equation can be solved. Try the solution

$$a_n(t) = e^{i(kn - \omega t)}, \tag{8.2}$$

where k and ω are some unknown parameters. We immediately find that this is a solution if we accept the *dispersion relation*[2]

$$\omega(k) = s + \sigma \, \cos \, k. \tag{8.3}$$

The latter two equations imply that motion of population in the Chebychev ladder is a wave phenomenon. Eq. (8.3) is similar to the dispersion relation for the discrete lattice.[3] A discrete lattice is a sequence of vibrating masses connected by taut, massless strings. However, the Chebychev ladder and the discrete lattice are not quite identical. The Chebychev ladder has a first-order differential equation of motion. The discrete lattice has a second-order differential equation of motion. A lattice of masses m, separated by a distance ℓ, with string tension T, has the dispersion relation

$$\omega(k)^2 = \frac{4T}{m\ell} \, \sin^2 \, \frac{k}{2} \, .$$

For a given value of k, there is an ambiguity in the sign of for the discrete lattice, but not for the Chebychev ladder. Thus, a given value of k can give either a right-going or a left-going wave in the discrete lattice. In the Chebychev ladder, upward-moving waves are confined to the region $k \in (-\pi, 0)$, while downward-moving waves have $k \in (0, \pi)$.

[2] A. P. French, *Vibrations and Waves* (MIT Press, Cambridge, 1971), Ch. 7; W. Pauli, *Pauli Lectures in Physics* (MIT Press, Cambridge, 1973), Vol. 2, Ch. 2.

[3] N. Ashby and S. Miller, *Principles of Modern Physics* (Holden Day, San Francisco, 1970), §12.5-6.

The Chebychev ladder can support wave packets.[4] The group velocity is calculated by finding the extrema of

$$\frac{\partial}{\partial k}\,\omega(k) = -\sigma\,\sin\,k. \tag{8.4}$$

The group velocity must be an extremum in order to insure minimal spreading of the wave-packet. Clearly, the group velocity is

$$v_{\rm G} = \pm\sigma. \tag{8.5}$$

To have $v_{\rm G} = \sigma$, the wave-numbers in the packet must be bunched around $k = -\frac{\pi}{2}$. To have $v_{\rm G} = -\sigma$, they must be bunched around $k = \frac{\pi}{2}$. Eq. (8.3) is not a free-space dispersion relation so there will always be some spreading of the wave packet.

Such wave action is consistent in every respect with the sample calculations from previous chapters. Those calculations clearly revealed constant-velocity wave packets spreading slightly in time. It is easy to verify now by inspection of the figures in the previous chapter that the speed of those wave packets was truly σ, a fact which we did not recognize at the time.

This result has significance in terms of recurrences in discretized systems. The rough calculations in Chapter V and the exact calculations in Chapter VI together hinted that the δ-truncated system is accurate only up to a time $\tau_{\rm R} = \frac{2\pi}{\delta}$, where δ is the maximum level separation of the discretized $(1, {\rm N})$ system as obtained from Gaussian integration. (We used the notation "ω" rather than "δ" in Chapter V, but this conflicts with the notation already employed in the present chapter.) By no coincidence, $\tau_{\rm R}$ is a quantity known as the *recurrence time* of a $(1, {\rm N})$ system with levels evenly spaced by δ.[5] Of course, since the Chebychev ladder is not the $(1, {\rm N})$ form of the discretized system, we cannot directly apply the formula $\tau_{\rm R} = \frac{2\pi}{\delta}$ to give a time-limit on the utility of the δ-truncated Chebychev ladder, unless we can apply a little thought to relate the quantity δ to known parameters of the Chebychev ladder.

Now, in Chapter V we found that a pure Chebychev bandshape [eq. (3.18)] can alternately be discretized by Gauss-Legendre integration (as opposed to being band-diagonalized). In so doing, the continuous band is replaced by a sequence of discrete energy levels, and the $(1, {\rm CONTINUUM})$ system becomes a $(1, {\rm N})$ system. For a Chebychev continuum, the positions of the energy levels are just the roots of the ${\rm N}$-th Chebychev polynomial of the first kind.[6] [These roots must be adapted to the interval $(s-\sigma, s+\sigma)$ as opposed to the standard interval $(-1, 1)$.] This discretized system is equivalent (by similarity transformation) to the δ-truncated Chebychev ladder, according to the discussion of Chapter VI. As it happens, the n-th root of the ${\rm N}$-th Chebychev polynomial is

$$x_n^{({\rm N})} = s + \sigma\,\cos\,\frac{(2n-1)\pi}{2{\rm N}}. \tag{8.6}$$

[4] L. Landau and E. Lifshitz, *The Classical Theory of Fields* (Pergamon, Oxford, 1975), Ch. 7.

[5] A. Makarov, V. Platonenko, and V. Tyakht, *Sov. Phys. JETP* **48**, 1044 (1978).

[6] U. Hochstrasser in *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), Ch. 22.

The widest level separation is between $n = [\mathrm{N}/2] + 1$ and $n = [\mathrm{N}/2]$, where the brackets indicate the integer function. To make things easy, suppose that N is a large even integer. Then, applying a couple of trigonometric identities,

$$\begin{aligned} \delta &= x^{(\mathrm{N})}_{[\mathrm{N}/2]} - x^{(\mathrm{N})}_{[\mathrm{N}/2]+1} \\ &= 2\sigma \sin \tfrac{\pi}{2\mathrm{N}} \\ &\approx \tfrac{\pi\sigma}{\mathrm{N}} \text{ , for } \mathrm{N} \text{ large.} \end{aligned} \tag{8.7}$$

Therefore, the reasoning of Chapter V would seem to imply a recurrence time of

$$\tau_{\mathrm{R}} = \frac{2\pi}{\delta} \approx \frac{2\mathrm{N}}{\sigma} \,. \tag{8.8}$$

Unfortunately, the time limit $\tau_{\mathrm{R}} = \frac{2\pi}{\delta}$ found in Chapter V was based on rather loose reasoning, and the resulting equation (8.8) is therefore suspect. It would be good to verify eq. (8.8) independently, in terms of our understanding of the dynamics of the Chebychev ladder. This is easily done.

Consider a wave-packet of population moving up the Chebychev ladder at a constant speed of σ. Although it has not been shown (mathematically) here, when the wave-packet eventually reaches the δ-truncation point of the Chebychev ladder, it reflects and subsequently moves down the ladder at speed σ until it reaches the ground-state. Up to this point, the population has been decreasing as it leaks out in the Chebychev ladder. Now, population will instead pour from the wave-packet back into the ground-state, causing a rapid revival of the ground-state population. If the δ-truncated ladder has N levels, this entire process will take a time of about

$$\frac{\text{number of levels moved}}{\text{speed of the wave packet}} = \frac{2\mathrm{N}}{\sigma}.$$

Clearly, there is perfect agreement between this result and eq. (8.8).

8.3. Non-Hermitian δ-Truncation of the Chebychev Ladder

§8.2 represents both good news and bad news. The good news is an enhanced understanding of the dynamics of the Chebychev band. The bad news is that pure δ-truncation is proven to be computationally inefficient for long times.

Suppose that accurate knowledge of only the ground-state probability amplitude (as opposed to knowledge of all levels) is required, and that our interest extends only to the time interval from $t = 0$ to $t = \tau$. According to eq. (8.8), the number of levels kept in the Chebychev ladder must be

$$\text{required number of levels} = \frac{\sigma\tau}{2}.$$

If the Chebychev ladder populations must additionally be accurate, twice as many levels are needed. In either case, the computation time for each integration step is $\mathrm{O}(\mathrm{N}) = \mathrm{O}(\tau)$. Clearly, the number of integration steps is also $\mathrm{O}(\tau)$. Thus, for the entire calculation,

$$\text{CPU time} \propto \tau^2.$$

Naturally, we would prefer to have a method with a computation time of $\mathrm{O}(\tau)$ rather than $\mathrm{O}(\tau^2)$.

The culprit is the wave-packet reflected from the δ-truncation point. If wave-packets reaching the top of the ladder could somehow simply disappear rather than being reflected (and eventually returning to the ground state), there would be no recurrence problem and δ-truncation would be good for essentially unlimited time intervals.

How may the reflection of the wave-packet from the δ-truncation point be averted? Non-Hermitian modifications to the Hamiltonian might achieve this objective. Such modifications would be analogous to adding damping to the discrete lattice,[7] or to matching impedances in electrical transmission lines.[8] Non-Hermitian termination of a tridiagonal Hamiltonian has already been employed by other investigators to good advantage in computing eigenvalues and eigenvectors.[9] We will actually present two essentially different solutions to this problem in this section and in §8.4.

Suppose that $a_{\mathrm{N}}(t)$ is the final probability amplitude kept in the δ-truncated system. The only explicit requirement of our hypothetical population trap is that it must insure the correctness of da_{N}/dt. If da_{N}/dt approximates the correct value for an untruncated system, then a_{N} will be correct, and $a_{\mathrm{N}-1}$, $a_{\mathrm{N}-2}$, *etc.*, will also automatically be correct. Thus, what we would like to do is find an *alternate equation of motion* for a_{N}, but not for any of the other probability amplitudes in the system.

The analysis will prove easier if rather than $a_n(t)$ we consider the quantities

$$b_n(t) = i^n \, e^{ist} a_n(t). \tag{8.9}$$

These quantities have the advantage of obeying the simpler equation of motion

$$\frac{d}{dt}\, b_n(t) = \frac{\sigma}{2}\, b_{n-1}(t) - \frac{\sigma}{2}\, b_{n+1}(t). \tag{8.10}$$

The basic solution of eq. (8.10) is still

$$b_n(t) = e^{i(kn-\omega t)}, \tag{8.11}$$

but the b_n have a slightly different dispersion relation than the a_n:

$$\omega(k) = \sigma \, \sin \, k. \tag{8.12}$$

An advantage of the b_n, due to eq. (8.12), is that wave-packets with speed σ have wavenumbers grouped near $k = 0$, $\omega = 0$. b_{n+1} has approximately the same phase as b_n. Of course, all results for b_n can be translated as results in terms of a_n by the use of eq. (8.9).

Our difficulty is that db_{N}/dt still depends on $b_{\mathrm{N}+1}$, an unknown quantity when the system is δ-truncated. We really would like to find an (approximate) expression for db_{N}/dt

[7] Physically this can be accomplished by immersing the discrete masses in liquid, for instance.

[8] W. L. Cooley in *Electronics Engineers' Handbook*, second edition, ed. by D. Fink and D. Christiansen (McGraw-Hill, New York, 1982), Ch. 3, §54.

[9] For example, see R. Haydock in *Solid State Physics*, ed. by E. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1980), Vol. 35, p. 215.

depending entirely on $b_{\rm N}$, $b_{\rm N-1}$, $b_{\rm N-2}$, *etc*. The first step in finding such an expression is to derive a somewhat odd alternative equation of motion for the Chebychev probability amplitudes.

Since the basic solution to eq. (8.10) is given by eq. (8.11), the general solution must be given by a superposition of the form[10]

$$b_n(t) = \int_{-\pi}^{\pi} b(k)\, e^{i(kn-\omega t)} dk. \tag{8.13}$$

$b(k)$ is some function characteristic of the wave-packet. An immediate consequence is that

$$\frac{d}{dt}\, b_n(t) = \int_{-\pi}^{\pi} -i\,\omega(k)\, b(k)\, e^{i(kn-\omega t)} dk \tag{8.14}$$

Now, $\omega(k)$ is an analytic function. That is, it can be written as a power series in the variable k. Consequently, in the integrand $\omega(k)$ can be replaced by the operator expression $\omega\left(-i\,\frac{\partial}{\partial n}\right)$, which can subsequently be removed to the outside of the integral. In this way, eq. (8.14) can be rewritten in terms of the following operator calculus expression:[11]

$$\begin{aligned} \frac{d}{dt}\, b_n(t) &= -i\,\omega\left(-i\,\frac{\partial}{\partial n}\right) b_n(t) \\ &= -\sigma\,\sinh\left(\frac{\partial}{\partial n}\right) b_n(t). \end{aligned} \tag{8.15}$$

The identity $\sin(i\theta) = \sinh(\theta)$ has been used. Eq. (8.15) may alternately be derived from the operator calculus equation

$$\mathcal{E} - \mathcal{E}^{-1} = \exp\left(\frac{\partial}{\partial n}\right) - \exp\left(-\frac{\partial}{\partial n}\right) = 2\,\sinh\left(\frac{\partial}{\partial n}\right),$$

where $\mathcal{E}$ is the unit displacement operator.[12] (That is, $\mathcal{E} a_n = a_{n+1}$.) Naturally, the operator $\frac{\partial}{\partial n}$ is not meaningful if b_n is defined only for integral values of n. However, eq. (8.14) makes sense even for non-integral values of n. We can regard eq. (8.14) as a definition of b_n for non-integral n. With this understanding, eq. (8.15) is a valid alternative equation of motion. Naturally, eq. (8.15) is used only for $n = {\rm N}$. Eq. (8.10) still applies for all $n < {\rm N}$.

Eq. (8.15) is useful because the derivatives $\frac{\partial}{\partial n}$ in $\sinh\left(\frac{\partial}{\partial n}\right) b_{\rm N}$ can be calculated entirely from a knowledge of b_n for $n \leq {\rm N}$. This is most easily done by regarding $\sinh\left(\frac{\partial}{\partial n}\right)$ as a *linear functional*. It operates on a set $\{b_n :\, n \in (-\infty, {\rm N})\}$ and returns a scalar value $db_n(t)/dt$. The $\sinh\left(\frac{\partial}{\partial n}\right)$ operator has a number of amusing but trivial properties, summarized in Appendix §8.7. Chapter V touched on the fact that linear functionals may be approximated as the weighted sum of function values at various sample points, and that there is a standard way of doing so.[13] In our case, the problem can be stated thus: For a given number of sample points ${\rm L}$, find coefficients B_0, B_1, ..., $B_{\rm L}$ so that

[10] J. Marion, *Classical Dynamics of Particles and Systems*, §4.5.
[11] V. Bush, *Operational Circuit Analysis* (Wiley, New York, 1946).
[12] A short summary of difference calculus may be found in P. Davis and I. Polonsky in Ref. 3, Ch. 25.
[13] R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1962).

$$\sinh\left(\frac{\partial}{\partial n}\right) b_{\rm N} \approx B_0 b_{\rm N} + B_1 b_{\rm N-1} + ... + B_{\rm L} b_{\rm N-L}\ , \tag{8.16}$$

for general sequences $\{b_n\}$. There is no best way of doing this, but with the proper choice of the B_ℓ (and large enough L) we should be able to make eq. (8.16) as accurate as we like (except for pathological wavefunctions, which are bound to exist). Since we know that the actual $b_n$vary fairly slowly in n, a reasonable approach is to insist that eq. (8.16) should be exact for the test functions $b_n = n^0$, $b_n = n^1$, ..., $b_n = n^{\rm L}$. There are also competing candidates for sets of test functions, but we will not discuss them.

In order to solve for the coefficients B_ℓ we must insert the test functions into eq. (8.16) and get a set of coupled linear equations for B_ℓ. When this is done, it is quickly ascertained that the B_ℓ coefficients satisfy

$$\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots \\ 0 & 1 & 2 & 3 & \cdots \\ 0 & 1 & 4 & 9 & \cdots \\ 0 & 1 & 8 & 27 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ B_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 0 \\ -1 \\ \vdots \end{bmatrix} . \tag{8.17}$$

Table (8.1) in Appendix §8.7 is helpful in verifying eq. (8.17). The matrix is (almost) a Vandermonde matrix, and is therefore non-singular.[14] It is fairly easy to build a short table of solutions to eq. (8.17) for various L:

$\underline{L}$	$\underline{B_0}$	$\underline{B_1}$	$\underline{B_2}$	$\underline{B_3}$	$\underline{B_4}$
0	0				
1	1	-1			
2	$\frac{3}{2}$	-2	$\frac{1}{2}$		
3	**3**	$-\frac{7}{2}$	2	$-\frac{1}{2}$	
4	$\frac{5}{2}$	$-\frac{11}{2}$	5	$-\frac{5}{2}$	$\frac{1}{2}$

A more complete table (up to $\mathrm{L} = 15$) appears in Appendix §8.7.

The altered Schrödinger equation for $b_{\rm N}$ is then just

$$\frac{d}{dt}\, b_n(t) = -\sigma\ \left(B_0 b_{\rm N} + B_1 b_{\rm N-1} + ... + B_{\rm L} b_{\rm N-L}\right). \tag{8.18}$$

It is possible to write down a formula describing the error in eq. (8.18) in terms of high-order time derivatives of $b_{\rm N}$,[15] though such an exercise is rather fruitless since these derivatives are not known. Unfortunately, in practice there is no known good estimate of the accuracy of eq. (8.16) or eq. (8.18) short of simply inspecting the numerical or graphic output for reflection from the δ-truncation point.

[14] An algorithm for inverting a Vandermonde matrix is given in the preceding reference.
[15] This is a general characteristic of such approximation formulae.

Eq. (8.18) is transformed into an equation for a_n by using eq. (8.9). Substituting for b_n gives

$$\frac{d}{dt}\,a_n(t) = -i\,s\,a_n(t) - \sigma\,\left(B_0 a_{\rm N} - i\,B_1 a_{\rm N-1} + ... + (-i)^{\rm L} B_{\rm L} a_{\rm N-L}\right). \tag{8.19}$$

This correction can be taken into account by modifying the Hamiltonian. Rather than the normal $[H_0]_{\rm NN} = s$ and $[H_0]_{\rm N,N-1} = \frac{\sigma}{2}$, we have

$$[H_0]_{\rm NN} = s - i\,B_0\sigma\ ,$$

$$[H_0]_{\rm N,N-\ell} = (-i)^{\ell+1} B_\ell\,\sigma\ ,\ \ \ell = 1, ..., {\rm L}.$$

Eq. (8.19) was simply multiplied by i to give these values. The transposed matrix elements $[H_0]_{\rm N-\ell,N}$ are *not* changed in the same way. Rather, they (and H_{nm} for $n, m < {\rm N}$) retain their normal values.

In keeping with the terminology in previous chapters, this approximation will be referred to as λ-*termination* of the δ-truncated ladder.

To test the concept of λ-termination, a simple numerical example is in order. As a test case, let's simply adopt the semi-infinite Chebychev band. The equation of motion is then eq. (8.1) with n confined to $0, 1, 2, ...$ (and $a_{-1} = 0$). We'll choose the initial condition $a_0(0) = 1$. We'll also set $s = 0$ and $\sigma = 1$, both of which can actually be done without loss of generality. Figure (8.1) displays the motions of the exact populations of the lowest 50 levels in a pure Chebychev ladder. The δ-truncation point is simply so high on the ladder that no reflection occurs. The solutions were calculated for $t = 10$, $t = 20$, $t = 30$, and $t = 40$. Since $\sigma = 1$, the wave packet has hit level 10 at time $t = 10$, level 20 at time $t = 20$, and so forth.

The same curves are depicted in figure (8.2), along with solutions computed using λ-termination of the Chebychev ladder. 20 levels were retained in the ladder, and there were ${\rm L} = 10$ terminating levels. That is, the probability amplitudes of levels 10 through 20 are used to compute the time derivative of $a_{20}(t)$. There is no discernable difference between the correct solution and the λ-terminated solution. If no λ-termination had been used, the bulk of the wave packet would already have begun to reflect at time $t = 20$. At time $t = 30$ the reflected wave would be more than halfway back to the ground state, and at time $t = 40$ it would again be relecting. No such effect is seen. The λ-termination simply absorbs the wave packet.

Figures (8.3,4) look at the error more generally. Here we see a Chebychev ladder of 40 levels, viewed at time $t = 60$. At this point the bulk of the wave packet (85%) has passed the truncation point, and the total error is computed for various numbers of terminating levels L. From Fig. (8.4), the error is seen to decrease approximately exponentially with L. The "reflection coefficient" in Fig. (8.4) [and in Fig. (8.5) later] is calculated as follows. Denoting the "exact" solution by $a_n(t)$ and the λ-terminated solution by $a'_n(t)$, the reflection coefficient is computed as the ratio of the "reflected population"

$$R = \sum_{n=0}^{39} |e_n|^2 = \sum_{n=0}^{39} \left| |a'_n|^2 - |a_n|^2 \right|$$

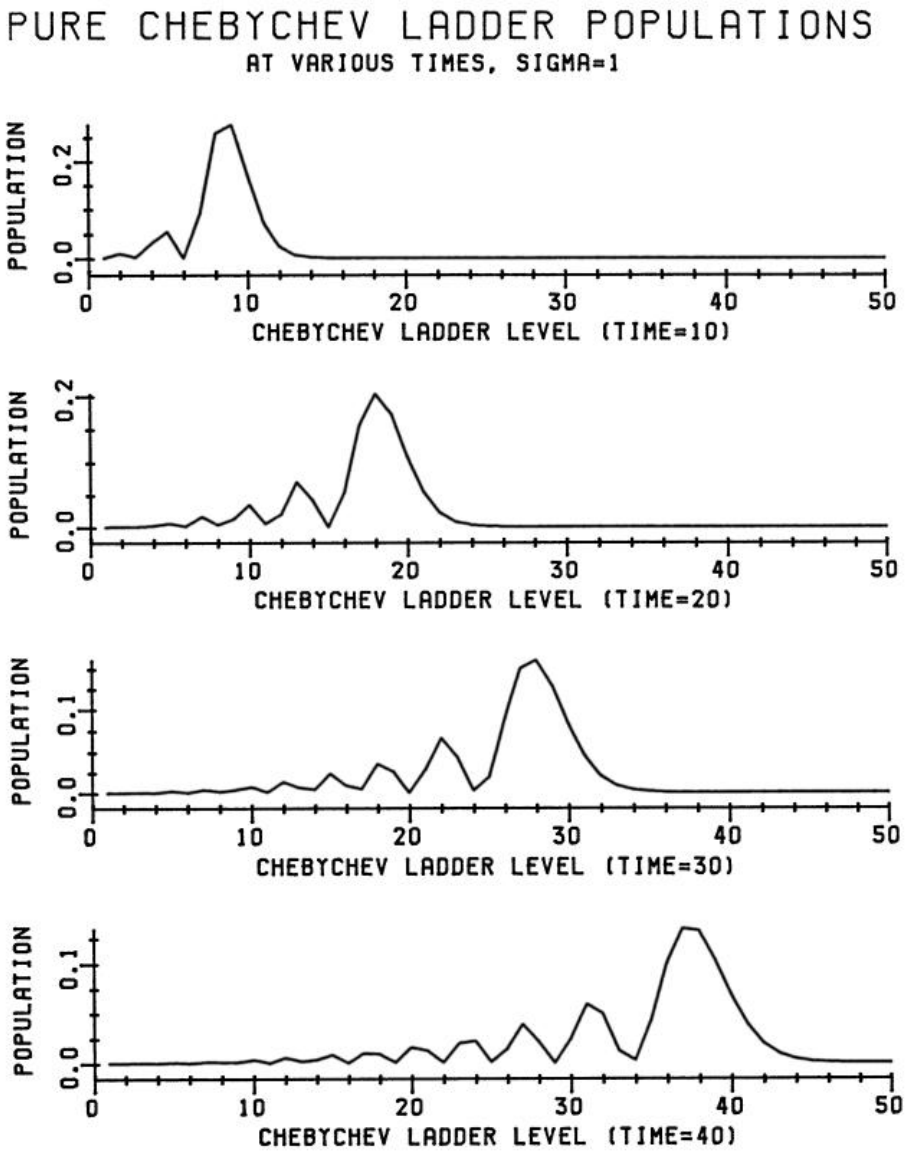

FIGURE 8.1

Lowest 50 levels in a pure Chebychev ladder system, with $s = 0$, $\sigma = 1$, at times $t = 10$, $t = 20$, $t = 30$, and $t = 40$. As expected, the wave-packet of population reaches approximately level t at time t.

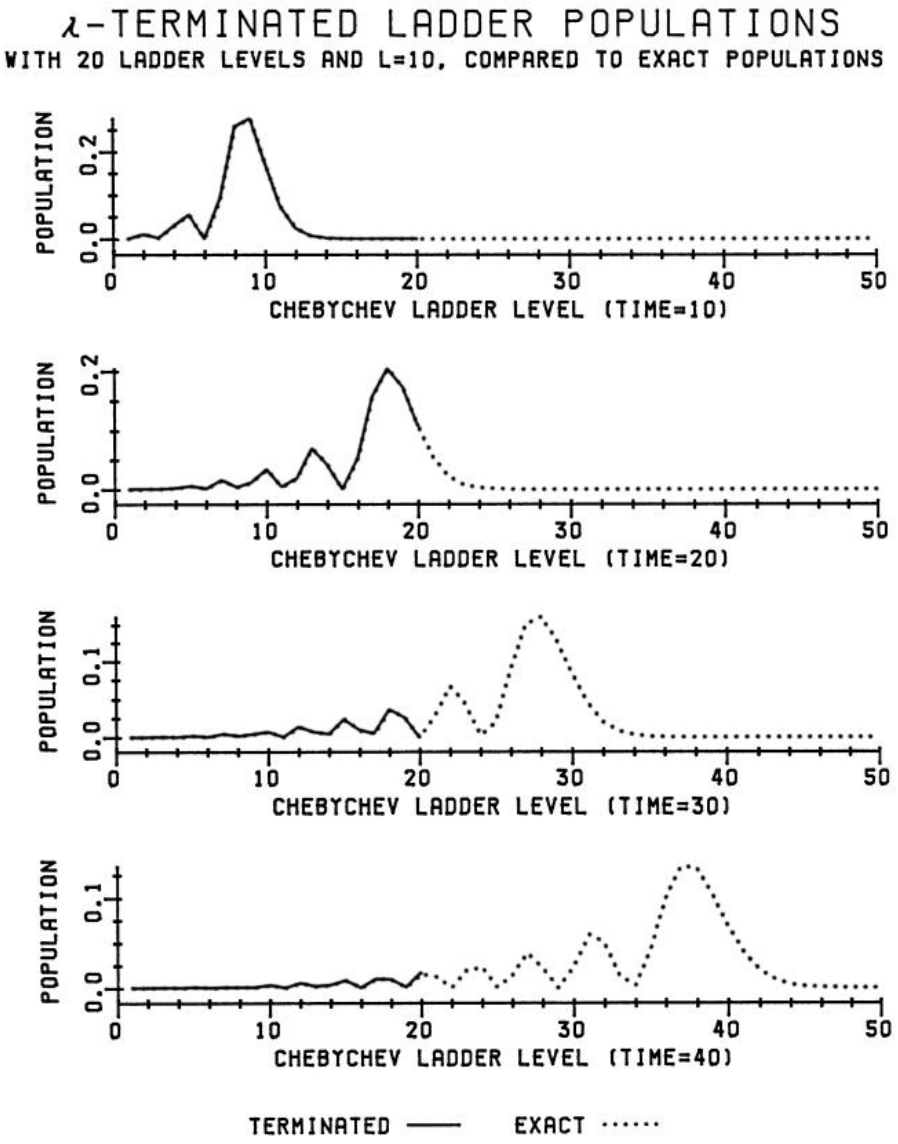

FIGURE 8.2

Exact Chebychev ladder populations (dotted lines), compared with approximate populations (solid lines) computed using λ-termination. As before, $\sigma = 1$, $s = 0$. In the λ-terminated system, 10 "pure" ladder levels were retained, followed by 10 levels used for the non-Hermitian termination of the ladder. There is no visual discrepency.

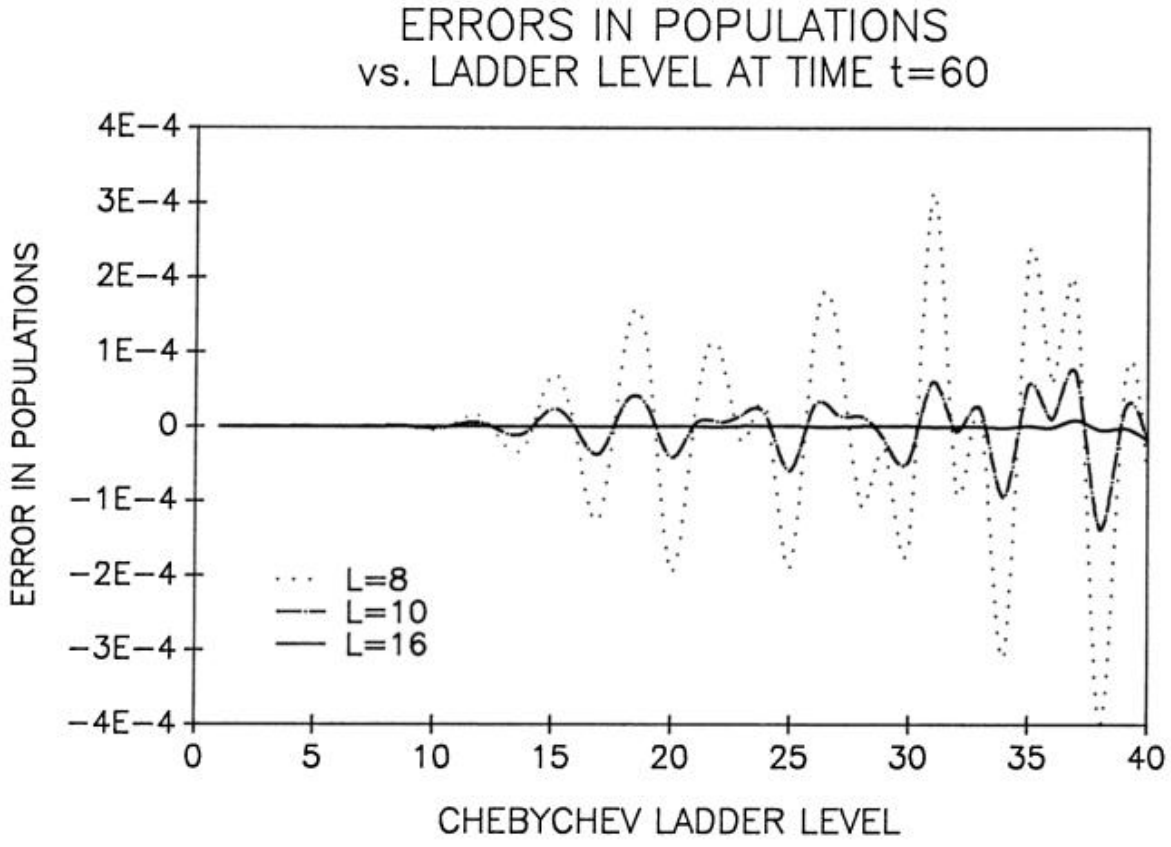

FIGURE 8.3

Error in the λ-termination of a 40-level pure Chebychev ladder system. The system is as before, with $s = 0$ and $\sigma = 1$, and the error is considered at time $t = 60$. The error measures used are described in the text. Shown is the population error in each level.

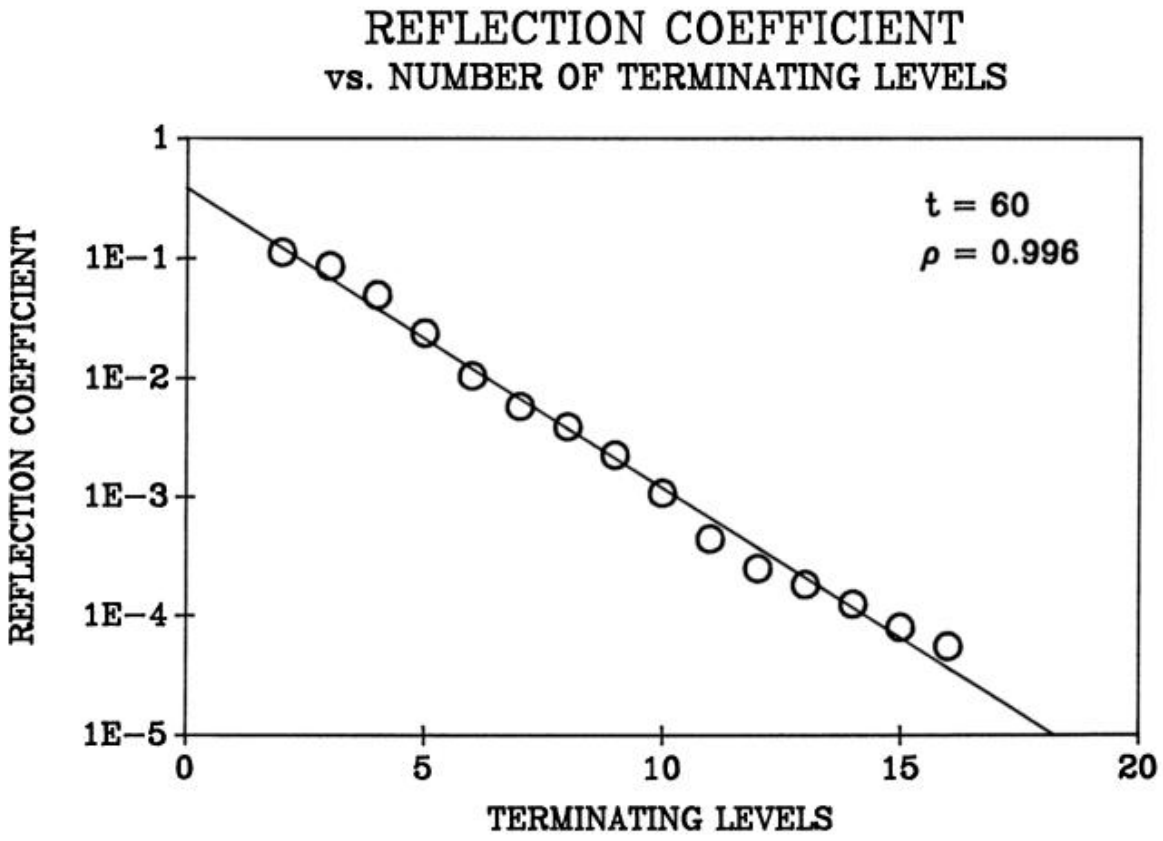

FIGURE 8.4

Error in the λ-termination of a 40-level pure Chebychev ladder system. The system is as before, with $s = 0$ and $\sigma = 1$, and the error is considered at time $t = 60$. The error measures used are described in the text. Shown is the error (averaged over all levels) for various numbers L of terminating levels. The total error is seen to decrease exponentially as L increases.

and the "transmitted population"

$$T = \sum_{n=40}^{\infty} |a_n|^2.$$

That is,

$$\text{Reflection Coefficient} = \frac{R}{T}.$$

The choice of this quantity as a representation of the "error" is rather arbitrary, of course. Figure (8.3) simply displays the quantity $|a'_n|^2 - |a_n|^2$ (at $t = 60$) so that we can see the error level-by-level.

These test calculations are encouraging, but caution should be observed in interpreting them. Increasing L tends to give higher accuracy, but we can't expect this to go on for indefinitely large L. From the table of B_ℓ coefficients in Appendix §8.7, we see that the coefficients become quite large. The largest coefficient is of the same order as 2^{L}. The value of the weighted sum is kept in check only because of cancellation of rather large numbers. Thus, we can only increase L to a certain point. Beyond this point (which depends on the accuracy of the arithmetic and of the numerical methods used to solve our differential equations), the large values of the B_ℓ coefficients will unacceptably amplify the error and cause the numerical solution to become unstable. This, of course, is a general problem with numerical differentiation formulas. Numerical integration formulas need not suffer the same flaw. A similar approximation for an integrating operator would typically have all positive coefficients summing to unity, and would pass more gracefully to the large L case. (See Ref. 13.) Naturally, we would usually like to make L as small as possible to reduce the number of energy levels in the system and thereby reduce our computation effort.

Of course, we are mainly interested in how well this approximation works for the eigenfunctions e^{ikn}. We have found numerically (but won't show here) that approximation (8.16) works quite well for L as small as 4, for the test functions e^{ikn} with $|k|$ limited to values less then $\frac{\pi}{4}$. (That is, for upward-moving waves.) On the other hand, for $k \approx \frac{\pi}{2}$ (downward-moving waves), even setting $\mathrm{L} = 10$ is not adequate. Therefore, we must conclude that our terminating method is not necessary universally adequate. One possible change is to use a different set of test functions for defining the weight coefficients B_ℓ, thus giving different values for B_ℓ. We will not attempt this, but will instead look at a radically different termination method in the next section.

By the way, we have been somewhat deceptive in figure (8.3), in choosing the δ-truncation point to be (the rather high) level 40. After all, we never use more than 16 terminating levels, so we seemingly needn't truncate the Chebychev ladder higher than level 16 or 17. Unfortunately,this is not the case. If, for example, we had truncated at level 30, we would have seen the following effect: Our error curve would indeed decrease exponentially until about $\mathrm{L} = 12$, at which point the error would begin increasing slightly! This is actually an "edge" effect. The formulas developed in this section have depended on the fact that eq. (8.10) has eigenfunctions given by eq. (8.11). However, eq. (8.11) is correct only for an infinite Chebychev ladder. The truncation of the ladder at the *top* has been accounted for by our calculations, but the truncation at the *bottom* has not. The

true eigenfunctions correspond those given in eq. (8.11) for large n, but at small n there are increasingly large discrepencies between the exact eigenfunctions and eq. (8.11). This leads to increasingly large errors if the λ-termination formula is applied too close to the bottom of the Chebychev ladder. Thus, the lowest terminating level $a_{\mathrm{N}-\mathrm{L}}$ must not be too close to the bottom of the ladder. [In a more realistic example, of course, the "bottom" of the ladder is at the top of the μ-truncation region rather than at the "ground state".]

How far from the bottom of the ladder must the terminating levels begin? Obviously, in practice we would like to minimize N (the number of Chebychev levels), while maintaining a given degree of accuracy. We do not want a marked disparity between the error from the edge effect and the error from λ-termination. If the edge-effect error dwarfs the λ-termination error, then we are just wasting computer resources with too many λ-terminating levels. Conversely, if the λ-termination error dwarfs the edge-effect error, then we are wasting computer resources by providing too big a "buffer zone" below the λ-termination region. Each must conform to the desired accuracy. Empirically, the error associated with each kind of truncation has been found to be of the same order of magnitude. Thus, choosing $\mathrm{L} \approx \mathrm{N} - \mathrm{L}$ is not a bad rule of thumb. (Of course, in figure 8.3 we *wanted* the edge-effect error to be tiny in order to unambiguously compute the error curve due to λ-termination, so we chose N somewhat bigger than $2\mathrm{L}$.) Unfortunately, time does not allow any further exploration of the "buffer zone" concept.

8.4. Rational λ-Termination

Though based on an interesting concept, and producing a usable system, the non-Hermitian Chebychev-ladder termination-method discussed in the previous section has certain flaws. The chief flaws are two in number: First, there is no obvious *a priori* way to bound the error. Second, the necessity of having a "buffer zone" of pure Chebychev levels is unfortunate. Using this method, it would not be unusual to replace each Chebychev ladder in the system with 10-20 levels (half buffer zone and half non-Hermitian termination). In most cases, we would prefer to use less levels, even with lower quantitative accuracy, if we could guarantee proper qualitative operation. In this section, we will present an entirely different ladder-termination method that meets these requirements.

Let's consider more closely what we are doing when we throw away part of a Chebychev ladder using δ-truncation. Clearly, what we are throwing away in this process is an entire semi-infinite Chebychev ladder. This ladder is entirely "pure", in the sense that there are no transitions between these levels and the remainder of the system, except for the connection between the lowest level in the discarded ladder and the highest level a_{N} retained in the full system.

In Chapter VI we demonstrated, among other things, that a $(1, \mathsf{CONTINUUM})$ system can be converted to a ladder system by means of a similarity transformation, and *vice-versa*. Thus, by means of a suitable similarity transformation we should be able to convert the entire discarded ladder into a continuum which interacts only with the highest retained level a_{N}. This is illustrated in Fig. (8.5).

It may be supposed that the continuum so produced (using the methods of §6.3) is what we have called the Chebychev band, defined in eq. (3.18). This is not so. In fact,

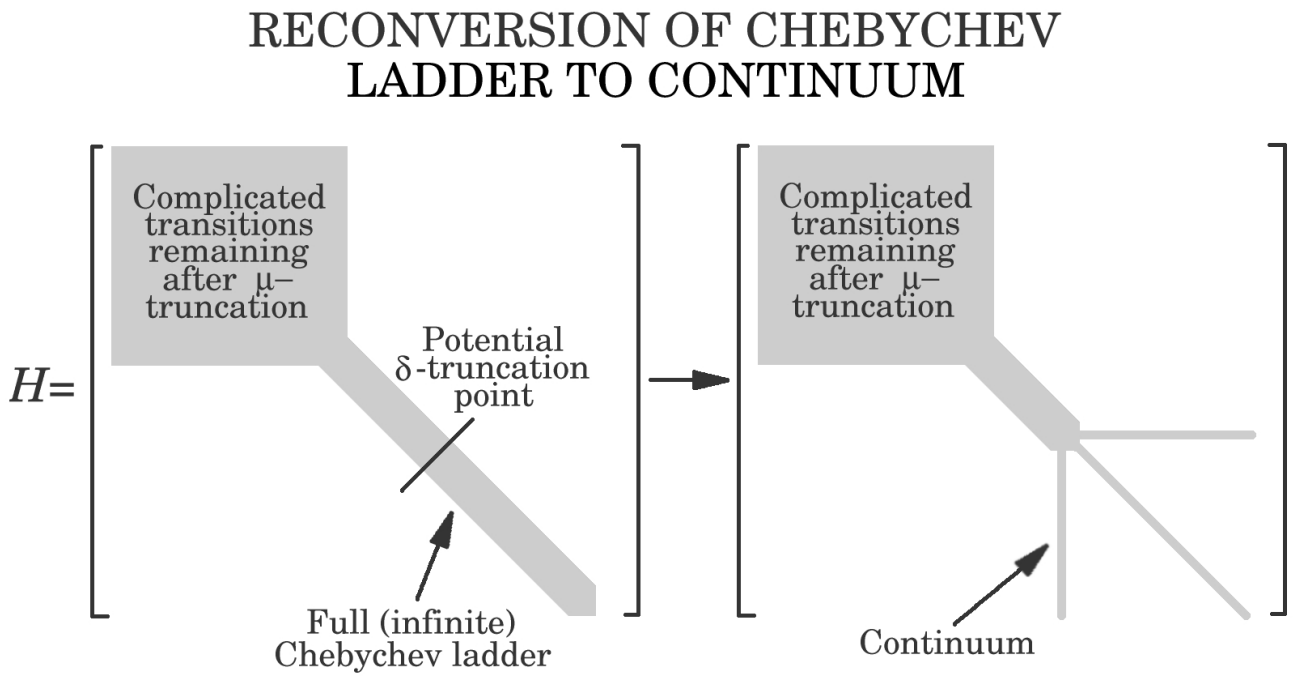

FIGURE 8.5

Conversion of the Chebychev ladder levels discarded by δ-truncation into a continuum. This occurs *via* the similarity transformation described in §6.3. The Hamiltonian is depicted schematically. This might be described as *continuation* since it is the opposite to *discretization*.

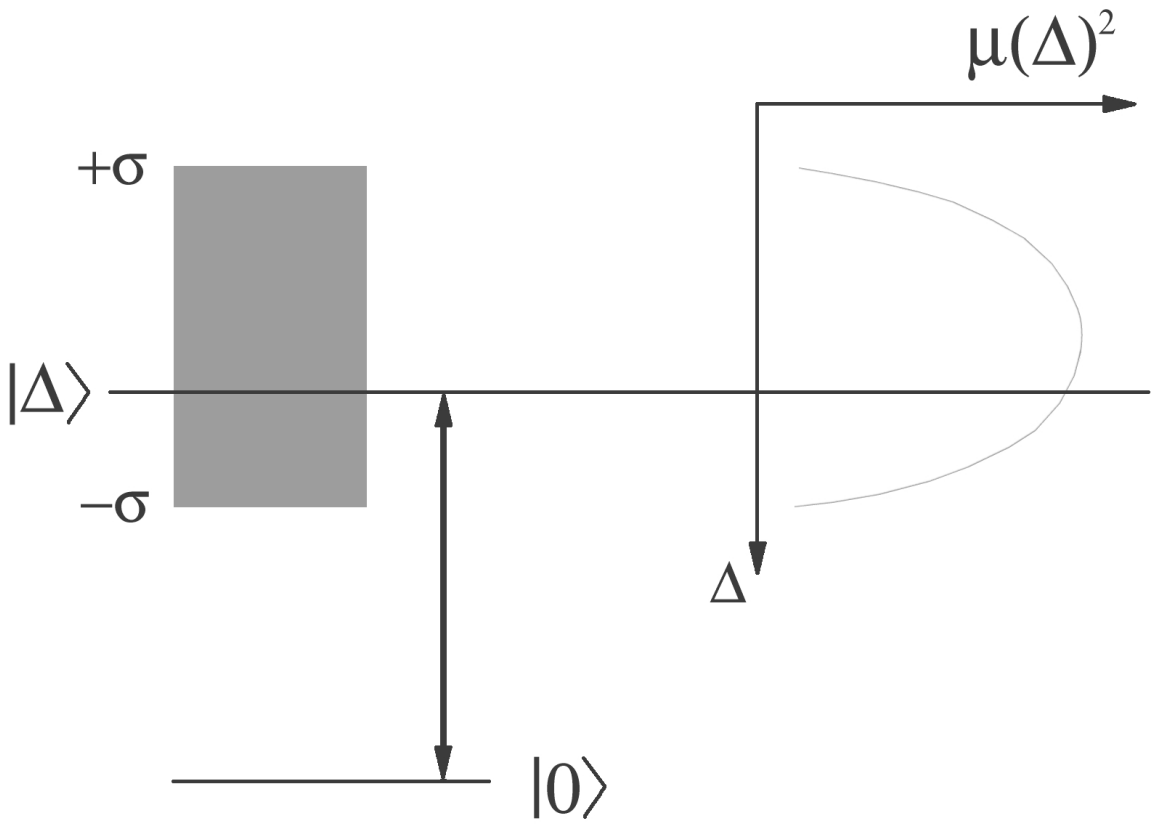

FIGURE 8.6

The $(1, \text{CHEBYCHEV 2ND KIND})$ system. The Chebychev bandshape of the second kind (so called because it is the weight function for Chebychev polynomials of the second kind) differs greatly from the normal Chebychev bandshape, as seen in Fig. (3.3).

what is produced is the *very different* bandshape defined by eq. (3.18'): The Chebychev bandshape of the second kind. The Chebychev bandshape of the second kind, depicted in Fig. (8.6), differs from the true Chebychev bandshape of Fig. (3.3c) in that it slightly resembles a Lorentzian bandshape [Fig. (3.3d)]. This being the case, perhaps we can use the *rational-band* techniques discussed in §5.4 and in §5.8 to efficiently approximate just this part of the system.

Recall that the first step in such an approximation is to find a good rational-function approximation [*i.e.*, an approximation of the form $\frac{p(\Delta)}{q(\Delta)}$, with p and q polynomials] of the $\mu(\Delta)^2$ function, in this case

$$\mu(\Delta)^2 = \frac{\sigma}{2\pi}\sqrt{1-\frac{(\Delta-s)^2}{\sigma^2}}. \tag{8.20}$$

The discrepency between eq. (8.20) and eq. (3.18') is explained by this: the matrix elements governing transitions between the highest retained level in our system (a_{N}) and the lowest discarded level ($a_{\mathrm{N}+1}$) are equal to $\frac{\sigma}{2}$ in the case under consideration, whereas they would be $E(t)\gamma$ in the ladder system generated from a true $(1, \mathsf{CONTINUUM})$ system. Thus, we must replace $E\gamma$ by $\frac{\sigma}{2}$ in eq. (3.18'). $\mu(\Delta)^2$ is, of course, supposed to be identically zero for $|\Delta - s| > \sigma$.

Undoubtedly it is possible to produce a highly optimized rational approximation for eq. (8.20), and this would probably be a good thing to do if very time-consuming calculations were to be carried out. However, we do not want to extend too far the discussion of what is, after all, a peripheral topic. For ourselves, therefore, we will simply adopt the suggested approximation of eqs. (5.62-5.67). This is a family of approximations, in which the degrees of the numerator and denominator polynomials are separately adjustable. The numerator is created by truncating the Taylor series of $\mu(\Delta)^2$, while the denominator is a window function used to insure that the approximated $\mu(\Delta)^2$ becomes very small for $|\Delta - s| > \sigma$. To get L terminating levels, one chooses the degree of the denominator to be $2\mathrm{L}$.

The rough behavior of this approximation can be seen from Fig. (5.10), which envisages a system little different from the one (or part of one) we are considering. (The value "n" in that figure is what we are calling "L".) The qualitative behavior of this approximation is good even for very small L, though empirically we find $\mathrm{L} = 1$ slightly too drastic. A reasonable compromise is to use $\mathrm{L} = 4$, or

$$\mu(\Delta)^2 \approx \frac{\sigma}{2\pi}\,\frac{1-\frac{(\Delta-s)^2}{2\sigma^2}}{1+\left(\frac{(\Delta-s)^2}{\sigma^2}\right)^8}\,. \tag{8.21}$$

The resulting λ-terminated Hamiltonian is

$$H(t) = \begin{bmatrix} \ddots & & & & & & & \\ & s & \frac{\sigma}{2} & & & & & \\ & \frac{\sigma}{2} & s & \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \\ & & \gamma_1 & \Delta_9 & & & & \\ & & \gamma_2 & & \Delta_{11} & & & \\ & & \gamma_3 & & & \Delta_{13} & & \\ & & \gamma_4 & & & & \Delta_{15} & \end{bmatrix},$$

where the symbols Δ_n and γ_n are defined by eqs. (5.63) and (5.67), respectively. Since all of these λ-termination coefficients are obtained from simple formulae, we have not bothered to create a table of such coefficients, as we did for polynomial λ-termination coefficients.

Approximations of this kind have none of the chief flaws mentioned for the method of the previous section. While we have not presented any specific error bounds, it is clear that any error in the calculation of the probability amplitudes of the system must be closely related to the error in rational approximations like those of eq. (8.21). This error is, of course, quantifiable. Moreover, the approximation is clearly qualitatively correct, since is merely represents a tiny modification to the shape of the continuum. Finally, no "buffer zone" is required, and the ladder-termination region can begin immediately above the δ-truncation level. This is clear since the approximation is entirely aimed at simulating what has been removed from the system, rather than at somehow using the remaining parts of the system for double-duty.

In Fig. (8.7), we see the results of calculations on the same 20-level model system used for Fig. (8.2), but using the rational-band λ-termination method rather than the polynomial λ-termination method. Though no buffer-zone is required, we have retained the 10-level buffer zone of the earlier calculation, merely in order to compare the results of the two calculations. As we might have expected, there is no visually ascernible error resulting from the approximation.

8.5. The Rest of the Story

Although the discussion above tells us a lot about the dynamics of the Chebychev ladder, and explains most of the effects we saw previously in our sample calculations, some of the story is still missing—particularly at high field strengths. What is missing are the effects due to the fact that the Chebychev ladder is not truly infinite ($n = 0, \pm 1, \pm 2, ...$) as modelled in §8.2, but is only semi-infinite ($n = 0, 1, 2, ...$).

Eq. (8.2) is a useful *approximation* for the eigenfunctions of the semi-infinite Chebychev ladder when n is large, but much less adequate for n small. We saw this already in §8.3 when we encountered "edge effects" in our non-Hermitian termination of the Chebychev ladder.

How can we understand the effect of the semi-infinite ladder better? It turns out that we can use our knowledge of the Chebychev ladder to find an analytic solution to the $(1, \mathsf{CHEBYCHEV\,2ND\,KIND})$ system (including the true eigenstates), in the case of a constant field $E(t)$. By understanding the properties of the analytic solution we will come to understand the Chebychev ladder somewhat better.

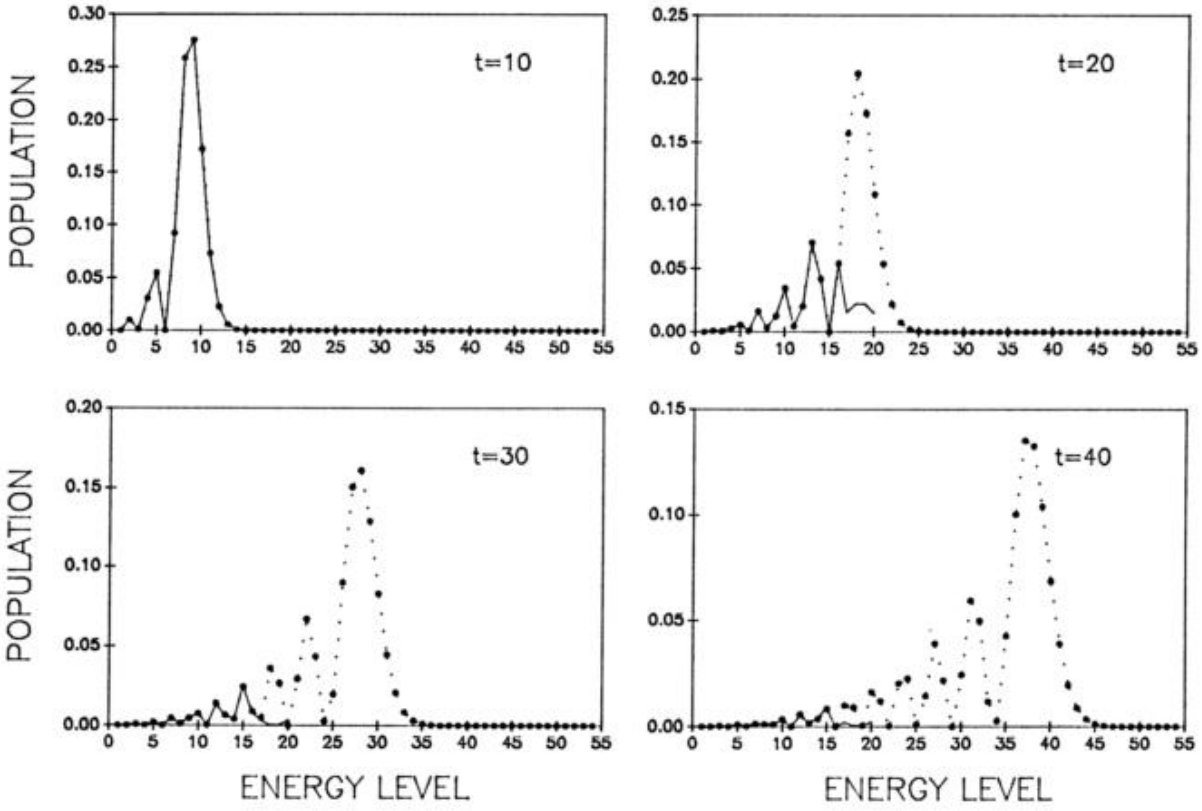

FIGURE 8.7

Calculation of λ-terminated populations as compared to the true Chebychev ladder populations, as in Fig. (8.2). Here, only four terminating levels were used, but the rational-band λ-termination was used rather than the polynomial λ-termination of the previous section. As usual, we have put $s = 0$ and $\sigma = 1$.

The Schrödinger equations of this system are, of course,

$$i\,\frac{d}{dt}\,a_0(t) = \Omega\,a_1(t)\,, \tag{8.22}$$

$$i\,\frac{d}{dt}\,a_1(t) = \Omega\,a_0(t) + \frac{\sigma}{2}\,a_2(t)\,, \tag{8.23}$$

$$i\,\frac{d}{dt}\,a_n(t) = \frac{\sigma}{2}\,a_{n-1}(t) + \frac{\sigma}{2}\,a_{n+1}(t)\,,\ n>1. \tag{8.24}$$

Here, the conventional symbol Ω is used in place of $E\gamma$ to simplify our expressions. Moreover, we continue to use the initial conditions

$$a_0(0) = 1\ ,\ \ a_{n>0}(0) = 0\,. \tag{8.25}$$

Solving these equations is conceptually simple. If we can find the true eigenfunctions of the system, and expand the initial conditions in terms of a superposition of these eigenfunctions, then we will have written down the solution at all times. While the eigenfunctions are not as simple as those given by eq. (8.2), it would be reasonable to suppose that the eigenfunctions might consist of a superposition of an upward-going wave and a downward-going wave, both of the form of eq. (8.2). In fact, we easily find that the eigenfunctions

$$a_n^{(\mathrm{II})}(k,t) = e^{-i\omega t}\begin{cases} 1 & ,\ n=0 \\ \tau(k)\,e^{ikn} + \tau(-k)\,e^{-ikn} & ,\ n>0 \end{cases} \tag{8.26}$$

do satisfy eqs. (8.22)-(8.24). (The purpose of the superscript Roman numeral will become clear in a moment.) As usual, $\omega(k)$ is defined by eq. (8.3), while

$$\tau(k) = \left(1+\lambda^{-2}\right)^{-\frac{1}{2}}\ \frac{e^{ik}-\lambda^{-2}e^{-ik}}{e^{ik}-e^{-ik}}. \tag{8.27}$$

where λ is a positive number defined by

$$\lambda^2 = \frac{\frac{\sigma^2}{4}}{\Omega^2 - \frac{\sigma^2}{4}}\,. \tag{8.28}$$

Actually, for our purposes it is slightly more convenient to express Ω interms of λ, rather than *vice versa*:

$$\Omega^2 = \frac{\sigma^2}{4}\,\left(1+\lambda^{-2}\right). \tag{8.29}$$

In fact, λ will be a basic parameter throughout the remainder of the chapter.

Now, for low field strengths ($|\lambda|>1$) these expressions are perfectly satisfactory. Without much effort, we can find a superposition of $a_n^{(\mathrm{II})}(k,t)$ that satisfies the initial conditions (8.25), and hence represents the solution at all times:

$$a_n(t) = \int_{-\pi}^{\pi}\left(\frac{-\lambda^2}{2\pi}\,\frac{e^{2ik}-1}{1-\lambda^2 e^{2ik}}\right)a_n^{(\mathrm{II})}(k,t)\,dk\ ,\ \ |\lambda|>1 \tag{8.30}$$

Though this formula was obtained primarily by trial-and-error,[16] it can be easily verified by evaluation at $t = 0$.[17] Alternatively, though there is no closed-form expression for $a_n(t)$ at arbitrary times t, we can still expand $a_n(t)$ conveniently in terms of a power series in λ^{-1}:

$$a_0(t) = \frac{2}{\sigma t}\left(\mathrm{J}_1(\sigma t) - 3\,\lambda^{-2}\,\mathrm{J}_3(\sigma t) + 5\,\lambda^{-4}\,\mathrm{J}_5(\sigma t) - ...\right), \tag{8.31}$$

$$a_{n>0}(t) = \sqrt{1+\lambda^{-2}}\,\frac{2(-i)^n}{\sigma t}\left((n+1)\,\mathrm{J}_{n+1}(\sigma t) - (n+3)\,\lambda^{-2}(n+3)\,\mathrm{J}_{n+3}(\sigma t) + ...\right), \tag{8.32}$$

where the J_n are Bessel functions. This result is obtained from eq. (8.30) by expanding the denominator of the integrand as a power series and then applying various Bessel-function identities.[18] Notice that $a_0(t)$ can actually be obtained from eq. (8.32), if the leading radical factor is omitted.

For small λ^{-1} at least, eqs. (8.31) and (8.32) have exactly the characteristics we have learned to expect. Each $a_n(t)$ is individually of order $t^{-\frac{3}{2}}$ for large times t, thus approaching zero as the wave packet of population moves to higher levels in the Chebychev ladder. Since $\mathrm{J}_n(z)$ has its maximum value near $z \cong n$, we see that $a_n(t)$ has its maximum value near $\sigma t \cong n$. Thus, the wave-packet is truly moving up the ladder at a speed of σ. By the way, "very small" λ^{-1} does not correspond to $\Omega \ll \sigma$. In fact, $\lambda^{-1} = 0$ corresponds to $\Omega = \frac{\sigma}{2}$.[19] To get $\Omega < \frac{\sigma}{2}$ we must allow λ to become purely imaginary (though still $|\lambda^{-1}| < 1$). Thus, $\Omega \to 0$ as $\lambda \to i$. There are several cases in which the infinite series in eqs. (8.31) and (8.32) collapse to a single term or just a few terms. Perhaps the most interesting of these is the case $\lambda \to \infty$, for which $\Omega = \frac{\sigma}{2}$. We find

$$a_n(t) = \frac{2(-i)^n}{\sigma t}\,(n+1)\,\mathrm{J}_{n+1}(\sigma t).$$

[16] "Trial and error" means that $a_n^{(\mathrm{II})}(k)$ is expanded in powers of e^{ik}; its multiplier function in the integrand is also written in terms of such a series, with undetermined coefficients. These coefficients are determined (by inspection), and the resulting expression is integrated (and compared against the initial conditions) as a check.

[17] The technique for evaluating integrals of this kind is quite simple. Just introduce a new integration variable $z = e^{ik}$ (or e^{-ik}, if it produces a simpler expression). This converts the line integral into a contour integral of a rational function on the unit circle $|z| = 1$.

[18] Helpful identities in expanding the integral are:

$$\int_{-\pi}^{\pi} e^{-iz(\cos k)} e^{ink} dk = 2\pi\,(-i)^n\,\mathrm{J}_n(z).$$

$$\mathrm{J}_{n-1}(z) + \mathrm{J}_{n+1}(z) = \frac{2n}{z}\,\mathrm{J}_n(z).$$

For verifying that the resulting expressions are indeed solutions of Schrödinger's equation, we use the identity

$$n\,\frac{d}{dz}\,\mathrm{J}_n(z) = \frac{n\,\mathrm{J}_n(z)}{z} + \frac{1}{2}\,(n-1)\,\mathrm{J}_{n-1}(z) - \frac{1}{2}\,(n-1)\,\mathrm{J}_{n+1}(z).$$

[19] The printed version said "$\Omega = \sigma/\sqrt{2}$", but this clearly contradicts eq. (8.29)—RSB, 3/2003.

This expression, which is even good if $n = 0$, is thus the closed-form solution of the sample system we solved numerically in §8.3 and §8.4.

For high field strengths ($|\lambda| < 1$), we do not have such an easy time of it. Not only is eq. (8.30) no longer adequate, but eq. (8.26) no longer even provides a complete set of eigenstates. The missing eigenfunctions, which we will denote by $a_n^{(\mathrm{I}+)}(t)$ and $a_n^{(\mathrm{I}-)}(t)$ are given by the expression

$$a_n^{(\mathrm{I}\pm)}(t) = e^{\mp i\omega' t} \begin{cases} \left(1+\lambda^{-2}\right)^{-\frac{1}{2}} & , \ n = 0 \\ (\pm\lambda)^n & , \ n > 0, \end{cases} \tag{8.33}$$

where

$$\omega' = \frac{\sigma}{2}\left(\lambda + \lambda^{-1}\right). \tag{8.34}$$

Unlike the eigenfunctions (8.26), these two eigenfunctions are not standing waves, but are merely constant population distributions! Although the phases of the probability amplitudes oscillate at a frequency $\pm\omega'$ (approximately $\pm\Omega$ for $\Omega \gg \sigma$), there is no movement of population in the ladder when the system is in one of these eigenstates.

With these two new eigenfunctions, trial-and-error again suffices to reveal the necessary superposition giving $a_n(t)$:

$$a_n(t) = \sqrt{1+\lambda^{-2}}\,\frac{1-\lambda^2}{2}\left(a_n^{(\mathrm{I}+)} + a_n^{(\mathrm{I}-)}\right) - \int_{-\pi}^{\pi}\left(\frac{\lambda^2}{2\pi}\,\frac{e^{2ik}-1}{1-\lambda^2 e^{2ik}}\right) a_n^{(\mathrm{II})}(k,t)\,dk. \tag{8.35}$$

As above, this can be evaluated as a power series in λ:

$$a_0(t) = \left(1-\lambda^2\right)\cos\,\omega' t + \frac{2}{\sigma t}\left(\lambda^2 \mathrm{J}_1(\sigma t) - 3\lambda^4\,\mathrm{J}_3(\sigma t) + 5\,\lambda^6 \mathrm{J}_5(\sigma t) - ...\right), \tag{8.36}$$

$$\begin{aligned} a_{n>0}(t) \;=\; & \sqrt{1+\lambda^2}\left(\frac{1-\lambda^2}{2}\,\lambda^{n-1}\left((-1)^n\,e^{i\omega' t} + e^{-i\omega' t}\right) + \right. \\ & \left. + \frac{2i^n}{\sigma t}\left((1-n)\,\lambda\,\mathrm{J}_{1-n}(\sigma t) - (3-n)\,\lambda^3 \mathrm{J}_{3-n}(\sigma t) + ...\right)\right). \end{aligned} \tag{8.37}$$

(Again, a_0 actually satisfies the formula for $a_{n>0}(t)$ if the radical factor is replaced simply by λ.) If the field strength Ω is so large that we can ignore terms of order λ^4, eq. (8.36) reduces to just

$$a_0(t) \cong \left(1-\lambda^2\right)\cos\,\omega' t + \frac{2}{\sigma t}\,\lambda^2 \mathrm{J}_1(\sigma t). \tag{8.38}$$

Similarly, we find that

$$a_1(t) \cong -i\,\left(1-\lambda^2\right)\,\sin\,\omega' t. \tag{8.39}$$

All of the other probability amplitudes are of order λ.

Even if λ is not "very small" (but still satisfies $|\lambda| < 1$), from eqs. (8.36) and (8.37) we can write down the asymptotic probability amplitudes as $t \to \infty$, since any given Bessel

function goes to zero as $1/\sqrt{t}$ for t large. We find simply that the $a_n^{(\mathrm{I}\pm)}(t)$ portions of the wave function survive and that the $a_n^{(\mathrm{II})}(t,k)$ portions do not:

$$a_n(t) \to \sqrt{1+\lambda^{-2}}\,\frac{1-\lambda^2}{2}\,\left(a_n^{(\mathrm{I}+)} + a_n^{(\mathrm{I}-)}\right)\ ,\ \text{for}\ t\,\text{large}. \tag{8.40}$$

The conclusion to be drawn from these expressions is remarkable: At high field strengths, *only a limited amount of population is absorbed by the continuum*. Most of the population *permanently* oscillates between the ground state and the lowest state of the Chebychev ladder at a frequency of $\omega' \cong \Omega$. An alternative way of saying this is that for $\Omega \gg \sigma$, the eigenstates we have called $a_n^{(\mathrm{I}+)}$ and $a_n^{(\mathrm{I}-)}$ (which represent a fixed distribution of population in the continuum) dominate the eigenstates $a_n^{(\mathrm{II})}(t,k)$ (which represent population waves in the continuum).

The total amount of permanently oscillating population can be quantified by computing the total population in the states $a_n^{(\mathrm{I}+)}$ and $a_n^{(\mathrm{I}-)}$, [in eq. (8.37)] as compared to a total system population of unity. We find simply

$$\sum_{n=0}^{\infty}\left|\sqrt{1+\lambda^{-2}}\,\frac{1-\lambda^2}{2}\,\left(a_n^{(\mathrm{I}+)} + a_n^{(\mathrm{I}-)}\right)\right|^2 = 1-\lambda^2. \tag{8.41}$$

This result is entirely at variance with what we would expect to find in, for example, a $(1, \mathsf{LORENTZIAN\ CONTINUUM})$ system. From eq. (5.42), we know that the (analytically exact) effective Hamiltonian for such a system is

$$H = \begin{bmatrix} 0 & \Omega \\ \Omega & -i\sigma \end{bmatrix}. \tag{8.42}$$

This gives us a two-level system that can be solved for the ground-state probability amplitude in a straightforward manner:

$$a_0(t) = \frac{\lambda_+ e^{\lambda_- t} - \lambda_- e^{\lambda_+ t}}{\lambda_+ - \lambda_-}, \tag{8.43}$$

where

$$\lambda_\pm = -\frac{\sigma}{2} \pm i\sqrt{\Omega^2 - \frac{\sigma^2}{4}}. \tag{8.44}$$

Thus, the ground-state probability amplitude does oscillate at a frequency of approximately Ω, but it also decays exponentially (to zero) at a rate $\frac{\sigma}{2}$.

Why should there be such a discrepency between the time behaviors of these two continua? Apparently, it arises from the following considerations. Although the Chebychev and Lorentzian bands considered here both have "width" σ, there is an important qualitative difference between them. Specifically, though its dipole matrix elements $\mu(\Delta)$ are small for $|\Delta| > \sigma$, the Lorentzian band actually has energy levels at all values of the detuning Δ. On the other hand, the Chebychev band simply has no energy levels at all for $|\Delta| > \sigma$. Why should this make a difference? If you will recall the discussion of continuum-continuum population trapping for the Lorentzian continuum (in §4.6.2), we found that the eventual population distribution in the continuum was bunched into two

lobes near $\Delta = \pm\Omega$. This is possible for the Lorentzian continuum, but not for the Chebychev continuum since there are no energy levels near $\Delta = \pm\Omega$ when $\Omega > \sigma$. Apparently, since the population cannot move into the energy levels it likes, it simply doesn't move anywhere.

Fortunately, this unexpected result at higher field-strengths does not hurt our previous development of ladder termination methods in §8.3 and §8.4. These were mathematically based on the equations of motion and only intuitively related to the wave-packet behavior of the Chebychev ladder.

By the way, this result is interesting in terms of the work of many investigators on the subject of *deviations* from exponential decay (see Chapter II). Many investigators have found small deviations from expontential decay, and it is known that such deviations are of the order of $\frac{1}{t}$ when the background continuum has an energy bounded from below.[20] Now we can see that the "deviations" are much greater when the background continuum is additionally bounded from above, since there need not be any decay (exponential or otherwise) at all!

Note that in Ref. 5, Makarov *et al*. demonstrated that the strictly limited continuum has a real eigenvalue when the interaction energy is outside the range of the energy levels in the continuum. This also implies that pure oscillation without damping can occur.

8.6. $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ Population Trapping in Strictly Limited Continua

Obviously, the discussion of the previous section is relevant not merely to the $(1, \mathsf{CONTINUUM})$ system, but to continuum-continuum population trapping as well. We have already discussed population trapping for *broad* continua ($\Omega < \sigma$) and *narrow* continua ($\Omega > \sigma$, but $\Delta \to \pm\infty$). For broad continua, we found that population was trapped in the initial continuum at high field strengths. For narrow continua, we found that at high field strengths the population initially oscillated between the continua at frequency Ω, but eventually settled down into a steady-state distribution equally divided between the two continua.

Now let's consider *strictly limited* continua ($|\Delta| < \sigma$) and see whether (as we may expect from the previous section) population oscillates between the continua without damping. As above, we'll use the Chebychev continuum of the 2nd kind as a model for strictly limited continua.[21] Of course, in the $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ system we have two such continua which, as usual, we call continuum 0 and continuum 1. Let us suppose for simplicity that both continua are of width σ and are centered at $\Delta = s = 0$.

Referring to eq. (6.29), we know that the Schrödinger equations of motion for the system are

$$i\,\frac{d}{dt}\,a_{n<-1}(t) = \frac{\sigma}{2}\,a_{n-1}(t) + \frac{\sigma}{2}\,a_{n+1}(t) \tag{8.45}$$

[20] L. Khalfin, *Sov. Phys. Dokl.* **1**, 671 (1956); **2**, 340 (1957); *Sov. Phys. JETP* **6**, 1053 (1958).

[21] Most of the results below can be found in R. Burkey, A. Glosson, and C. D. Cantrell, *Phys. Rev. A*, in publication.

$$i\,\frac{d}{dt}\,a_{-1}(t) = \frac{\sigma}{2}\,a_{-2}(t) + \Omega\,a_1(t) \tag{8.46}$$

$$i\,\frac{d}{dt}\,a_1(t) = \Omega\,a_{-1}(t) + \frac{\sigma}{2}\,a_2(t) \tag{8.47}$$

$$i\,\frac{d}{dt}\,a_{n>1}(t) = \frac{\sigma}{2}\,a_{n-1}(t) + \frac{\sigma}{2}\,a_{n+1}(t). \tag{8.48}$$

(Recall that for convenience we simply have no energy level labelled a_0.)

In place of eq. (8.26), it is natural to try the eigenfunctions

$$a^{(\mathrm{II})}_{n<0}(t,k) \propto e^{i(kn-\omega t)} + \rho\, e^{i(-kn-\omega t)}, \tag{8.49}$$

$$a^{(\mathrm{II})}_{n>0}(t,k) \propto e^{i(kn-\omega t)}, \tag{8.50}$$

with our normal dispersion relation, namely $\omega = \sigma\,\cos\,k$. Thus, we have a wave moving from continuum 0 towards continuum 1, a wave reflected from the continuum 1 back into continuum 0 (with reflection coefficient ρ), and a wave transmitted from continuum 0 into continuum 1.

We find that eqs. (8.49)-(8.50) do actually solve eqs. (8.45)-(8.48), resulting in eigenfunctions of

$$a^{(\mathrm{II})}_n(t,k) = e^{-i\sigma(\cos\,k)t}\begin{cases} \frac{\sigma^2}{4}\,\sin\,kn - \Omega^2 e^{ik}\sin\,k(n+1) & ,\ n<0 \\ -\frac{\sigma\Omega}{2}\,(\sin\,k)\,e^{ikn} & ,\ n>0. \end{cases} \tag{8.51}$$

In the interest of simplicity (and for comparison with our previous results) let's stick to the initial conditions used in Chapter VI: namely,

$$a_{-1}(0) = 1\,,\ a_{n\neq -1}(0) = 0. \tag{8.52}$$

As we may suspect, the solution of Schrödinger's equation follows the same pattern as that of the $(1,\mathsf{CONTINUUM})$ system in §8.5. The full solution is a superposition of the eigenfunctions, but with the cases $\Omega < \frac{\sigma}{2}$ and $\Omega > \frac{\sigma}{2}$ requiring separate treatment.

The low field-strength case $\Omega < \frac{\sigma}{2}$ is somewhat the simpler of the two. We find, by the same methods as in §8.5,

$$a_n(t) = \frac{i}{\pi}\int_{-\pi}^{\pi} \frac{e^{ik}}{\frac{\sigma^2}{4} - \Omega^2 e^{2ik}}\,a^{(\mathrm{II})}_n(t,k)\,dk \tag{8.53}$$

$$= \begin{cases} i^{n+1}\frac{2}{\sigma t}\,\left((-n)\mathrm{J}_{-n}(\sigma t) - \lambda^{-2}(2-n)\mathrm{J}_{2-n}(\sigma t) + ...\right) & ,\ n<0 \\ (-i)^n\frac{2}{\sigma t}\,\left(\lambda^{-1}(n+1)\mathrm{J}_{n+1}(\sigma t) - \lambda^{-3}(n+3)\mathrm{J}_{n+3}(\sigma t) + ...\right) & ,\ n>0. \end{cases} \tag{8.54}$$

The parameter

$$\lambda = \frac{\sigma}{2\Omega} \tag{8.55}$$

is similar in purpose (though not identical in value) to the parameter used in §8.5. This parameter agrees with our previously defined λ parameter in the limit $\Omega \gg \sigma$.

This solution is already sufficient to investigate the special cases $\lambda = 1$ ($\Omega = \frac{\sigma}{2}$) and $\lambda = \infty$ ($\Omega = 0$). For $\Omega = \frac{\sigma}{2}$ we find simply

$$a_n(t) = \begin{cases} i^{n+1} \mathrm{J}_{-(n+1)}(\sigma t) & , \ n < 0 \\ (-i)^n \mathrm{J}_n(\sigma t) & , \ n > 0 \end{cases} \tag{8.56}$$

while for $\Omega = 0$ we find

$$a_n(t) = \begin{cases} i^{n+1} \frac{2}{\sigma t} (-n) \, \mathrm{J}_{-n}(\sigma t) & , \ n < 0 \\ 0 & , \ n > 0 \end{cases} \tag{8.57}$$

Thus, for $\Omega = \frac{\sigma}{2}$, the population simply divides into two equal wave-packets. One wave-packet moves up the Chebychev ladder of continuum 1, while the other moves down the ladder of continuum 0. The two continua unrecoverably absorb a equal amounts of population. When $\Omega = 0$, on the other hand, continuum 1 naturally receives no population. All of the population is unrecoverably dephased into continuum 0, as the wave-packet moves down the Chebychev ladder.

It should come as no suprise, however, that the set of $a_n^{(\mathrm{II})}$ eigenfunctions is not complete in the high field-strength case $\Omega > \frac{\sigma}{2}$—*i.e.*, $\lambda < 1$. The additional eigenfunctions needed for the case $\Omega > \frac{\sigma}{2}$ are

$$a_n^{(\mathrm{I}\pm)}(t) = e^{\mp i\omega' t} \begin{cases} (\pm\lambda)^{-n} & , \ n < 0 \\ \pm (\pm\lambda)^n & , \ n > 0 \end{cases} \tag{8.58}$$

where

$$\omega' = \Omega \left(1 + \lambda^2\right). \tag{8.59}$$

As in the $(1, \mathsf{CONTINUUM})$ case, these eigenfunctions are simply constant population distributions with phase oscillating at a frequency of $\omega' = \Omega$. Even without precisely constructing the initial state (8.52) from $a_n^{(\mathrm{I}\pm)}$ and $a_n^{(\mathrm{II})}(k)$, we can see that these eigenfunctions will dominate those of eq. (8.51) when $\Omega \gg \sigma$ since the linear combination

$$\frac{a_n^{(\mathrm{I}+)} - a_n^{(\mathrm{I}-)}}{2\lambda}$$

is already equal to the initial state at time $t = 0$, up to terms of order $\frac{\sigma}{\Omega}$.

More precisely, we find that

$$a_n(t) = \frac{1-\lambda^2}{2\lambda} \left(a_n^{(\mathrm{I}+)} - a_n^{(\mathrm{I}-)}\right) + \frac{8\lambda^2}{2\pi i \sigma^2} \int_{-\pi}^{\pi} \frac{e^{-ik}}{1 - \lambda^2 e^{-2ik}} \, a_n^{(\mathrm{II})}(t,k) \, dk \tag{8.60}$$

$$= \begin{cases} \frac{1-\lambda^2}{2\lambda} \lambda^{-n} \left(e^{-i\omega' t} - (-1)^n e^{i\omega' t}\right) + \frac{2(-i)^{n+1}}{\sigma t} \left(\lambda^2 (n+2) \mathrm{J}_{n+2}(\sigma t) - \lambda^4 (n+4) \mathrm{J}_{n+4}(\sigma t) + \ldots\right) & n < 0 \\ \frac{1-\lambda^2}{2\lambda} \lambda^n \left(e^{-i\omega' t} + (-1)^n e^{i\omega' t}\right) + \frac{2(-i)^n}{\sigma t} \left(\lambda (n-1) \mathrm{J}_{n-1}(\sigma t) - \lambda^3 (n-3) \mathrm{J}_{n-3}(\sigma t) + \ldots\right) & n > 0. \end{cases} \tag{8.61}$$

Interestingly, the solutions for $a_{n>0}(t)$ (*i.e.*, the probability amplitudes in continuum 1) we have found here are closely related to those found in the previous section for the $(1, \mathsf{CONTINUUM})$ system. The only difference (for equal λ) is that in the previous section there was an additional factor of $\sqrt{1+\lambda^2}$. This holds for *both* the $\lambda < 1$ and $\lambda > 1$ cases. That is, aside from a constant factor, the time evolution of the upper continuum is identical in the $(1, \mathsf{CONTINUUM})$ and $(\mathsf{CONTINUUM}, \mathsf{CONTINUUM})$ systems.

At any rate, the qualitative conclusions of the previous section are not altered at high field strengths. A portion of the population permanently oscillates between the two continua, while another portion unrecoverably dephases into the continua. Remarkably, eq. (8.41) (giving the total oscillating population in the limit $t \to \infty$) remains correct:

$$\text{Total oscillating population} = 1 - \lambda^2. \tag{8.62}$$

As before, when $\Omega \gg \sigma$ we have $\lambda \ll 1$, and consequently most of the population does not dephase into the continua.

What steps would be necessary to extend these results to the case of an arbitrary initial population distribution in continuum 0? This could be done by altering our initial conditions to

$$a_m(0) = 1 \ , \ \ a_{n\neq m}(0) = 0, \tag{8.63}$$

where m is an unspecified negative integer. If the resulting wave-functions $a_n(t)$ has the properties we have outlined above regardless of the value m chosen, then we would know that any initial population distribution has these properties also. [Since the wavefunction resulting from an arbitrary initial distribution can be expressed as as a superposition of wavefunctions resulting from eq. (8.57)]. However, as one may guess from the complexity of the calculations in this section and the previous one, this work has not yet been done.

8.7. Appendix A: Tables

This Appendix presents tables of λ-termination coefficients. It also presents tables of $\sinh \frac{\partial}{\partial n}$ calculations. All of the latter results are entirely trivial. However, they are useful when investigating new sets of test functions and λ-termination coefficients, as well as being fun.

To simplify the following table, the notation $\xi = \cosh \frac{\partial}{\partial n}$, $\zeta = \sinh \frac{\partial}{\partial n}$ will be employed. The symbol $\binom{j}{k}$ represents the number of combinations of j objects, taken k at a time. λ is a constant.

$\underline{f(n)}$	$\underline{\xi\, f(n)}$	$\underline{\zeta\, f(n)}$
$A_n + B_n$	$\xi\, A_n + \xi\, B_n$	$\zeta\, A_n + \zeta\, B_n$
λ	0	0
$\lambda\, A_n$	$\lambda\, \xi\, A_n$	$\lambda\, \zeta\, A_n$
$A_n\, B_n$	$(\xi\, A_n)\ (\xi\, B_n) + (\zeta\, A_n)\ (\zeta\, B_n)$	$(\xi\, A_n)\ (\zeta\, B_n) + (\zeta\, A_n)\ (\xi\, B_n)$
n^j	$\sum_{\text{even}\, k \le j} n^{j-k} \binom{j}{k}$	$\sum_{\text{odd}\, k \le j} n^{j-k} \binom{j}{k}$
$e^{\lambda n}$	$\cosh(\lambda)\, e^{\lambda n}$	$\sinh(\lambda)\, e^{\lambda n}$
$(-1)^n$	$(-1)^{n+1}$	0
$(\pm i)^n$	0	$(\pm i)^{n+1}$
$(-1)^n A_n$	$(-1)^{n+1} \xi\, A_n$	$(-1)^{n+1} \xi\, A_n$
$(\pm i)^n A_n$	$(\pm i)^{n+1} \xi\, A_n$	$(\pm i)^{n+1} \xi\, A_n$
$\cos\ \lambda n$	$\cos(\lambda)\ \cos(\lambda n)$	$-\sin(\lambda)\ \sin(\lambda n)$
$\sin\ \lambda n$	$\cos(\lambda)\ \sin(\lambda n)$	$\sin(\lambda)\ \cos(\lambda n)$

Table 8.1: $\cosh\ \frac{\partial}{\partial n}$ and $\sinh\ \frac{\partial}{\partial n}$ operator action.

From eq. (8.17), a table of exact B_n coefficients for λ-termination has been calculated by means of a symbolic algebra computer program:[22]

[22] muMath, from Microsoft Consumer Products.

L	B_0	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}	B_{11}	B_{12}	B_{13}	B_{14}	B_{15}
0	0															
1	1	-1														
2	$\frac{3}{2}$	-2	$\frac{1}{2}$													
3	2	$-\frac{7}{2}$	2	$-\frac{1}{2}$												
4	$\frac{5}{2}$	$-\frac{11}{2}$	5	$-\frac{5}{2}$	$\frac{1}{2}$											
5	3	-8	10	$-\frac{15}{2}$	3	$-\frac{1}{2}$										
6	$\frac{7}{2}$	-11	$\frac{35}{2}$	$-\frac{35}{2}$	$\frac{21}{2}$	$-\frac{7}{2}$	$\frac{1}{2}$									
7	4	$-\frac{29}{2}$	28	-35	28	-14	4	$-\frac{1}{2}$								
8	$\frac{9}{2}$	$-\frac{37}{2}$	42	-63	63	-42	18	$-\frac{9}{2}$	$\frac{1}{2}$							
9	**5**	-23	60	-105	126	-105	60	$-\frac{45}{2}$	5	$-\frac{1}{2}$						
10	$\frac{11}{2}$	-28	$\frac{165}{2}$	-165	231	-231	165	$-\frac{165}{2}$	$\frac{55}{2}$	$-\frac{11}{2}$	$\frac{1}{2}$					
11	6	$-\frac{67}{2}$	110	$-\frac{495}{2}$	396	-462	396	$-\frac{495}{2}$	110	-33	6	$-\frac{1}{2}$				
12	$\frac{13}{2}$	$-\frac{79}{2}$	143	$-\frac{715}{2}$	$\frac{1287}{2}$	-858	858	$-\frac{1287}{2}$	$\frac{715}{2}$	-143	39	$-\frac{13}{2}$	$\frac{1}{2}$			
13	7	-46	182	$-\frac{1001}{2}$	1001	$-\frac{3003}{2}$	1716	$-\frac{3003}{2}$	1001	$-\frac{1001}{2}$	182	$-\frac{91}{2}$	7	$-\frac{1}{2}$		
14	$\frac{15}{2}$	-53	$\frac{455}{2}$	$-\frac{1365}{2}$	$\frac{3003}{2}$	$-\frac{5005}{2}$	$\frac{6435}{2}$	$-\frac{6435}{2}$	$\frac{5005}{2}$	$-\frac{3003}{2}$	$\frac{1365}{2}$	$-\frac{455}{2}$	$\frac{105}{2}$	$-\frac{15}{2}$	$\frac{1}{2}$	
15	8	$-\frac{121}{2}$	280	-910	2184	-4004	5720	-6435	5720	-4004	2184	-910	280	-60	8	$-\frac{1}{2}$

Table 8.2: λ-Termination Coefficients Based on Polynomial Test Functions.

CHAPTER IX
SUMMARY

9.1. Why a Summary?

A large number of facts has been presented. Hopefully, an outline summary of the more interesting results may serve to reduce any little confusion caused by this situation.

9.2. Low Driver-Rank

Our main concern has been with what we have called systems of *low driver-rank*. These are (model) quantum systems having a Hamiltonian operator

$$H(t) = H_0 + H'(t)$$

where the *matrix rank* M of $H'(t)$ is a small positive integer. By contrast, we have generally assumed H_0 to be a diagonal matrix. For the sake of discussion, let us suppose that the system has N energy levels, where we may have $\mathrm{N} = \infty$. In all cases, we suppose that $\mathrm{M} \ll \mathrm{N}$. Except where stated otherwise, all results pertain to the case of a time-varying driver $H'(t)$.

9.3. Exact Methods

9.3.1. Constant $H'(t)$—Eigenvalues and Eigenvectors

Computing the eigenvalues and eigenvectors of the Hamiltonian involves diagonalization of an $\mathrm{N} \times \mathrm{N}$ matrix in the general case, if approximations such as perturbation theory are not used. For systems of low driver-rank, we have found that diagonalization of a mere $\mathrm{M} \times \mathrm{M}$ matrix is needed. This has the novel effect of reversing the normal roles of the eigenvalues and the electric field (or other external parameter).

9.3.2. Constant $H'(t)$—Laplace Transform

Computing the Laplace transform of the probability amplitudes requires inversion of an $\mathrm{N} \times \mathrm{N}$ matrix in the general case. For systems of low driver-rank, we have found that

inversion of a mere $\mathrm{M} \times \mathrm{M}$ matrix is needed. In fact, if only the ground-state probability amplitude is of interest, we need merely invert an $(\mathrm{M}-2) \times (\mathrm{M}-2)$ matrix.

9.3.3. Time-Varying $H'(t)$—Integral Equations

The N coupled Schrödinger differential equations can be converted to N coupled integral equations in the general case. For systems of low driver-rank, we have found that the behavior of the system can be encompassed in a mere M coupled integral equations. For a general N-level system whose levels interact with a background continuum, a set of N exact integro-differential equations has been derived.

9.3.4. Time-Varying $H'(t)$—Band-Diagonalization

While the Hamiltonian $H(t)$ cannot be simply diagonalized in the general case, it can be *band-diagonalized* for a system of low driver-rank, using a similarity transformation independent of time. The band-diagonal Hamiltonian has $\leq \mathrm{M}$ distinct co-diagonals.

9.4. Consequences of the Exact Methods

9.4.1. Rational Continua

If the matrix elements of $H'(t)$ are expressed by rational functions of the energy-level index, though the system has continuous bands of energy levels it may be exactly represented by an effective non-Hermitian Hamiltonian with only finitely many levels. An example is the $(1, \mathsf{LORENTZIAN\,CONTINUUM})$ system, which is exactly representable by a two-level system. For a constant external field, this effective two-level system can be solved in closed form. Moreover, many results concerning two-level systems can be immediately generalized to the $(1, \mathsf{LORENTZIAN\,CONTINUUM})$ system.

9.4.2. The $(1, \mathsf{DISCRETE\,LORENTZIAN})$ System

The $(1, \mathsf{DISCRETE\,LORENTZIAN})$ system can be exactly represented (prior to the recurrence time $t = \tau_{\mathrm{R}}$) as a non-Hermitian three-level system. This three-level system also represents a discrete level coupled to two Lorentzian continua, one of *positive* width and one of *negative* width.

9.4.3. Weisskopf-Wigner Approximations (Langevin Equations)

For *broad* continua, one can apply a Markov approximation to the M coupled Schrödinger integral equations using the mean value theorem of Calculus. This gives M coupled differential equations—*i.e.*, an effective M-level Hamiltonian. This can be used either in replacing a continuum by a detailed reservoir model, or else for obtaining generalized forms of the Weisskopf-Wigner or Golden Rule approximations, or for explicitly computing a Langevin equation.

9.4.4. Gaussian Discretization of the Continuum

By means of Gaussian integration, a continuum can be modelled by an effective discrete *Hermitian* Hamiltonian. This approximation is very good for small times, but becomes useless for times greater than the recurrence time τ_{R}. The larger the number of discrete levels used, the longer the recurrence time.

9.4.5. Tridiagonalization of the $(1, \mathsf{CONTINUUM})$ System

The $(1, \mathsf{CONTINUUM})$ system can be exactly tridiagonalized by a similarity transformation independent of time. The matrix elements of the Hamiltonian are given by a formula involving recursion coefficients of orthogonal polynomials.

9.4.6. The $(1, \mathsf{CHEBYCHEV\ 2ND\ KIND})$ System

The $(1, \mathsf{CONTINUUM})$ system with a Chebychev continuum of the second kind has been analytically solved in terms of Bessel functions. So has the $(\mathsf{CHEBYCHEV\ 2ND\ KIND}, \mathsf{CHEBYCHEV\ 2ND\ KIND})$ system.

9.5. Approximate Low Driver-Rank

9.5.1. Approximate Tridiagonalization of the Hamiltonian

In all cases, a continuum may be approximately represented as a *ladder* of energy levels, with a few additional transitions to the remaining states of the system. We call this ladder the *Chebychev Ladder*. This holds true whether the transitions to be modelled are between discrete states and the continuum, between two continua, or within a single continuum.

9.5.2. Wave Packets in the Chebychev Ladder

The time-evolution of the populations in the Chebychev ladder is a wave-phenomenon, exactly described, in which wave packets of population move up and down the ladder at a constant speed.

9.5.3. Non-Hermitian Ladder Termination

In order to render numerical calculation efficient, approximate methods have been provided for eliminating many Chebychev ladder energy levels.

9.6. (CONTINUUM, CONTINUUM) Population Trapping

9.6.1. The Broad-Continuum Case

For broad, featureless continua in which population is initially confined to a single one of the continua, the population can be permanently trapped there. This happens *either* when the interaction between the continua is very weak *or* very strong! (In the case of a time-varying interaction, the population-trapping is even more pronounced.)

9.6.2. The Narrow-Continuum Case

For continua whose matrix elements are large only in a region (HWHM) smaller than the interaction strength, this isn't true—when the interaction strength becomes large, the population is unrecoverably split evenly between the two continua. (See §9.4.1.)

9.6.3. The Limited-Continuum Case

When the continua are bounded in energy both from above and below, this isn't true either. For large interaction strengths, the population simply oscillates between the two continua without unrecoverably dephasing (or "decaying")! (See §9.4.6.)

[1]9.6.5. The (CONTINUUM, CONTINUUM, CONTINUUM) System

For broad, featureless three-continua systems, the results are similar to those of two-continua systems. Population initially in the middle continuum is trapped there for large or small interaction strengths. Population initially in an end continuum is trapped there if the *ratio* of the interaction strengths (between the middle and outer continua) is large or small.

9.7. Population Non-Decay

Population in a discrete state coupled to a background continuum of states *need not* decay exponentially (or *at all*) into the continuum. If the continuum is bounded in energy both from above and below, the population can simply oscillate between the discrete state and the continuum at high interaction strengths. (See §9.4.6.)

9.8. What Remains to be Done

I believe that the mathematical development of low-driver-rank theory is fairly complete, but there are several directions in which useful extensions can be made.

[1] Oops! There is no section 9.6.4.—RSB, 3/2003.

All of the theory presented herein is based on solving Schrödinger's equation for the probability amplitudes of the system. The theory can probably be applied also to density-matrix equations of motion, but this has not be done so far. Such a development would be useful since (see Chap. II) the density-matrix approach is a generalized superset of the state-vector approach. Effects such as collisional damping which can be considered very naturally in a density-matrix setting cannot be dealt with as easily in a state-vector setting.

We have also limited ourselves to the semi-classical case, but it seems that these methods could be applied in the case of quantized electromagnetic fields as well. This could allow simplified generalizations to the Jaynes-Cummings models or improved methods of deriving Langevin equations in the quantum theory of damping.

Though we have considered only one-dimensional continua, we know that the low-driver-rank approach can be applied also to the case of multi-dimensional continua. This would be interesting, since the more casual approach of collapsing a multi-dimensional continuum to one of a single dimension (by introduction of a "density of states" function) does some violence to our idea of the structure of the system.

The main areas of extension, however, involve physical applications. I must admit that there is more of mathematical method than of physics in this dissertation. This was not originally intended. However, as the ramifications of the idea of low driver-rank became apparent, it seemed to me that presentation of the many methods derived from this idea was of more immediate importance than presentation of applications of those methods. Whether or not this was the *correct* choice, the mere physical bulk of this document demonstrates that presenting both the methods and extensive applications together was not practical.

The motivation of most of the methods presented here was reduction of computer time and memory costs, with the idea of incorporating model systems with dense bands of energy levels into propagation calculations. In propagation calculations, one must solve the coupled Maxwell-Schrödinger equations at a large number of points in space and time, and consequently requires such time and memory economies. Thus, these methods seem well-suited to modeling vibrational bands of polyatomic molecules in propagation calculations such as those of M. Crenshaw (see review in Chapter II).

Theoretical Intra-Molecular Relaxation models also deal with dense bands of energy levels, and thus would prove a good area of application.

Finally, I suggest that low-driver-rank methods would be ideal for studying the properties of the Quasi-Continuum (QC). Quasi-continua are dense bands of levels with transitions allowed within the band. In fact, by definition, one assumes that transitions of any *given* frequency are allowed. QC studies in the literature do mimic the dense energy-level spacings of "true" quasi-continua, but generally omit the many allowed transitions. Low-driver-rank theory can accomodate easily calculable models with both properties and should therefore be applied to model QC problems.

VITA

Ronald Steven Burkey, the only child of John Eugene Burkey and Josephine Cecilia Sharpe Burkey, was born in Columbus, Ohio, on March 24, 1957. He graduated *cum laude* with a B.S. in mathematics from the Ohio State University in 1978. After working as an actuary for a year, he switched his field of emphasis to physics. He received his M.S. degree in 1983 and his PhD. in 1989 from the University of Texas at Dallas. He is a member of *Phi Beta Kappa*, *Phi Kappa Phi*, and *Sigma Xi*. Since 1986 he has been employed by Heads Up Technologies, Inc., in the capacity of electrical engineer, and holds the title of Senior Engineer.