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- DISCRETIZATION IN THE QUASI-CONTINUUM

- MULTICHANNEL EXCITATION OF THE QUASI-CONTINUUM

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Discretization in the quasi-continuum

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Straightforward discretization of the equations of motion of a quasi-continuum interacting with an electromagnetic field often leads to physical and numerical difficulties. We derive two distinct methods for reducing the number of energy levels that must be treated explicitly in such calculations. One of these applies to bands of quasi-continua with slowly decreasing shoulders; the other, to bands with rapidly decreasing shoulders.

INTRODUCTION

Beginning with Rice in 1929, many authors have considered a model of the so-called "quasi-continuum" in which a distinguished ground state is coupled to a band of N upper states that are not coupled to one another (see Fig. 1). These efforts are summarized well by Shore.[1] The $(1, N)$ system allows many analytic results to be derived because it has a simple eigenvalue equation[2] and because it is susceptible to analysis using the Laplace transform.[3-5] In the special case (the Rice model) of evenly spaced sublevels of the upper band, Schrödinger's equation can be transformed into a delay-differential equation[6,7] and hence exhibits recurrences in which the ground-state probability experiences quasi-periodic growth and decay.

In general, previous investigations dealt with the case of the known (simple, classical) form of the electric field acting on a two-level system, or else with a constant electric field. [The case of a sinusoidal field under the rotating-wave approximation (RWA) and the case of a suddenly turned-on field, although physically different from the constant-field case, are mathematically identical to it for times later than the switch-on time.] For an investigation of a laser pulse passing through a medium,[7] these assumptions about the electric field may not be justified owing to reshaping of the initial pulse as a result of propagation, so it is necessary to consider the case of a time-varying field. Peterson *et al.*[8] have studied the adiabatic case, in which the field is turned on slowly rather than suddenly, and have shown that on laboratory time scales even quite fast pulses can sometimes be in the adiabatic rather than the sudden regime.

Yeh *et al.*,[4] in contrast to Peterson *et al.*, have recently dealt with the quasi-continuum in the case of a time-varying-field envelope in their "interrupted coarse-graining" theory. They also limit the electric field to be slowly varying. In fact, for the weak-field case their limitation on the pulse turn-on time is just that given in Ref. 8 as a condition for adiabaticity. Thus, for weak fields at least, Yeh's procedure appears to be somewhat akin to the adiabatic approximation; yet it also has features distinct from the adiabatic approximation since continua are not normally considered to possess an adiabatic regime.

Witriol *et al.*[9] have considered the problem of reducing the number of levels in a model of a laser-stimulated molecular species reacting to form another species that is removed from the population. This model is, in some ways, more general than the $(1, N)$ model, but the level-reduction scheme is strongly dependent on values of the various system parameters.

We address the same problem as in Ref. 4, namely, that of reducing the difficulty of performing calculations in the $(1, N)$ model of a quasi-continuum with a large number of levels. As in Ref. 9, we reduce a continuum or quasi-continuum of levels to the physically more appealing and computationally cheaper problem of a discrete band with only a few levels. Our techniques are characterized by two properties. First, the field may vary in a totally general way: It may be quantized or classical, and in the latter case the RWA may be applied or not. Second, we strive for high (if not perfect) accuracy rather than merely approximate agreement between the given and reduced systems.

Some of the major questions in laser-induced chemistry in recent years have concerned the nature of intramolecular relaxation (IMR) and the methods by which IMR can be studied experimentally. Recently we pointed out that our preliminary results[10] for the time dependence of the expectation value of the dipole moment (or other off-diagonal observables) are useful in the context of IMR. Although we do not address the question of IMR in this paper, we intend to do so in a future publication.

INTRODUCTION OF THE THEORY

Consider a quantum system interacting with an electric field according to the Hamiltonian

$$H(t) = H_0 + E(t)\mu,$$

where the operators H_0 and μ are independent of time. If we assume that the RWA has been made, then H_0 represents a matrix of detunings $\Delta = n\omega - E/\hbar$, rather than a matrix of energies, and $E(t)$ (which absorbs a constant of $1/2\hbar$) represents the envelope of the electric field rather than the oscillating field itself. We do not assume that the field envelope is constant. In fact, our main concern is to discover the effects of a nonconstant $E(t)$ on the evolution of the system. Thus the RWA is not forced on us; indeed, we may even allow the field to be quantized. If the RWA is not made we must replace the plus in the definition of $H(t)$ by a minus, or else μ will represent the negative of the dipole matrix.

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Fig. 1. A typical $(1, N)$ system. Transitions are allowed from the ground state to the upper band, not within the upper band itself.

We concern ourselves here only with the special case in which the system consists of a nondegenerate ground state interacting with a band of upper levels but in which the upper levels are not coupled directly among themselves. As far as the results that we will derive are concerned, the band may be discrete, continuous, or a combination of the two. However, for simplicity, in our discussion and notation we will generally assume that we are dealing with a pure continuum. For such a system we employ the following notation: The ground-state amplitude is denoted by $a(t)$. Upper levels are indexed by the quantity $\Delta = \omega - E/\hbar$, which represents the detuning of the level that it indexes. The probability amplitudes for the upper levels are denoted by $b(t, \Delta)$. The only nonzero elements of the dipole matrix are those coupling the ground state to the upper states, $\mu(\Delta)$, which we assume to be real. For completeness, we also introduce a function $g(\Delta)$, which gives the density of states in the upper band. This allows us to let Δ vary over the continuous range $(-\infty, \infty)$ even in the discrete case by letting $g(\Delta)$ behave appropriately, e.g., as a delta function in the case of a single discrete level.

The problem that we address is this: Given a system as described above and some simple initial conditions [which we typically choose to be $a(t_0) = 1$ and $b(t_0, \Delta) = 0$, where t_0 is a time before which the incident field $E(t)$ vanishes] how can we [for arbitrary fields $E(t)$] solve for the time evolution of the system when there may be a large number (possibly an uncountable infinity) of levels in the system? The answer that we envisage for this problem is a reduction of the system in some sense to a system with a much smaller number of levels. In an ideal (and extreme) case we could, perhaps, reduce the number of levels to two or three and solve the system analytically; in a less ideal case we still might be able to reduce the number levels sufficiently to make numerical solutions quite inexpensive.

This, of course, is no new idea. Converting complicated systems to two-level systems (on the grounds that most of the levels do not matter) is not uncommon. However, because of the special system that we have chosen to consider, we try a somewhat different approach to the problem than has been employed in the past.

In our notation, Schrödinger's equations can be written as

$$\frac{d}{dt}a(t) = iE(t)\int_{-\infty}^{\infty}\mu(\Delta)g(\Delta)b(t,\Delta)d\Delta, \tag{1.1}$$

$$\frac{d}{dt}b(t,\Delta) = i\Delta b(t,\Delta) + iE(t)\mu(\Delta)a(t). \tag{1.2}$$

Integrating Eq. (1.2) and substituting into Eq. (1.1) gives the integrodifferential equation

$$\frac{d}{dt}a(t) = -E(t)\int_{t_0}^{t}E(t')a(t')\chi(t-t')dt', \tag{2}$$

where

$$\chi(t) = \int_{-\infty}^{\infty}\mu(\Delta)^2 g(\Delta)e^{i\Delta t}d\Delta. \tag{3}$$

All the integrals become sums in the discrete case since the density function becomes a sum of delta functions.

Consider Eq. (1.1) for the time development of $a(t)$, which is the quantity of primary interest given that $b(t, \Delta)$ may be found straightforwardly if $a(t)$ is known. Then it seems natural, in order to discretize Eq. (1.1), to try to replace $b(t, \Delta)$ with some other quantities [in particular, a discrete set of functions $b_1(t)$, $b_2(t)$, etc.] that have known equations of motion and that give an equation of motion for $a(t)$ but that are not necessarily intuitively related to the actual function $b(t, \Delta)$. In particular, we may suppose that there exist numbers $\Delta_1, \Delta_2, \Delta_3, \ldots$ and $\mu_1, \mu_2, \ldots$ such that

$$\frac{d}{dt}a(t) = iE(t)\sum_{n>0}\mu_n b_n(t), \tag{4.1}$$

$$\frac{d}{dt}b_n(t) = i\Delta_n b_n(t) + iE(t)\mu_n a(t). \tag{4.2}$$

From the similarity of these equations to Eqs. (1.1) and (1.2) and from Eqs. (2) and (3), it is easy to see that the b_n will exist if and only if

$$\chi(t) = \sum_{n>0}\mu_n{}^2\exp(i\Delta_n t), \tag{5}$$

where $\chi(t)$ is as defined earlier. In the sections that follow, we discuss at some length the possibility of finding numbers μ_n and Δ_n for a given system and hence guaranteeing the reduction of Eq. (1.1) to Eq. (4.1). A preliminary discussion of a different but related technique based on tridiagonalization of the Hamiltonian is given in the following section.

Note that we have not assumed in any way that μ_n and Δ_n are real. Thus, even though Eqs. (4.1) and (4.2) superficially resemble Schrödinger's equations, it may be that the system for which these would be Schrödinger's equations would not have a Hermitian Hamiltonian and hence could not exist in the real world. This should not bother us since the b_n were introduced merely as a mathematical convenience. However, this realization leads us to ask if the discretized equations of motion (4.1) and (4.2) allow us to compute any quantities of physical interest other than the ground-state amplitude $a(t)$. In fact, they do. The complex polarization Φ, defined[7] as

$$\Phi = 2iN\int_{-\infty}^{\infty}a^*(t)\mu(\Delta)g(\Delta)b(t,\Delta)d\Delta, \tag{6}$$

is easily computed in the discretized system. Multiplying Eq. (1.1) by $2Na^*(t)/E(t)$ is seen to give the complex polarization; on the other hand, substituting for the time derivative of $a(t)$ from Eq. (4.1), we get an expression involving only $a(t)$ and $b_n(t)$. Therefore

$$\Phi = 2iN\sum_{n>0}a^*(t)\mu_n b_n(t). \tag{7}$$

It is fortunate that Φ is so easily calculated in the discretized system, since Φ is the quantity that couples Schrödinger's equation to Maxwell's equations in the differential equations

that describe the behavior of an optical field in a bulk material.

From Eqs. (2) and (3) it is clear that the system is completely characterized by the function $\mu(\Delta)^2 g(\Delta)$, which we call the shape of the band and refer to as $w(\Delta)$ for convenience. We must make a distinction between two cases: whether $w(\Delta) \sim |\Delta|^{-n}$ (for some n) as $|\Delta| \to \infty$ or whether $w(\Delta)$ dies away faster than every such power. The reason for this distinction is that we have found methods of dealing with either case but have found no method that can deal with both cases. A deeper reason for the existence of these two disparate cases is not evident.

SLOWLY DYING BANDS

First, consider the case in which $w(\Delta)$ dies away like $|\Delta|^{-n}$ for some integer n as $|\Delta| \to \infty$. If this is true, then the function $w(\Delta)$ can be approximated as a rational function, i.e., as a ratio of two polynomials in Δ:

$$w(\Delta) \approx \frac{p(\Delta)}{q(\Delta)} \qquad [p(\Delta), q(\Delta) \text{ polynomials}]. \tag{8}$$

If such a relation holds, we say that we have a rational band.

Suppose, in fact, that approximation (8) holds strictly rather than approximately. Our main result of this section can be expressed in the following theorem.

Theorem

If $\mu(\Delta)^2 g(\Delta)$ is a rational function (with simple poles) of form (8), then a reduction of Eqs. (1) to Eqs. (4) exists. The Δ_n are just the roots of $q(\Delta)$ that lie in the upper half complex Δ plane, whereas the μ_n can be expressed by the formula

$$\mu_n = \left[2\pi i\frac{p(\Delta_n)}{q'(\Delta_n)}\right]^{1/2}, \tag{9}$$

where the prime on $q(\Delta)$ represents differentiation.

Proof

Compute $\chi(t)$ according to Eq. (3). $w(\Delta)$ must die away at least as fast as $|\Delta|^{-2}$ or else the total dipole moment [the integral of $w(\Delta)$] would not exist. The integral in Eq. (3) can be written, therefore, as the limit of the complex line integral around a large semicircle in the upper half Δ plane and consequently as a sum of the integrals around the singularities in the upper half-plane (since the integrand is analytic except at those points). Therefore

$$\chi(t) = \sum_{\Delta_n}\exp(i\Delta_n t)\,p(\Delta_n)\oint_{\Delta_n}\frac{d\Delta}{q(\Delta)},$$

where the sum is to be taken over the upper half-plane roots Δ_n of $q(\Delta)$ and the integrals are evaluated around those points. Since $q(\Delta)$ has no repeated roots, the square of Eq. (9) is the value of the integral as given by complex variable theory. Therefore Eq. (5) is valid (for these values of μ_n and Δ_n), and so the reduction exists. Q.E.D.

The simplest example of a rational band is the Lorentzian band.

$$w(\Delta) = \mu(\Delta)^2 g(\Delta) = \mu^2\frac{\sigma}{\pi}\frac{1}{(\Delta - s)^2 + \sigma^2}, \tag{10}$$

where σ is the width of the band, s is the offset of the center of the band, and μ is the total dipole moment. This function has exactly one pole in the upper half Δ plane, namely, $\Delta = s + i\sigma$, and the application of formula (9) gives the reduced dipole-matrix element μ. Thus the reduced equations of motion for the Lorentzian-band system are

$$\frac{d}{dt}\begin{bmatrix}a(t)\\ b(t)\end{bmatrix} = i\begin{bmatrix}0 & E(t)\mu\\ E(t)\mu & s + i\sigma\end{bmatrix}\begin{bmatrix}a(t)\\ b(t)\end{bmatrix}. \tag{11}$$

These equations are often seen as the result of an approximation that is applied when Eq. (2) has been derived but has not been found to be solvable. In fact, these are formally identical with the equations obtained from the Weisskopf–Wigner approximation. It should be remembered, however, that according to the derivation above they are exact for a Lorentzian band in an arbitrarily varying field. There is no approximation here except possibly the RWA or the approximations inherent in supposing a semiclassical interaction with the electric field. This result has been seen in analytic Lorentzian-band solutions for the case of $E(t)$ constant[2] and for $E(t)$ exponentially increasing.[10] Furthermore, it can be applied to give the exact Lorentzian-band solution for any $E(t)$ function for which the two-level solution is known. For example, in Ref. 10 we gave the solution for $a(t)$ for a system of two discrete levels when $E(t)$ is semiexponentially increasing, i.e., when it increases from zero and goes to a constant value in a particular way (see Fig. 2). Now we can immediately generalize that result to obtain $a(t)$ when the upper level is a Lorentzian band. By replacing the detuning in that formula[10] by the quantity $s + i\sigma$, which includes both the detuning and the bandwidth, we immediately get the desired solution:

$$a(\tau) = \exp(i\xi_- \tau)M\left[i\frac{(s + i\sigma)\xi_-}{2\lambda\alpha}, -i\frac{s + i\sigma}{\lambda}, 2i\alpha\tau\right],$$

where

$$\xi_- = \frac{s + i\sigma}{2\epsilon_\infty} - \alpha$$

and

$$\alpha = \left[\left(\frac{s + i\sigma}{2\epsilon_\infty}\right)^2 + \left(\frac{\mu_{01}}{2}\right)^2\right]^{1/2}.$$

Here, M is the confluent hypergeometric function.

We conclude this section with a result that is not an application of the rational-band theorem but that is nonetheless

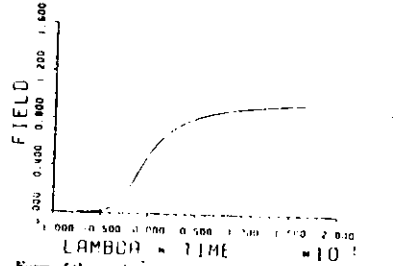

Fig. 2. Form of the semiexponential pulse. Initially ($t = -\infty$) the field envelope increases as $e^{2\lambda t}$, but eventually it goes to a constant value.

related to the Lorentzian-band result given above. Imagine that, *instead* of a continuous band of levels, we have an otherwise similar band of evenly spaced discrete levels. In the case of a Lorentzian-band shape, expression (10) must be replaced by

$$\mu_n^2 = \frac{\sigma\delta}{\pi}\frac{1}{(n\delta - s)^2 + \sigma^2}\left(\tanh\frac{\pi\sigma}{\delta}\right)\mu^2,$$

where δ is the spacing between levels. (In this instance only, μ_n refers to the nth level of the given system rather than the reduced system.) If $\chi(t)$ is computed using formula (3), we find[1] that for $t < 2\pi/\delta$ (the recurrence time of the system)

$$\chi(t) = \mu^2\frac{1 + \tanh\frac{\pi\sigma}{\delta}}{2}\exp[i(s + i\sigma)t] + \mu^2\frac{1 - \tanh\frac{\pi\sigma}{\delta}}{2}\exp[i(s - i\sigma)t].$$

Therefore, so long as we confine our attention to times less than the recurrence time, the discrete Lorentzian system can be reduced *exactly* to a three-level system with detunings $s \pm i\sigma$ and dipole-matrix elements given by the square roots of the coefficients of the exponentials in the equation above. If we compare this with the result seen in the case of a continuous Lorentzian band, we will notice that this three-level reduction is equivalent to replacing the discrete Lorentzian band by two continuous Lorentzian bands. Mathematically, one of the continuous bands has width σ and the other has the negative width $-\sigma$. Presumably it is this negative-width band that causes the breakdown of the reduction at the first recurrence. When $\tanh(\pi\sigma/\delta) \approx 1$, the negative-width band is almost decoupled from the rest of the system, and only the positive-width band remains. This is reasonable since when the spacing δ is less than the bandwidth σ we might expect that the levels in the discrete Lorentzian would be dense enough to justify a continuum approximation.

QUICKLY DYING BANDS

Consider the case in which $w(\Delta)$ dies away as $|\Delta| \to \infty$ faster than $|\Delta|^{-n}$ for any n. If this is true, then it is possible to define orthogonal polynomials $f_n(\Delta)$ with respect to the weight function $w(\Delta)$:

$$\int_{-\infty}^{\infty} w(\Delta)f_n(\Delta)f_m(\Delta)\mathrm{d}\Delta = \delta_{nm}.$$

Given that it is possible to define orthogonal polynomials, there is a systematic procedure for developing approximation formulas for the class of integrals

$$\int w(\Delta)f(\Delta)\mathrm{d}\Delta,$$

where $f(\Delta)$ is to be an arbitrary function as far as the formula is concerned.[11,12] Furthermore, there is a systematic procedure for deriving the error terms of such formulas.[13] In general, one finds a linear approximation formula of the form

$$\int_{-\infty}^{\infty} w(\Delta)f(\Delta)\mathrm{d}\Delta \approx \sum_{n>0} w_n f(\Delta_n), \tag{12}$$

where the Δ_n are the roots of one of the orthogonal polynomials $f_n(\Delta)$ and the w_n are weight factors. The error term (which is not shown) involves a high-order derivative of $f(\Delta)$. If we apply approximation (12) to the case $f(\Delta) = e^{i\Delta t}$, we get

$$\chi(t) \approx \sum_{n>0} w_n \exp(i\Delta_n t), \tag{13}$$

which is of the form of Eq. (5). Consequently, a quickly dying band can be approximately discretized by putting levels at the positions of the roots of one of the orthogonal polynomials and using as dipole-matrix elements the square roots of the weight factors that would be needed for an approximate integration formula based on the orthogonal polynomial.

The error in a calculation of the ground-state probability amplitude using such a scheme can be approximated by applying mean-value integral formulas to integrodifferential Eq. (2). If $E(t)$ does not become too large within the decay time of $\chi(t)$, it can be shown that the maximum error in the ground-state amplitude on the time interval $[0, t]$ is less than

$$\delta\chi \int_0^t \int_0^{t'} E(t')E(t'')\mathrm{d}t''\mathrm{d}t', \tag{14}$$

where $\delta\chi$ is the maximum error in $\chi(t)$ on this interval. The units in this expression are correct if we recall that $E(t)$ is taken to include a factor of $1/2\hbar$.

A more obvious way to discretize a continuous band would be simply to replace the continuum by a set of evenly spaced levels with dipole-matrix elements that are roughly the same as (or proportional to) the value of the $\mu(\Delta)$ at the corresponding position. (For convenience, we refer to this procedure as Rice discretization since equally spaced levels are involved.) Rice discretization is not the best choice for precisely the same reason that choosing equally spaced sample points in approximation formula (12) is not the best choice. There is also a physical reason for avoiding Rice discretization. Equally spaced levels cause the phenomenon of recurrences, in which constructive and destructive interference create a quasi-periodic oscillation in the ground-state amplitude. We saw earlier in the case of the discrete Lorentzian band that the reduction to a three-level system worked until the first recurrence time, but then it broke down. The approach of using expression (13) as a prescription for discretization avoids this trap and optimizes the discretization at the same time.

Expression (14) for the error in $a(t)$ that is due to the error in $\chi(t)$ implies that our version of the discretization also breaks down eventually. In fact, since the error term of expression (13) involves a derivative of $f(\Delta)$ (which is $e^{i\Delta t}$), the error in $\chi(t)$ must have a polynomial dependence on t. Thus the reduction does fail in time, but the error expression gives us a means to estimate the time range for which the approximation is valid.

As an example, consider a uniform continuous band of width $2\Delta_0$ in which $w(\Delta)$ is $\mu^2/(2\Delta_0)$ for $|\Delta| < \Delta_0$ and is zero outside this range. For this band shape, the orthogonal polynomials are Legendre polynomials. The discretized system therefore has a ground state and a band of discrete levels positioned according to the roots (times Δ_0) of a Legendre polynomial; the dipole-matrix elements are proportional (by a factor of $\mu/\sqrt{2}$) to the square roots of the weight factors for Gaussian integration and connect the levels in the band to the ground state but not to other levels in the band. The error formula for Gaussian integration[11] guarantees a bound on the error in $\chi(t)$. If there are to be N levels in the discretized band, the error in $\chi(t)$ is given by

$$|\delta\chi| \le \frac{2^{2N+1}(N!)^4}{(2N+1)[(2N)!]^3}(\Delta_0 t)^{2N}.$$

As a numerical example, take the case $\Delta_0 = 0.3\ \mathrm{cm}^{-1}$, with $\mu E(t)$ ramping linearly from zero to $0.05\ \mathrm{cm}^{-1}$ at $t = 1/30$ nsec and remaining constant thereafter. We adopt the goal of providing six-figure accuracy for the ground-state probability amplitude on the time interval $t < 1/3$ nsec. As may be expected, expression (14) actually gives a slightly pessimistic estimate for the necessary number of discretized levels. We have integrated Schrödinger's equation using 16 discretized levels chosen as discussed above. The resulting ground-state probability amplitude (which is real) is depicted in Fig. 3. In contrast, consider the Rice discretization, which involves replacing the band by a set of evenly spaced discrete levels connected to the ground state by equal dipole-matrix elements. Figure 4 displays the error in the ground-state probability amplitude calculated from Rice discretizations with 16, 32, 64, and 128 evenly spaced levels, compared with the "correct" ground-state amplitude calculated from the system as discretized by our method described above (using 16 levels). Among the Rice discretizations, only the 128-level case attains six-figure accuracy. In Fig. 4, notice that the ground-state probability amplitudes as obtained from the Rice discretizations appear to coincide periodically (and simultaneously) with the true ground-state amplitude. The reason for this novel feature is not entirely clear to us.

Although the technique of approximating $\chi(t)$ using orthogonal-polynomial methods of quadrature obviously leads to quite satisfactory results compared with simpler discretization schemes, the application of formula (13) has two inconvenient aspects. First, and most important, we have to have an effective method of computing the roots of the orthogonal polynomials and a method of computing the weight factors. Second, we cannot build a more accurate discretization from a less accurate one. That is, if we decide that we must have more accuracy, then there is no alternative to using an orthogonal polynomial of higher degree, computing its

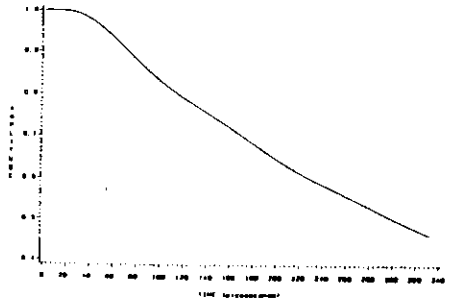

Fig. 3. Ground-state probability amplitude for a uniform rectangular band of full width $0.6\ \mathrm{cm}^{-1}$, as calculated by our technique using 16 levels in the discretized band. This result is accurate to about six decimal places.

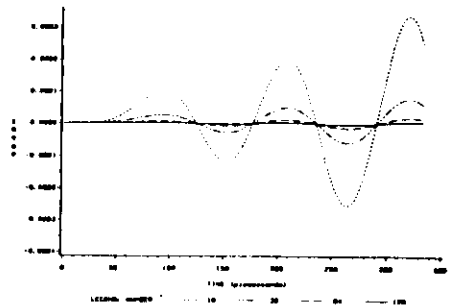

Fig. 4. Error resulting from Rice discretizations of 16, 32, 64, and 128 evenly spaced levels in the calculation of the of full width $0.6\ \mathrm{cm}^{-1}$. The zero point of errornd is taken to be the amplitude calculated using our method (see Fig. 3).

roots, etc. We cannot simply take the less accurate discretization, add a few more levels, and try again.

This is all that we have to say on discretization within the framework of Eq. (5). As it happens, however, there is another approach to the discretization of quickly dying bands that, although it is based on a completely different premise about how discretization should be performed, uses similar mathematical machinery to that discussed above, and in a more convenient way.

The alternative approach to discretization can be summed up in the following theorem.

Theorem

The Hamiltonian of any system (of the type that we are discussing in this section) can be tridiagonalized by a similarity transformation that is independent of $E(t)$. The diagonal elements of the Hamiltonian are

$$0, \quad -\frac{d_0}{e_0}, \quad -\frac{d_1}{e_1}, \quad -\frac{d_2}{e_2}, \ \ldots,$$

and the codiagonal elements are

$$E(t)\,\mu, \quad \frac{1}{e_0}, \quad \frac{1}{e_1}, \quad \frac{1}{e_2}, \ \ldots,$$

where the d_n and e_n come from a recurrence formula[12] of the orthogonal polynomials f_n with respect to $w(\Delta)$,

$$f_{n+1}(\Delta) = (d_n + e_n\Delta)f_n(\Delta) - c_n f_{n-1}(\Delta).$$

Proof

We explicitly give the similarity transformation. Note that, although our vectors may have many elements, we represent them as having just two components, a scalar and a function of Δ; the scalar represents the ground-state component, and the function represents the upper-level components. With this notation, the new basis vectors are

$$\begin{bmatrix}1\\0\end{bmatrix}, \quad \begin{bmatrix}0\\ \dfrac{\mu(\Delta)}{\mu}f_0(\Delta)\end{bmatrix}, \quad \begin{bmatrix}0\\ \dfrac{\mu(\Delta)}{\mu}f_1(\Delta)\end{bmatrix}, \ \ldots.$$

Given the exact form of these vectors, the Hamiltonian matrix

is easily seen to be as stated in the theorem. That the vectors are orthogonal and form a complete set is a trivial consequence of the orthogonality and completeness of the orthogonal polynomials. Q.E.D.

This theorem puts us in a much better position than that in which we were left by the previous method since, even though we still need to know the orthogonal polynomials, we no longer need to know the roots and weight factors. Further, successively more accurate discretizations can now be built up recursively.

The manner in which the total dipole strength and the band shape figure independently in the tridiagonal Hamiltonian is astonishing. Only two matrix elements depend on $E(t)$ and μ. All other nonzero elements in the matrix are somehow geometric constants that depend only on the shape (and not on the strength) of the band. To compute the complex polarization we need only the first two probability amplitudes. Hence any approximation that we make regarding the elimination of the higher levels affects the polarization (which is the only physical quantity other than the population that interests us) only indirectly.

If we were to truncate the Hamiltonian matrix, keeping just the low levels, we would find that the remaining matrix is actually similar to the discretized Hamiltonian derived earlier in this section, in which the detunings are the roots of some orthogonal polynomial and the dipole-matrix elements are the square roots of the weight factors of an approximate integration scheme based on the orthogonal polynomial. This is perhaps not surprising since the mathematics of orthogonal polynomials permeates the entire subject. Nevertheless, this observation serves to connect what we have found here to the general framework of discretization embodied in Eq. (5). Furthermore, since the previous method of discretization in this section permitted the derivation of error formulas, we can obtain estimates from these formulas of the error involved in truncating the tridiagonal Hamiltonian.

The notion that the mathematics of orthogonal polynomials may be useful in solving the dynamics of quantum systems, particularly in the tridiagonal case, is not new.[7,14,15] Orthogonal polynomials have generally been seen as a tool for computing the dressed-state eigenvalues and eigenvectors of a system experiencing a constant-amplitude field (or perhaps a field that has been suddenly switched on). What we have found is valid for a field varying in an entirely general way.

References 7 and 14 nevertheless present results relevant to the tridiagonal method of discretization. These authors *start* with a tridiagonal Hamiltonian (which is truncated for the sake of computer calculations) and solve (in the case of a constant field) for the populations. The matrix elements of the Hamiltonian are chosen as recursion coefficients for the Chebyshev, Hermite, Legendre, or Laguerre orthogonal polynomials. Thus, in light of the theorem given above, we see that the numerical results given in Ref. 14 can be viewed as approximations (in the case of a constant field) to populations in systems containing continuous bands of various shapes—among which are included the Gaussian band shape and the uniform rectangular band shape.

We do not discuss the tridiagonal method of discretization further here. In a future publication, we will show that the method can be vastly generalized. The detailed discussion of the method is more appropriate in that context than in this.

SUMMARY AND DISCUSSION

We have considered the discretization of systems in which there is a ground state and a band of levels that interact with the ground states but not with each other. This band is envisaged as a continuum, and the problem is to introduce in place of the band a discrete set (it is hoped that the set will be finite) of quantities that can be used to calculate the ground-state amplitude and the complex polarization. This is not the same problem as computing the eigenvalues and eigenvectors since we want our discretization to be useful in the case of a time-varying electric field $E(t)$. In fact, only reductions that are good in the case of a totally general $E(t)$ have been discussed, and hence the results derived can be coupled with a numerical-differential-equation solver to solve Schrödinger's equation for the type of system that we have considered.

We have found two essentially separate cases. In the one case, in which $w(\Delta) = \mu(\Delta)^2 g(\Delta) \sim |\Delta|^{-n}$ (for some integer n) as $|\Delta| \to \infty$, we have found that $w(\Delta)$ can be approximated as a rational function $p(\Delta)/q(\Delta)$. We have shown how to find N quantities [where the degree of $q(\Delta)$ is $2N$] for which we know the equations of motion and in terms of which we can express the equation of motion of the ground-state amplitude $a(t)$. These equations of motion resemble those for an $(N+1)$-level Schrödinger equation, except that the Hamiltonian need not be Hermitian. There is no approximation in these equations beyond the rational approximation, and the ground-state amplitude and complex polarization can be computed [for arbitrary fields $E(t)$] after arbitrarily long times in the reduced system.

In the second case, where $w(\Delta)$ dies to zero faster than any power of $|\Delta|$ as $|\Delta| \to \infty$, we have found a similarity transformation that tridiagonalizes the Hamiltonian. The tridiagonal Hamiltonian is discrete but infinite, and the only approximation involved is in the truncation of this matrix to give a finite system. The similarity transformation is completely independent of time, so that once again the reduced system can be used in the case of a time-varying field. Furthermore, the only elements of the Hamiltonian matrix that depend on the field connect the ground state with the next higher level. Thus only these two levels have to be accurately known to compute the complex polarization. Since any truncation of the Hamiltonian (or, possibly, replacement of the upper states by a reservoir) will leave the equations of motion of these levels unchanged (though altering the actual values of some of the probability amplitudes entering into them), the effect of such an approximation on the ground-state amplitude or the complex polarization can only be indirect. We have also given the matrix obtained from a certain similarity transformation of the truncated tridiagonal Hamiltonian and shown how it can be used to give an expression for the error involved in the truncation.

ACKNOWLEDGMENTS

We thank Daniel R. Adams and C. B. Collins for help in producing Figs. 3 and 4 and R. E. Wyatt for drawing our attention to the work of Roger Haydock.

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Note Added in Proof. Witriol[16] advocates direct numerical solution of integrodifferential equation (2). This a form of coarse graining in the time domain. We do not mean to imply that we have a method of attack for every possible case. If, for example, one shoulder dies as $|\Delta|^{-n}$ while the other dies as $|\Delta|^{-m}$ with $n > m$, then Eq. (8) is invalid and the approach that follows it fails.

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Multichannel excitation of the quasi-continuum

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For a quantum system in which a continuous or quasi-continuous band of levels is excited by means of several dipole interaction channels, we develop a mathematical theory that simplifies the numerical solution of the Schrödinger equation. The theory allows time-varying electric fields (or electric-field envelopes). It also takes into account the exact shape of the band as well as the fact that different excitation channels see different band shapes. Accuracy of the results can be as high as desired. We show that the dephasing of the quasi-continuum probability amplitudes in the conventional continuum basis corresponds to the propagation of well-defined waves in the new basis that we introduce.

1. INTRODUCTION

Actual calculations involving real quantum systems can be difficult in the sense that so many levels interact in such a complicated way that calculations can require vast quantities of computer time. It is therefore common in quantum optics to construct simplified models in which one can easily study certain phenomena without necessarily trying to mimic any real system with the model. These phenomena include passage of optical pulses through media, intramolecular relaxation (IMR), and laser-induced dissociation.

One popular model is the $(1, N)$ system, in which a special state, the ground state, can interact with a band of N levels but the N levels cannot interact among themselves. These efforts are summarized by Shore.[1] In this model, dense bands of levels absorb population from the ground state, making the model useful for the study of IMR. Another popular model is the ladder system, in which a series of states can interact with adjacent states but not with any other state. The first investigation employing the ladder-system model was that of Göppert-Mayer in 1931.[2] In this model, multiphoton absorption can occur, making it possible (for example) to study questions of laser chemistry. Haydock[3] showed that, in the case of a constant electric field (envelope), all discrete systems can be converted into ladder systems with reasonable ease. We have shown[4] that the $(1, \text{band})$ system can be converted into a ladder system even if the band is continuous and the electric field varies and that this can be done with a similarity transformation independent of time. Thus there is a certain degree of unity in the two models.

However, these two models do not by themselves cover (even conceptually) all phenomena of interest. In particular, phenomenological damping is often added to the models. Lefebvre and Savolainen[5] have developed a complicated model combining features of both $(1, N)$ systems and ladder systems, with many adjustable parameters. Witriol[6] has also developed such models. Galbraith *et al.*[7] generalized the treatment of $(1, N)$ systems in another way by coupling two $(1, N)$ systems [or, alternatively, by using a $(1, N)$ system in which each level is replaced by two degenerate levels]; they found that many of the results and methods previously applied to the $(1, N)$ case can be extended to cover this case as well.

Rather than a complex model, we present a mathematical theory that aids in the accurate reduction of models containing a continuous (or dense discrete) band of levels to a computable form. By this we mean that the Schrödinger equation is put into such a form that one can use a numerical differential-equation solver on a computer to determine the time evolution of the probability amplitudes. Our method of reduction has two basic virtues. First, time-varying electric fields are welcome. Second, continuous bands of levels may be present. For various reasons, some of which are discussed in Section 2, the replacement of richly structured bands by phenomenological damping may not be entirely satisfactory. Therefore we not only take into account the exact band shape but also actually allow each level not in the band to perceive the band as having a different shape. (By the shape of the band we mean the functional form of the dipole operator matrix. Thus we do not force the dipole matrix into a specific form.)

Yeh *et al.*[8] have considered another method for taking the band shape into account in their interrupted coarse-graining theory of $(1, \text{band})$ systems. They easily derive qualitative information about the evolution of the system, given that the electric field is constrained to be slowly varying. On the other hand, our approach to the solution of (N, band) systems has no such constraint and was designed to produce highly accurate quantitative information.

We also present results of a numerical application of this technique. This example is interesting because some features of it are both analogous to and *explainable by* classical wave theory. Because of this, despite our comments in the above paragraph, our method can provide qualitative insight as well as quantitative information regarding the time evolution of the system.

All the approaches mentioned above, including our own approach, deal with the time evolution of the system as dictated by the Schrödinger equation for state vectors. Some phenomena, such as collisional damping, simply cannot be dealt with in this framework, requiring density-matrix equations of motion for adequate treatment. It may be possible to extend our method to cover this case, but, if so, we do not know how to do it at the present time. Therefore, although we state that the electric field may vary arbitrarily in time, it should be noted that the time of variation of the field (as well as the time interval of interest) is shorter than the collisional damping time.

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2. THEORY

We present a method of dealing with continuous bands of levels, and we constantly refer to continuous bands throughout the paper. Actually, our results hold, to a large degree, for discrete bands (such as dense quasi-continuous bands). We speak this way, however, because the concepts that we use are more familiar in the continuous case and because we want to distinguish the band that we are simplifying from other (presumably discrete) levels in the system. Moreover, we speak of a classical electric field even though our results are good for a quantum field. With this in mind, consider a system consisting of N discrete levels and a continuous band of levels. We allow dipole transitions among the discrete levels or between the discrete levels and the band; however, no dipole transitions are allowed within the band itself (see Fig. 1). Schematically, the Hamiltonian of a quantum system interacting semiclassically with an electric field can be written as

$$H(t) = \delta + E(t)\mu.$$

Our notation assumes that the rotating-wave approximation has been made, although this is by no means required in our approach. The operator δ is diagonal in the matrix representation that we use and contains the detunings of the levels; the form of the dipole matrix μ reflects the selection rules mentioned above. The electric-field envelope $E(t)$ is allowed to vary in time.

How should the band be treated computationally if we are to solve the Schrödinger equation numerically? The continuous band is often taken to act qualitatively as a reservoir, absorbing population until none remains in the discrete states. It is not uncommon to eliminate the band by introducing phenomenological damping in the form of complex detunings of the discrete states.[6] This procedure is unsatisfactory in some ways, although the introduction of complex detunings is mathematically correct if the band has a Lorentzian shape.[4] Although Lorentzian bands do sometimes arise, the Lorentzian band shape can by no means be thought of as typical because of the extremely slowly decreasing shoulders of the band. It is not clear if the Lorentzian-band approximation is reasonable quantitatively unless *a posteriori* manipulation of the bandwidth (phenomenological damping rate) is allowed.

Consequently, we desire a more useful way of dealing with multichannel excitation of the continuum. Not only must any such method take the exact shape of the band into account in a more accurate way, but it also must not limit our ability to use a time-varying electric-field envelope $E(t)$.

Denote the detunings of the discrete levels by Δ_k (where $k = 1, \ldots, N$) and the detuning of a level in the band by Δ (where $\Delta_{\min} \le \Delta \le \Delta_{\max}$). Let μ_{jk} be the dipole matrix element connecting the jth and kth discrete levels, and let $\mu_k(\Delta)$ be the dipole matrix element connecting the kth discrete level and the Δth continuous level. In this basis, vectors and matrices are naturally partitioned into discrete and continuous parts. We will write our vectors, for instance, as having $N + 1$ elements: The first N elements are the actual elements of the vector corresponding to discrete levels, and the last element combines all the elements corresponding to levels in the band in the compact form of a function of Δ.

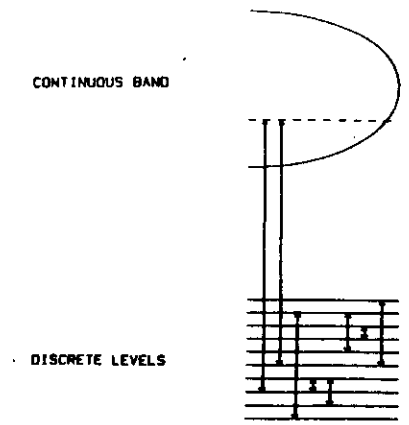

Fig. 1. A typical system in which a continuous band is excited through multiple channels. In general, the system may make any transition except those between two levels of the band.

There is no reason to suppose that $\mu_k(\Delta)$, which represents the shape of the band as seen by the kth discrete level, should be simply related to $\mu_j(\Delta)$ unless $j = k$. We will suppose, however, that there is a certain underlying shape $\mu(\Delta)$ *of* which all the $\mu_k(\Delta)$ are modifications. In particular, we assume that there are polynomials $p_k(\Delta)$ so that

$$\mu_k(\Delta) = \mu(\Delta)p_k(\Delta). \tag{1}$$

By assumption, $\mu(\Delta) = 0$ for $\Delta < \Delta_{\min}$ or for $\Delta > \Delta_{\max}$; thus $p_k(\Delta)$ need be accurate only in the interval $\Delta_{\min} \le \Delta \le \Delta_{\max}$. As an approximation, Eq. (1) can be made quite accurate, since by the Stone–Weierstrass theorem of real analysis theory,[9] a continuous function can be approximated by polynomials on a closed finite interval to any desired degree of accuracy. Furthermore, the actual *choice* of $\mu(\Delta)$ is somewhat arbitrary. For a given level of accuracy in the approximation of Eq. (1), how closely $\mu(\Delta)$ approximates $\mu_k(\Delta)$ merely influences the degree of $p_k(\Delta)$ and not our ability to make (in theory) the approximation. That is, if $\mu(\Delta)$ is chosen poorly, then $p_k(\Delta)$ will be of higher degree.

It is possible to define a set of polynomials $f_k(\Delta)$, orthogonal with respect to the weight function $\mu(\Delta)^2$ (Refs. 10 and 11):

$$\int_{\Delta_{\min}}^{\Delta_{\max}} \mu(\Delta)^2 f_k(\Delta) f_j(\Delta) \mathrm{d}\Delta = \delta_{jk}. \tag{2}$$

Such orthogonal polynomials have proven quite useful in other investigations.[3,4,12,13] We use them to define a new basis, in which the Hamiltonian will be conveniently simplified. Let our new basis be denoted by

$$\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N, \mathbf{u}_0, \mathbf{u}_1, \ldots,$$

where the $\mathbf{v}_k$ are the unmodified discrete states

$$v_1 = \begin{bmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \end{bmatrix}, \quad v_2 = \begin{bmatrix} 0 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \end{bmatrix}, \quad \ldots, \quad v_N = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 1 \\ 0 \end{bmatrix},$$

and the u_k are based on the orthogonal polynomials, which are defined above:

$$u_k = \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \mu(\Delta)/f_k(\Delta) \end{bmatrix}.$$

It should be mentioned that this basis does not actually span the entire state space; however, the space spanned by these vectors includes every vector that could be produced during a numerical solution of the Schrödinger equation with the population initially in the discrete states, so this basis is certainly good enough for our purposes. Clearly, this set of states is countably infinite, whereas the conventional continuum basis is *un*countably infinite.

Now we can write all the nonzero matrix elements of the Hamiltonian. By noting that all orthogonal polynomials satisfy a recurrence relation of the form[10,14]

$$f_{n+1}(\Delta) = (d_n + e_n\Delta)f_n(\Delta) - c_n f_{n-1}(\Delta), \tag{3}$$

we find that

$$\langle v_j|\delta|v_k\rangle = \Delta_j\delta_{jk}, \tag{4a}$$

$$\langle u_j|\delta|u_j\rangle = -d_j/e_j, \tag{4b}$$

$$\langle u_j|\delta|u_{j+1}\rangle = 1/e_j. \tag{4c}$$

Similarly, by noting that all polynomials can be written in terms of the orthogonal polynomials $f_k(\Delta)$, we have

$$p_k(\Delta) = \sum_{m=0}^{M} p_{km} f_m(\Delta) \tag{5}$$

for some numbers p_{km}, where $M = \max|\deg(p_k)|$. Therefore

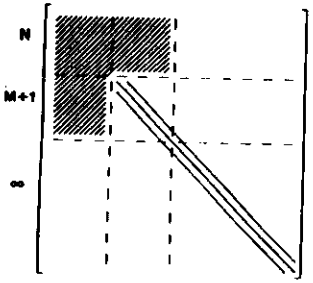

Fig. 2. Hamiltonian matrix, in our basis, is infinite but discrete. It is tridiagonal with a border that is not full. The tridiagonal elements are independent of the electric field.

$$\langle v_j|\mu|v_k\rangle = \mu_{jk}, \tag{6a}$$

$$\langle v_j|\mu|u_k\rangle = p_{jk} \quad \text{if } k \le M$$
$$= 0 \quad \text{if } k > M. \tag{6b}$$

Let us summarize what we have found so far. We have found a similarity transformation that is independent of time and of the field envelope $E(t)$ in which (1) the detuning matrix δ is tridiagonal, (2) the dipole matrix μ has only a few (i.e., a finite number) nonzero elements, and (3) all the matrix elements in the transformed system can be calculated easily. Put another way, in our basis the Hamiltonian is tridiagonal (and infinite) with a border that is not full [having only a finite number of nonzero elements, given by Eqs. (4a) and (6); see Fig. 2]. Since the transformation is independent of time, the Schrödinger equation can be solved (numerically, if desired) in the new basis. That is, for any quantum system containing a band of levels that do not interact among themselves, one can approximate uniformly the band shape to any desired degree of accuracy; furthermore, in the approximate system there is a similarity transformation that is independent of time for which the continuous band is converted into a ladder, of which only a finite number of the lowest levels are coupled to levels not in the ladder.

This result is a generalization of that for the $N = 1$, $M = 1$ case presented in Ref. 4. It is also a special case of an even more general result that we will present in a future publication.

As an example, consider the case of two-channel excitation of the Tchebychev continuum

$$\mu(\Delta)^2 = \frac{2}{\pi\sigma}\left[1 - \left(\frac{\Delta - s}{\sigma}\right)^2\right]^{1/2},$$

where s is the detuning of the center of the band and σ is the half-width; i.e., $\Delta_{min} = s - \sigma$ and $\Delta_{max} = s + \sigma$. Chebychev's name is attached to this shape since the orthogonal polynomials formed are Chebychev polynomials of the second kind. Aside from the fact that, intuitively, this shape does not seem unreasonable, our reason for choosing it is that the elements of the tridiagonal Hamiltonian are extremely simple.[14] Recall also that the choice of $\mu(\Delta)$ is arbitrary [if we are willing to accept the penalty of an increase in M for a poor choice of $\mu(\Delta)$]. Thus, regardless of our motives for choosing this overall band shape, we are entitled to do so whatever the actual shape of the band. In Eqs. (4b) and (4c) we get

$$1/e_n = \sigma/2$$

and

$$-d_n/e_n = s.$$

For a numerical example, we set $\sigma = 0.3\ \text{cm}^{-1}$, $s = \Delta_1 = \Delta_2 = \mu_{jk} = 0$, and $p_{10} = p_{11} = p_{20} = 1/\sqrt{2}$, $p_{21} = -1/\sqrt{2}$ (see Fig. 3). This represents two discrete levels that cannot interact with each other, one seeing the band as a modified Chebychev shape bunching up near Δ_{max} and the other seeing the band bunching up near Δ_{min}. We initially put all the population in the ground state. The field is initially at zero but ramps linearly to $0.05\ \text{cm}^{-1}$ at $t = 1/30$ nsec, remaining constant until $t = 1$ nsec and then suddenly going to zero again. In the conventional continuum basis there are uncountably infinitely many coupled differential equations. Therefore we work in the ladderlike basis of Fig. 2. Even here there are

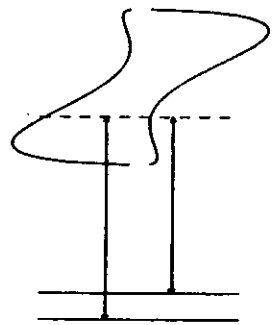

Fig. 3. A system in which a band of overall Chebychev shape is excited through two channels. The single continuous band is depicted twice to emphasize that the two discrete states see a different band shape.

(countably) infinitely many levels. For the purpose of the example, we truncate the system and retain only the lowest 100 levels in the ladder. Thus, in practice, there are two approximations made; Eq. (1) approximates the band shape (allowing introduction of a discrete basis), whereas the truncation makes the number of levels finite. The Schrödinger equation is integrated from $t = 0$. The results are shown in Fig. 4, in which population is plotted against level number; the ground state is on the extreme left-hand side of the graphs, and the topmost level retained in the ladder is on the extreme right-hand side. We see an apparent pulse of population that forms near the discrete states and moves at a constant velocity up the ladder. When the pulse reaches the point at which we have truncated the ladder, however, it reflects (with a great deal of interference) and moves back toward the discrete states. Subsequent activity is shown in Fig. 5, which explores what happens when our approximation of the truncation of the band becomes important. When the reflected pulse reaches the discrete states, the field has been turned off, and there is no interaction, so the pulse is reflected again. In fact, it continues to be reflected for a (relatively) long time. If we had retained, say, only 50 levels in our ladder, Fig. 4 would be identical (to the eye) with our Fig. 4 until about $t = 900$ psec, at which time the pulse would reach the top of the ladder and begin to reflect. Basically, there is so little population in the highest levels (until the pulse reaches that area) that the number of levels retained in the truncated system is of no consequence almost until reflection begins. If this wavelike behavior could be counted on (we will show below that it can be, at least for the Chebychev band shape), and if we know the speed of the pulses (which turns out to be σ), then we could easily determine the number of levels that must be kept in the ladder. If accurate probability amplitudes are desired for all levels, then the number of levels kept must be larger than the pulse speed multiplied by the time interval of interest. At the end of this time, however, the pulse reflects, and the truncation of the ladder becomes important. If, on the other hand,

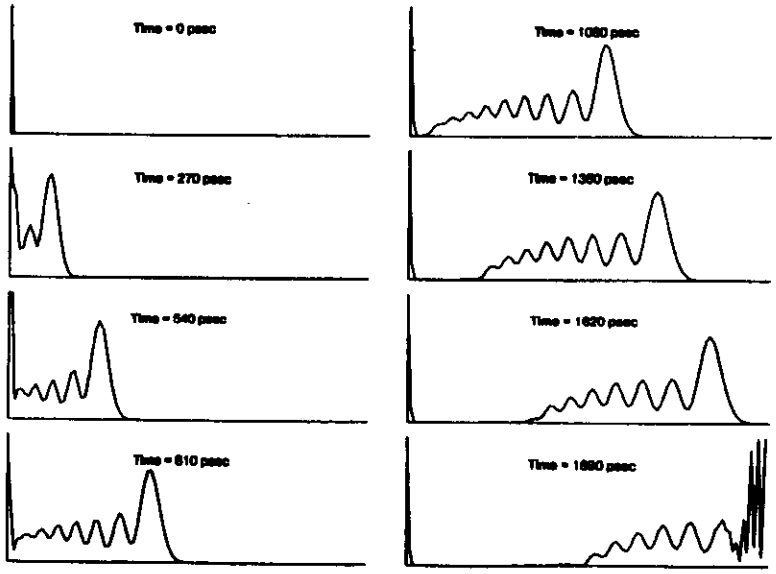

Fig. 4. Population versus level in the system of Fig. 3 in the ladder basis. The extreme left-hand level is the ground state, and the extreme right-hand level is the highest level kept in the ladder. The vertical scale runs from population = 0 to population = 1/15. (Any higher populations are truncated.) Apparently, a pulse of probability moves up the ladder. In the final frame ($t = 1890$ psec), the interference pattern caused by the beginning reflection of the pulse is seen.

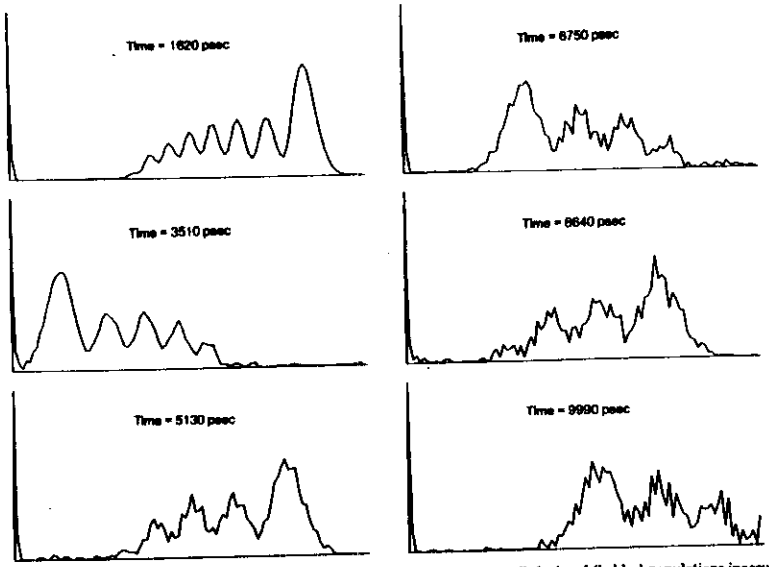

Fig. 5. Continuation of Fig. 4 for long times in which the truncation of the ladder makes all the band (ladder) populations inaccurate. The probability pulse continues to bounce around in the ladder, with one reflection occurring between successive frames.

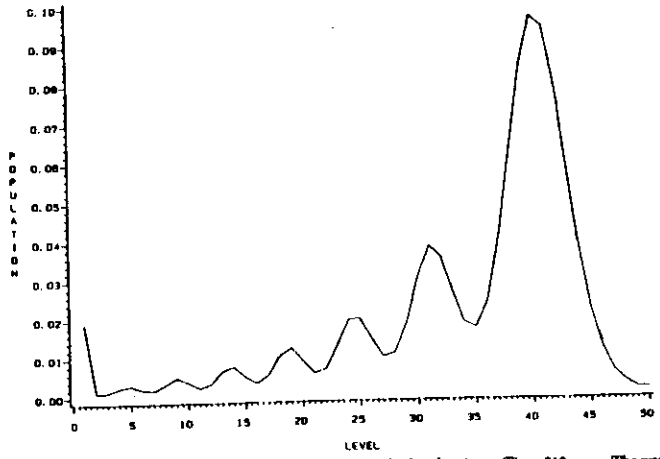

Fig. 6. Population versus level in a ladder basis, $N = 1$, $M = 1$ uniform rectangular band system. Time, 810 psec. The wave packet is moving to the right and has not yet reflected for the first time. HWHM of the band in the conventional continuum basis is 0.3 cm^{-1}; the band center is at resonance; $\mu E(t)/2\hbar$ ramps linearly from zero to 0.05 cm^{-1} at $t = 1/30$ nsec, remaining constant thereafter.

we are interested in maintaining only the accuracy of the amplitudes of the discrete states (or of the complex polarization,[4,13] which is almost the same thing), the requirements are less stringent. In this case, twice the number of retained levels must be less than the pulse speed multiplied by the length of time that the field remains on.

Although the Chebychev band shape was chosen for the simplicity of its tridiagonal detuning matrix, the effects seen above are not limited to the Chebychev band, as may be expected from the arbitrariness of $\mu(\Delta)$. For example, in Fig. 6 we see similar pulse propagation in the case of a uniform rectangular band with $N = 1$, $M = 1$. Nonetheless, the reason for this wavelike behavior is certainly easier to understand in the Chebychev case than in any other. Eberly *et al.*[13] discovered these effects in a closely related system (a finite ladder with constant field) but concluded that a wave analogy was not entirely appropriate. For the Chebychev band, however, the wave analogy is instructive.

Consider an infinite Chebychev medium in which the quantities a_n ($n = 0, \pm 1, \pm 2, \ldots$), which can be viewed as probability amplitudes, obey the equation

$$da_n/dt = i[(\sigma/2)a_{n-1} + \varepsilon a_n + (\sigma/2)a_{n+1}],$$

which is recognizably the Schrödinger equation for those levels in the Chebychev ladder that are not directly coupled to any discrete states. As a trial solution, use

$$a_n(t) = \exp[i(\omega t - kn)],$$

which gives us the dispersion relation

$$\omega = \varepsilon + \sigma \cos k, \tag{7}$$

from which follows an expression for the group velocity of wave packets[15,16]:

$$v_g = \partial\omega/\partial k = -\sigma \sin k.$$

Slowly spreading wave packets will, of course, have the maximum or minimum values, namely, $v_g = \pm\sigma$. Except for unimportant phase factors [which can be removed by an appropriate transformation of $a_n(t)$], Eq. (7) is the dispersion relation of a classical, transversely vibrating, massless string mounted with massive beads. Another equivalent classical problem is that of longitudinally vibrating masses connected by springs. Thus it is no surprise that wave packets apparently move up and down the ladder at constant velocity. There is one difference from the two classical cases just mentioned in that the Schrödinger equation is a first-order differential equation, whereas wave equations are of second order. This means that, for a given k, there is no sign ambiguity in the group velocity. This is of little consequence unless the ladder system is truncated (the ends of the Chebychev medium are tied down), causing eventual reflections. However, it can be shown that the reflected wave is conjugated, thus reversing k and the group velocity. In fact, it can be shown that the wave packets are distorted not by reflection but only by spreading. Thus, even if the electric field $E(t)$ is turned off, Chebychev wave packets can continue bouncing back and forth for a long time. Pulse spreading is exhibited in Fig. 5. The apparent cumulative degradation of the pulse is not due to the reflection of the pulse; rather, it is due to increasing interference with portions of the pulse that have spread but have not yet reflected. The motion need not represent any actual displacement of population in the band as seen in the conventional continuum basis; rather it represents an oscillation in the relative dephasing of the probability amplitudes in that basis. When the Chebychev pulse is near the top of the Chebychev ladder, the amplitudes are all dephased, and hence no process can extract population from the band; whether the field is on at this point is irrelevant. On the other hand, when the pulse is near the bottom of the ladder, the probability amplitudes of the band states in the original basis are nearly in phase, and hence the band can interact with the discrete states (if the field is turned on). Of course, if the field is turned off the populations in the band are always constant in the conventional continuum basis, regardless of changes in phase. The behavior of Chebychev-like waves could be considered to be the origin of recurrences in quantum systems.

Finally, we should make a remark about the choice of $\mu(\Delta)$ in practice. First, it is desirable to choose $\mu(\Delta)$ so as to minimize M (thus simplifying interaction of the discrete states with the band). Second, it is desirable to choose $\mu(\Delta)$ so as to exhibit Chebychev waves (thus simplifying application of our qualitative knowledge). In fact, these considerations are not mutually exclusive. The most convenient overall band shape in practice is the weight function for Chebychev polynomials of the *first* kind. For this shape, only the first recursion coefficients ($n = 0$) in Eq. (3) differ from those discussed above, so Chebychev waves propagate just as before. On the other hand, it is well known that in expansion of function in terms of polynomials, use of Chebychev polynomials of the first kind generally produces the fastest convergence. That is, in general, this choice of $\mu(\Delta)$ minimizes M.

3. SUMMARY

We have discussed multichannel excitation of the quasi-continuum disguised as its inverse problem: multichannel excitation of a discretized form of a continuum. The system that we have considered has several discrete levels that may interact with one another semiclassically by means of a dipole interaction or with a separate continuous band of levels. We say that this is a disguise of the problem because most of the results that we have obtained hold equally well if the band is discrete. Treatments of similar problems sometimes insist that the electric-field envelope be constant or at least change slowly, but we have allowed the field to vary without restrictions on the rate of change or on the size of the field. Furthermore, we have taken into account the exact shape of the band and have even allowed the various discrete levels to perceive the band as being of different shapes.

Our general result is that there is a similarity transformation independent of the electric field (i.e., of time) that simplifies the Hamiltonian (and hence numerical solution of the Schrödinger equation) drastically. In this basis, the Hamiltonian is mostly tridiagonal, except for a finite number of matrix elements proportional to the electric field. Thus the continuous band turns into an (infinite) discrete ladder with only a few of the lowest-lying levels coupled to the original discrete levels by means of a dipole transition. Transitions within the ladder, however, are independent of the field.

We find that pulses of probability are injected into the ladder from the original discrete states. These pulses move up the ladder forever in the case of a real continuum, but if only a finite number of levels are retained (because of the necessity of performing computer calculations), the pulses eventually reflect and move down the ladder again. This reflection could be viewed as the origin of both error in discretization of continua and of recurrences in quantum systems. In the case of an overall Chebychev band shape, we proved that these pulses of population travel up and down the ladder at constant speed and experience distortion because

of spreading but not because of reflections. The medium (i.e., the ladder) through which the wave packets move has the same dispersion relation as the classical, vibrating massless string on which are mounted massive beads. However, choice of the overall band shape is, to a large degree, arbitrary, so this effect is present in all systems with finite-width continuous bands.

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