IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Generalisation of the Landau-Zener calculation to three levels

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1986 J. Phys. A: Math. Gen. 19 1151

(http://iopscience.iop.org/0305-4470/19/7/017)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 31/05/2010 at 10:57

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. 19 (1986) 1151-1161. Printed in Great Britain

Generalisation of the Landau–Zener calculation to three levels

C E Carroll and F T Hioe

Department of Physics, St John Fisher College, Rochester, New York 14618, USA

Received 8 August 1985

Abstract. The Landau-Zener calculation, for avoided crossing of two energy levels, is generalised by putting in a third level, so that three levels approach one another. A three-level model of an atom, with two transitions driven by laser beams, can be transformed into our model by using the rotating-wave approximation. The resulting transition probabilities have a simple analytic form, like those of the original two-level model.

1. Introduction

Exact solutions of the time-dependent Schrödinger equation are useful in studying the dynamics of quantum systems. Landau (1932) and Zener (1932) found such a solution for the dynamical model corresponding to avoided crossing of two energy levels. The calculated transition probabilities have been applied in theories of atomic (Geltman 1969) and nuclear (Abe and Park 1983) collisions, and an application to quantum optics is outlined below. A generalisation of this calculation to treat avoided crossing of three or more energy levels would be useful. A simple three-level model is formulated and solved in this paper.

The Landau-Zener model includes only two quantum states. They are widely separated in energy at large negative and large positive times. The avoided crossing at times near zero gives a transition from one quantum state to the other, with probability given by a simple formula. Rubbmark *et al* (1981) have verified this calculation by measuring the probability of transition between two Rydberg states in lithium. Our simple and symmetric three-level model similarly gives simple formulae for transition probabilities, which might possibly be confirmed by experiments with laser-driven atomic transitions.

The models with two or three energy levels are specified precisely by writing the time-dependent Schrödinger equation for a two- or three-component wavefunction. The Hamiltonian appears as a 2×2 or 3×3 Hermitian matrix. The diagonal matrix elements are proportional to t, the time. Off-diagonal matrix elements are independent of t; they prevent crossing of eigenvalues of the Hamiltonian matrix, which are called energy levels. These time-dependent energy levels are shown in figure 1. The Schrödinger equations for the two- and three-level models are

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}a\\b\end{pmatrix}=\begin{pmatrix}rt & -\frac{1}{2}\Omega\\ -\frac{1}{2}\Omega^* & -rt\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} \tag{1}$$

and

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}a\\b\\c\end{pmatrix}=\begin{pmatrix}rt & -8^{-1/2}\Omega & 0\\ -8^{-1/2}\Omega^* & 0 & -8^{-1/2}\Omega\\ 0 & -8^{-1/2}\Omega^* & -rt\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix}. \tag{2}$$

Here, $\hbar=1$ and a, b, c are components of the wavefunctions; the components are

0305-4470/86/071151+11$02.50 © 1986 The Institute of Physics

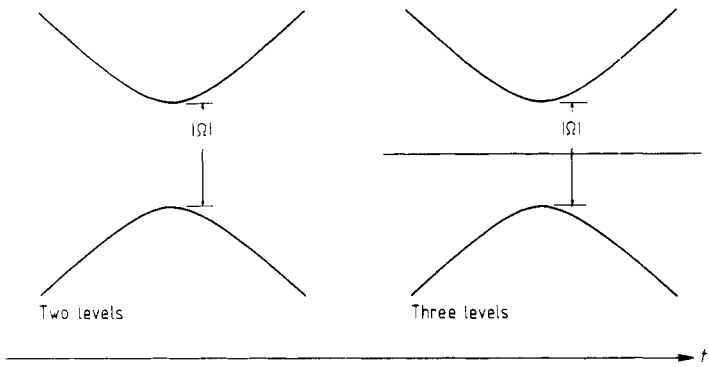

Figure 1. Eigenvalues of Hamiltonian matrix as functions of time. The minimum gap between two eigenvalues is $|\Omega|$ or $\frac{1}{2}|\Omega|$.

complex functions of t. The rate of sweeping through the avoided crossing is r, and $\pm r$ are the slopes of the asymptotes of the hyperbolae in figure 1. The off-diagonal elements of the Hamiltonian matrix in (1) and (2) are proportional to a parameter Ω, which may be complex. The coefficients of Ω in (1) and (2) are chosen so that $|\Omega|$ is the minimum separation between top and bottom energy levels in figure 1.

Although any 2×2 Hamiltonian matrix that is Hermitian and linear in t can be transformed into the form appearing in (1), there are many three-level generalisations to choose from. The Hamiltonian appearing in (2) is a simple generalisation of the time-independent Hamiltonian studied by Cook and Shore (1979). Solutions of (2) can be obtained by the method of Majorana (1932), but not for arbitrary initial conditions, nor for the initial conditions we shall use. On the other hand, a different generalisation of the Landau-Zener model has a 3×3 Hamiltonian matrix with one diagonal element proportional to t, the other eight matrix elements being constant. For such a Hamiltonian, the Schrödinger equation can be solved by the method of Demkov (1966). See Nikitin (1970) for applications of this three-level model to atomic collisions.

Solution of (1) or (2) must give transition probabilities that depend on $|\Omega|^2/r$, a dimensionless combination of the parameters appearing in (1) and (2). If $|r|$ is large, the atomic or molecular system can scarcely respond to the rapidly changing Hamiltonian, and occupation probabilities of the two or three quantum states are always close to their initial values. The transition probabilities can be increased by decreasing $|r|$, with fixed $|\Omega|$, or increasing $|\Omega|$, with fixed $|r|$. The adiabatic-following approximation (Messiah 1960, Abragam 1961) is applicable if $|\Omega|$ is large and $|r|$ is small, because no degeneracy of energy levels appears at any time; see figure 1.

In our treatment of (1) and (2), we shall ignore the trivial case of $r=0$, and number the rows and columns of the Hamiltonian matrix so that $r>0$. The dimensionless parameter is then defined by

$$s=\Omega/4r^{1/2}. \tag{3}$$

We shall derive the transition probabilities given in the last column of table 1. Their behaviour at small and large values of $|s|$ agrees with the above assertions. The probabilities of transition from one energy level to another, and of no transition, turn out to be quadratic polynomials in $\exp(-2\pi|s|^2)$. These results are remarkably simple, but we can derive them only by lengthy analysis.

Equation (2) describes a simple and symmetrical three-level model that can be related to an experiment in which two transitions in an atom are driven by two laser beams. This relation is shown in § 2. A brief description of our calculation is given in § 3 and the results are discussed in § 4. The method of solving (2) is fully described in the appendix.

2. Application to quantum optics

In this section, we describe two simple optical experiments, and sketch the approximations that lead to (1) or (2), respectively.

Suppose that transitions between atomic energy levels are driven by the optical-frequency electric fields of one or two lasers. The optical-frequency electric fields are described classically, and the effect of the atom on the applied fields is ignored. The atomic energy levels that are used are numbered from 1 to 2, or from 1 to 3; their energies appear as diagonal elements in the Hamiltonian matrix, as first written. Transitions between atomic levels with consecutive numbers are driven by the applied fields, which oscillate with constant amplitude. The Rabi frequency for each transition is defined as $2dE$, where d is the transition dipole moment and E is the amplitude of the oscillating electric field (Allen and Eberly 1975); we set $\hbar = 1$. The off-diagonal elements of the Hamiltonian matrix, as first written, oscillate at optical frequencies, and each is proportional to the corresponding Rabi frequency. Since dipole transitions between levels 1 and 3 are forbidden by Laporte's rule, zeros appear in two corners of the matrix in (2). Although the applied oscillating fields are described classically, they are supposed so weak that each drives only one transition, and only when its frequency is near resonance. We shall ignore the counter-rotating components of the oscillating electric fields; they are absent if circularly polarised light propagating along a magnetic field is used. This rotating-wave approximation (Allen and Eberly 1975) permits application of a unitary transformation that removes all optical-frequency oscillations from the Hamiltonian and wavefunction (see Einwohner *et al* 1976). The unitary matrix used in this transformation is diagonal and time dependent; hence, the numbering of the atomic levels is unaffected by this transformation. An important effect of the transformation is to reduce each off-diagonal element of the Hamiltonian matrix to a constant. This gives us the off-diagonal elements that appear in (1) and (2). In (1), Ω is the Rabi frequency but, in (2), both Rabi frequencies are equal to $2^{-1/2}\Omega$.

The effect of this transformation on the diagonal elements of the original Hamiltonian matrix is to replace each of them by a relatively small frequency difference, proportional to the detuning or equal to a linear combination of the two detunings. Each detuning is equal to the difference between the atomic resonance frequency and the frequency of the applied oscillating field that drives the transition. One of our simplifying assumptions is that each detuning is proportional to t, the time. A consequence of this is that the applied oscillating fields have a negligible effect on the atom when $|t|$ is sufficiently large; this can be seen from the usual models for dispersion or from the exact solutions of (1) and (2). Hence, our mathematical model need not describe turning on the lasers at an early time and turning them off at a late time.

The detunings that are proportional to t need not be produced by varying the frequencies of the laser beams. Stark or Zeeman shifts that are linear in t can be produced by appropriate external fields. Time-dependent Stark shifts were used to vary the detunings in an interesting experiment by Hulet and Kleppner (1983).

In the three-level model, any one of the three levels may be the ground level. The two atomic transitions are driven by two oscillating electric fields, and we assume that the frequencies of the applied oscillating fields both pass through resonance at $t=0$. The two energy-level differences may have different signs; their absolute values are equal to the resonant frequencies. If the two resonant frequencies are equal, the two oscillating applied fields may be derived from one laser.

We should also mention that the unitary transformation formulated by Einwohner *et al* (1976) can be arranged to yield a vanishing trace in the resulting Hamiltonian matrix. This possibility has been used to write (1) and (2) in the forms given.

This section has related the Schrödinger equations (1) and (2) to possible experiments in which atomic transitions are driven by laser beams. The rotating-wave approximation was used to simplify the time-dependent Hamiltonian matrix, and Laporte's rule was used to argue that zeros appear in two corners of the matrix in (2).

3. Solution of Schrödinger equation

Equation (1) can be solved by using confluent hypergeometric functions; different forms of the solution are given by Zener (1932) and Wannier (1965). Both papers cite Whittaker and Watson (1927), where many properties of confluent hypergeometric functions are stated and derived. Equation (2) can be solved by generalising the confluent hypergeometric functions. The required properties of the new functions must be derived; this is done in the appendix.

A simple preliminary step toward solution is to write (1) and (2) in dimensionless form. The dimensionless parameter s is defined by (3) and the dimensionless time variable is

$$\tau=(r/2)^{1/2}t.$$

Recall that $r>0$. We now want to solve

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix}a\\b\end{pmatrix}=\begin{pmatrix}2\tau & -8^{1/2}s\\ -8^{1/2}s^* & -2\tau\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} \tag{4}$$

and

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix}a\\b\\c\end{pmatrix}=\begin{pmatrix}2\tau & -2s & 0\\ -2s^* & 0 & -2s\\ 0 & -2s^* & -2\tau\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix}. \tag{5}$$

We can find integral representations of the solutions of these two equations; we integrate around a loop in the complex plane. The integral representations given in the appendix serve as a basis for writing the general solution of (4) or (5). We shall assume that one of the quantum states is occupied, with unit probability, in the limit as $\tau\to-\infty$, and calculate the resulting occupation probabilities in the limit $\tau\to+\infty$. These final occupation probabilities are diagonal elements of the density matrix; they are given in the last column of table 1 and plotted in figures 2 and 3.

Our analytic solutions of (5) are vector functions of τ; each vector has three complex components. These vectors have jump discontinuities at $\tau=0$. These discontinuities must be removed; the necessary calculations lengthen our appendix. As a by-product of these calculations, we find explicit formulae for the wavefunctions at

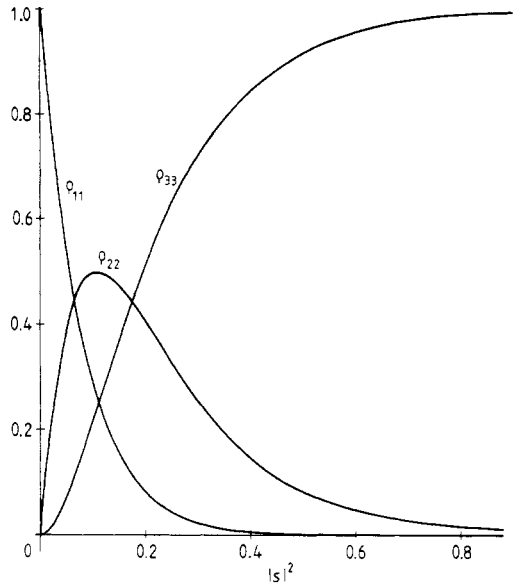

Figure 2. Occupation probabilities at large positive times, $\tau \to +\infty$. The initial condition is that level 1 is certainly occupied at large negative times.

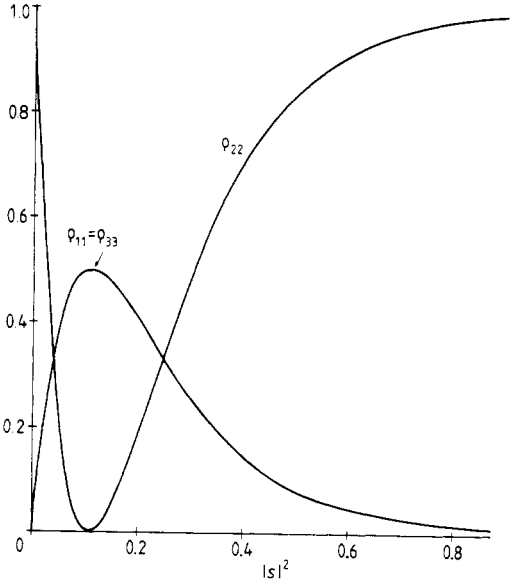

Figure 3. Occupation probabilities at large positive times, $\tau \to +\infty$. The initial condition is that level 2 is certainly occupied at large negative times.

$\tau = 0$. The resulting occupation probabilities at $\tau = 0$ are given in the second column of table 1.

We must emphasise that alternative methods of solution can be applied to (1) or (4), but not to (2) or (5). The method of Demkov (1966) gives integral representations of solutions of the Schrödinger equation, but it is not applicable to (5). The method of Majorana (1932) gives solutions of (5), but not solutions that satisfy the initial conditions we use.

Table 1. Changes of occupation probabilities, from large negative times to $t=0$ to large positive times. The initial conditions appear in the first column.

Limit of occupation probabilities as $t\to-\infty$	Occupation probabilities at $t=0$	Limits of occupation probabilities as $t\to+\infty$
1	$\frac{1}{2}[1+\exp(-2\pi\|s\|^2)]$	$\exp(-4\pi\|s\|^2)$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$1-\exp(-4\pi\|s\|^2)$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$1-\exp(-4\pi\|s\|^2)$
1	$\frac{1}{2}[1+\exp(-2\pi\|s\|^2)]$	$\exp(-4\pi\|s\|^2)$
1	$\frac{1}{4}[1+\exp(-\pi\|s\|^2)]^2$	$\exp(-4\pi\|s\|^2)$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$2[1-\exp(-2\pi\|s\|^2)]\exp(-2\pi\|s\|^2)$
0	$\frac{1}{4}[1-\exp(-\pi\|s\|^2)]^2$	$[1-\exp(-2\pi\|s\|^2)]^2$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$2[1-\exp(-2\pi\|s\|^2)]\exp(-2\pi\|s\|^2)$
1	$\exp(-2\pi\|s\|^2)$	$[1-2\exp(-2\pi\|s\|^2)]^2$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$2[1-\exp(-2\pi\|s\|^2)]\exp(-2\pi\|s\|^2)$
0	$\frac{1}{4}[1-\exp(-\pi\|s\|^2)]^2$	$[1-\exp(-2\pi\|s\|^2)]^2$
0	$\frac{1}{2}[1-\exp(-2\pi\|s\|^2)]$	$2[1-\exp(-2\pi\|s\|^2)]\exp(-2\pi\|s\|^2)$
1	$\frac{1}{4}[1+\exp(-\pi\|s\|^2)]^2$	$\exp(-4\pi\|s\|^2)$

4. Discussion

The final occupation probabilities shown in figures 2 and 3 have simple limits as $|s|\to 0$ and $|s|\to\infty$, which are given by the sudden approximation and the adiabatic-following approximation, respectively. The time-dependent eigenvalues of the Hamiltonian matrix and their minimum differences are shown in figure 1. The rate of change of the Hamiltonian has the dimensions of the square of a frequency or the square of an energy, and it should be compared with the square of an eigenvalue difference. The ratio is roughly $1/|s|^2$; the precise value depends on τ and on the choice of eigenvalue difference. If $|s|^2$ is small, the change of the Hamiltonian is rapid compared to the square of the eigenvalue difference, and the occupation probabilities are always close to their initial values; see table 1.

If $|s|^2$ is large, the occupation probabilities at any time are nearly those found from the adiabatic-following approximation. For adiabatic following, see the early experimental work of Phipps and Stern (1931) and later experiments by Bloch *et al* (1946) and Grischkowsky (1970). A physical interpretation is given by Abragam (1961) and a geometrical interpretation by Powles (1958). In order to state the adiabatic-following approximation in a precise form, and generalise it to the N-level problem, the approximate density matrix has recently been written as a polynomial in the Hamiltonian matrix (Hioe 1983). Our three-component wavefunctions, for $\tau=0$ and $|s|\to\infty$, give density matrices that agree with the three-level calculation by Hioe (1983). If Ω and s are real, the adiabatic-following limit, or $s^2\to\infty$ limit, of the density matrix is real and symmetric. The imaginary antisymmetric part of the density matrix falls off as $1/s^2$ when s^2 is large. However, in table 1, deviations from the adiabatic-following limit decrease exponentially as $s^2\to\infty$. We discuss the different behaviours of these deviations from the adiabatic-following limit in another paper (Carroll and Hioe 1986).

The final occupation probabilities, shown in figures 2 and 3, exhibit large changes as $|s|$ is increased from 0 to ∞. If level 1 is occupied with unit probability at large negative times, we can obtain final occupation probabilities of (0.25, 0.50, 0.25) for the three levels. $|s|^2 = (\ln 2)/(2\pi) \simeq 0.1103$ is the condition for this. The symmetric initial condition is that level 2 is occupied with unit probability at large negative times. This initial condition and the symmetry of our model imply that the occupation probability is transferred equally to the other two levels. If $|s|^2$ is large, figure 3 or the adiabatic-following calculation shows that the occupation probability is finally transferred back to level 2. But in the case of $|s|^2 = (\ln 2)/(2\pi) \simeq 0.1103$, the occupation probability of level 2 approaches zero at large positive times.

A simpler calculation of the three final occupation probabilities could be based on a two-level approximation, in which only two levels at a time are involved in an avoided crossing, while the other level is far away. Such a calculation can give any set of final occupation probabilities that add up to unity. But the symmetry of our three-level model demands that the two avoided crossings be similar, so that they give the same transition probabilities. Such a simplified calculation cannot give the specific results that we find for $|s|^2 = (\ln 2)/(2\pi)$. In any event, this two-level approximation is not applicable to our model, in which the three levels are closest together at $t = 0$.

5. Conclusion

The two-level dynamical model of Landau and Zener has been generalised to give a symmetrical three-level model. The wavefunctions for the new model, and the resulting transition probabilities, are analytically similar to those of the Landau-Zener model. This is to say that the transition probabilities are given by remarkably simple formulae. Our work could be used to predict transition probabilities in an optical experiment.

Acknowledgment

This work was partially supported by the US Department of Energy, Division of Chemical Sciences, under grant number DE-FG02-84 ER 13243.

Note added in proof. Some closely related calculations have recently appeared in *Journal of the Optical Society of America.*

Appendix

The general solution of the Schrödinger equation, (4) or (5), is derived in this appendix. Also, particular solutions are found and used to construct table 1.

Solutions of (4) and (5) can be written in terms of path integrals. In the vector V, each component is a complex function of τ, and is proportional to an integral along a certain path in the complex plane. A different path of integration can give a different solution; this allows us to find a complete set of orthonormal vectors V. Each basis vector V satisfies (4) or (5) when $\tau \neq 0$, but one component of each vector is discontinuous at $\tau = 0$. The general solution of the Schrödinger equation is continuous, of course; it is equal to a linear combination of the vectors V when $\tau < 0$, and equal tc a different linear combination when $\tau > 0$. We are obliged to find the unitary transformation that connects the basis vectors used for $\tau > 0$ with those used for $\tau < 0$.

For the two-level model, the general solution can be obtained in several other ways, some of which use the known properties of various confluent hypergeometric functions

(Whittaker and Watson 1927). Wannier (1965) gives a remarkably brief calculation, using large complex values of τ to get from the negative real τ axis to the positive real τ axis. We are not able to do a similar calculation for the three-level case, and τ is real throughout the following calculations.

Solutions of (4) and (5) can have the forms

$$\begin{pmatrix} \dfrac{is\exp(\frac{1}{2}\pi|s|^2)}{[2\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int (z+i)^{-1+i|s|^2}(z-i)^{-\frac{1}{2}-i|s|^2}\exp(z\tau^2)\,dz \\ \dfrac{\tau\exp(\frac{1}{2}\pi|s|^2)}{2[\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int (z+i)^{i|s|^2}(z-i)^{-\frac{1}{2}-i|s|^2}\exp(z\tau^2)\,dz \end{pmatrix} \tag{A1}$$

and

$$\begin{pmatrix} \dfrac{is\exp(\frac{1}{2}\pi|s|^2)}{2[\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int z^{-1/2}(z+i)^{-1+i|s|^2}(z-i)^{-i|s|^2}\exp(z\tau^2)\,dz \\ \dfrac{\tau\exp(\frac{1}{2}\pi|s|^2)}{2[\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int z^{-1/2}(z+i)^{i|s|^2}(z-i)^{-i|s|^2}\exp(z\tau^2)\,dz \\ \dfrac{is^*\exp(\frac{1}{2}\pi|s|^2)}{2[\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int z^{-1/2}(z+i)^{i|s|^2}(z-i)^{-1-i|s|^2}\exp(z\tau^2)\,dz \end{pmatrix} \tag{A2}$$

respectively. We have multiplied each of these vectors by a convenient scalar function of $|s|^2$; it will turn out to be a normalisation factor. To define the integrands precisely, we draw branch lines on or parallel to the negative real z axis; they run to the left from $\pm i$, or from 0 and $\pm i$. The same path of integration is used in all components of each vector V. Partial integration is used to show that (4) and (5) are satisfied; to make the integrated parts vanish, we assume that the path of integration does not cross a branch line, and that both ends are far to the left in the z plane, where $|\exp(z\tau^2)|$ is negligible. If $\tau \neq 0$, the integrals obviously converge, and the Schrödinger equation is satisfied exactly. Since a basis function that vanishes identically is of no use, the path of integration must enclose at least one branch point and the branch line drawn from it. We use a path of integration that encloses only one branch line and goes around the branch point in the usual counterclockwise direction.

We recognise that the integrals in (A1) have the same form as the path integral used to define the Whittaker function (Whittaker 1903). The integrals in (A2) are slightly more general. In either case, the precise form of the integrands could be found by Laplace's method.

We could define V_1, V_2 and V_3 by using (A2) and paths of integration that enclose $z=-i$, $z=0$ and $z=+i$, respectively. But a small modification of this definition is necessary; V_2 is defined by using a normalisation factor of $\exp(\pi|s|^2)$, in place of the $\exp(\frac{1}{2}\pi|s|^2)/[\sinh(\pi|s|^2)]^{1/2}$ that appears in each component of (A2). In the two-level case, we define V_1 by using (A1) and a path of integration that encloses $z=-i$; and we define V_2 by using

$$\begin{pmatrix} \dfrac{\tau\exp(\frac{1}{2}\pi|s|^2)}{2[\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int (z+i)^{-1/2+i|s|^2}(z-i)^{-i|s|^2}\exp(z\tau^2)\,dz \\ \dfrac{is^*\exp(\frac{1}{2}\pi|s|^2)}{[2\pi\sinh(\pi|s|^2)]^{1/2}}\displaystyle\int (z+i)^{-1/2+i|s|^2}(z-i)^{-1-i|s|^2}\exp(z\tau^2)\,dz \end{pmatrix}$$

and a path of integration that encloses $z=+i$.

We now find the asymptotic forms of these vectors as $\tau \to \pm\infty$, and use these forms to show that these vectors are normalised and orthogonal. The normalisation integral becomes, in this paper, a sum of the absolute squares of the two or three components. Similarly, the overlap integral becomes a sum of products; it involves one vector and the complex conjugate of another. Letting $\tau \to \pm\infty$, we find

$$V_1 \sim \begin{pmatrix} \exp(-i\tau^2 - i|s|^2 \ln(2\tau^2) + i \arg(s) + i \arg \Gamma(i|s|^2) - \frac{1}{4}i\pi) \\ 0 \\ 0 \end{pmatrix},$$

$$V_2 \sim \begin{pmatrix} 0 \\ i \operatorname{sgn}(\tau) \\ 0 \end{pmatrix}$$

and

$$V_3 \sim \begin{pmatrix} 0 \\ 0 \\ \exp(i\tau^2 + i|s|^2 \ln(2\tau^2) - i \arg(s) - i \arg \Gamma(i|s|^2) + \frac{1}{4}i\pi) \end{pmatrix}.$$

Terms of order $1/|\tau|$ are not shown here; we need only the leading term of the asymptotic series. Similar asymptotic forms are found in the two-level case. These asymptotic forms show that the vectors V are properly normalised when $|\tau|$ is sufficiently large. Then the Schrödinger equation (4) or (5) can be used to show that they are properly normalised for other values of τ, except for $\tau = 0$. Similarly, we can show that two vectors with different subscripts are orthogonal, except at $\tau = 0$.

This completes the exact solution of the Schrödinger equation, except for the difficulty at $\tau = 0$ and the resulting problem of connecting positive-τ solutions with negative-τ solutions. The first step toward overcoming this difficulty is to find the limits of the vectors V as $\tau \to 0$, from above and from below. The integrals all converge when $\tau \neq 0$, because $\exp(z\tau^2)$ appears in each integrand. In the components of each vector that do not contain a factor of τ outside the integral sign, the integrands behave like $z^{-3/2}\exp(z\tau^2)$ when $|z|$ is large. This behaviour gives uniform convergence of the integral, in an interval that includes $\tau = 0$. Uniform convergence implies that all such components are continuous at $\tau = 0$; thus, we have only to evaluate the integrals at $\tau = 0$. In the component of each vector that does contain a factor of τ outside the integral sign, the integrand behaves like $z^{-1/2}\exp(z\tau^2)$ when $|z|$ is large. This implies that the integral diverges when $\tau = 0$ but it is not difficult to find the limits of such a component as $\tau \to 0^+$ and as $\tau \to 0^-$. The two limits are not equal. The limits of our basis vectors V are collected in table 2. The ambiguous signs show components that have jump discontinuities at $\tau = 0$.

In each vector V, one component becomes dominant as $\tau \to -\infty$. This is useful if the initial condition is that one of the energy levels is occupied, with unit probability, at large negative τ. The corresponding occupation probabilities at $\tau = 0$, given in the middle column of table 1, are found from the limits as $\tau \to 0^-$, given in table 2. These limits are also used to compute the density matrices at $\tau = 0$; this computation is mentioned in § 4.

The general solution of the Schrödinger equation can now be written in terms of the basis vectors V, which form a complete orthonormal set. The general solution is equal to $A_1V_1 + A_2V_2 + A_3V_3$, or a similar expression with two terms. The coefficients A_1, A_2, A_3 are constant, so long as the vectors V satisfy (4) or (5). However, the

Table 2. Limits of basis vectors as $\tau \to 0^{\pm}$.

Vector	Limits
Two-level case	
V_1	$\begin{pmatrix} s[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(-\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(i\lvert s\rvert^2)}{\Gamma(\frac{1}{2}+i\lvert s\rvert^2)} \\ \pm i[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp(-\frac{1}{2}\pi\lvert s\rvert^2) \end{pmatrix}$
V_2	$\begin{pmatrix} \pm i[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp(-\frac{1}{2}\pi\lvert s\rvert^2) \\ s^*[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(-i\lvert s\rvert^2)}{\Gamma(\frac{1}{2}-i\lvert s\rvert^2)} \end{pmatrix}$
Three-level case	
V_1	$\begin{pmatrix} \frac{s}{2}[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(-\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(\frac{1}{2}+\frac{1}{2}i\lvert s\rvert^2)} \\ \pm i[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp(-\frac{1}{2}\pi\lvert s\rvert^2) \\ \frac{s^*}{2}[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(-\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(\frac{1}{2}+\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(1+\frac{1}{2}i\lvert s\rvert^2)} \end{pmatrix}$
V_2	$\begin{pmatrix} s\cosh\left(\frac{\pi}{2}\lvert s\rvert^2\right)\exp\left(\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(\frac{1}{2}-\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(1-\frac{1}{2}i\lvert s\rvert^2)} \\ \pm i\exp(-\pi\lvert s\rvert^2) \\ s^*\cosh\left(\frac{\pi}{2}\lvert s\rvert^2\right)\exp\left(-\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(\frac{1}{2}+\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(1+\frac{1}{2}i\lvert s\rvert^2)} \end{pmatrix}$
V_3	$\begin{pmatrix} \frac{s}{2}[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(\frac{1}{2}-\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(1-\frac{1}{2}i\lvert s\rvert^2)} \\ \pm i[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp(-\frac{1}{2}\pi\lvert s\rvert^2) \\ \frac{s^*}{2}[\sinh(\pi\lvert s\rvert^2)]^{1/2}\exp\left(\frac{i\pi}{4}-\frac{\pi}{2}\lvert s\rvert^2\right)\frac{\Gamma(-\frac{1}{2}i\lvert s\rvert^2)}{\Gamma(\frac{1}{2}-\frac{1}{2}i\lvert s\rvert^2)} \end{pmatrix}$

vectors V are discontinuous at $\tau = 0$. Hence, the general solution must be written as $A_1(\pm)V_1 + A_2(\pm)V_2 + A_3(\pm)V_3$, where the ambiguous sign is the sign of τ. The general solution is continuous (and analytic) at $\tau = 0$; this condition gives linear equations to determine $A_1(+)$, $A_2(+)$, $A_3(+)$ in terms of $A_1(-)$, $A_2(-)$, $A_3(-)$, or vice versa. These linear equations can be written explicitly, using the results in table 2, and the determinant does not vanish. In the two-level case, the linear equations and their solution involve ratios of gamma functions. In the three-level case, we find

$$\begin{aligned} A_1(+) &= \exp(-2\pi|s|^2)A_1(-) - 2[\sinh(\pi|s|^2)]^{1/2}\exp(-\tfrac{3}{2}\pi|s|^2)A_2(-) \\ &\quad -2\sinh(\pi|s|^2)\exp(-\pi|s|^2)A_3(-), \\ A_2(+) &= [1-2\exp(-2\pi|s|^2)]A_2(-) - 2[\sinh(\pi|s|^2)]^{1/2} \\ &\quad \times\exp(-\tfrac{3}{2}\pi|s|^2)[A_1(-)+A_3(-)] \end{aligned} \tag{A3}$$

and

$$\begin{aligned} A_3(+) &= -2\sinh(\pi|s|^2)\exp(-\pi|s|^2)A_1(-) - 2[\sinh(\pi|s|^2)]^{1/2} \\ &\quad \times\exp(-\tfrac{3}{2}\pi|s|^2)A_2(-) + \exp(-2\pi|s|^2)A_3(-). \end{aligned}$$

The coefficients in these formulae form a unitary matrix (the S matrix), because we have made a unitary transformation from one set of basis vectors to another. It seems remarkable that the S matrix is real and symmetric.

The transformation formulae (A3) may be used to continue the general solution of (5) from negative τ to positive τ. The simplest initial condition is that one of the three levels is occupied, with unit probability, in the limit as $\tau \to -\infty$. The asymptotic forms of the vectors V simplify computations with this initial condition. For example, if level 1 is occupied with certainty at large negative times, then $|A_1(-)| = 1$, $A_2(-) = A_3(-) = 0$, and the coefficients $A_j(+)$ are determined by (A3). In any case, the probability that level j is occupied at large positive times is $|A_j(+)|^2$. Using the transformation formulae (A3), and corresponding formulae for the two-level case, we find the results shown in the last column of table 1.

References

Abe Y and Park J Y 1983 *Phys. Rev.* C **28** 2316

Abragam A 1961 *The Principles of Nuclear Magnetism* (Oxford: OUP) pp 31-6

Allen L and Eberly J H 1975 *Optical Resonance and Two Level Atoms* (New York: Wiley)

Bloch F, Hansen W W and Packard M 1946 *Phys. Rev.* **70** 474

Carroll C E and Hioe F T 1986 *Phys. Rev.* A to be published

Cook R J and Shore B W 1979 *Phys. Rev.* A **20** 539

Demkov Yu N 1966 *Dokl. Akad. Nauk SSSR* **166** 1076 (*Sov. Phys.-Dokl.* **11** 138)

Einwohner T H, Wong J and Garrison J C 1976 *Phys. Rev.* A **14** 1452

Geltman S 1969 *Topics in Atomic Collision Theory* (New York: Academic)

Grischkowsky D 1970 *Phys. Rev. Lett.* **24** 866

Hioe F T 1983 *Phys. Lett.* **99A** 150

Hulet R G and Kleppner D 1983 *Phys. Rev. Lett.* **51** 1430

Landau L 1932 *Phys. Z. Sowj.* **2** 46

Majorana E 1932 *Nuovo Cimento* **9** 43

Messiah A 1960 *Mécanique Quantique* (Paris: Dunod) pp 637-46 (Eng. transl. J Potter (Amsterdam: North-Holland))

Nikitin E E 1970 *Theory of Elementary Atomic and Molecular Processes in Gases* (Moscow: Khimiya) (Eng. transl. M J Kearsley (Oxford: OUP))

Phipps T E and Stern O 1931 *Z. Phys.* **73** 185

Powles J G 1958 *Proc. Phys. Soc.* **71** 497

Rubbmark J R, Kash M M, Littman M G and Kleppner D 1981 *Phys. Rev.* A **23** 3107

Wannier G H 1965 *Physics* **1** 251

Whittaker E T 1903 *Bull. Am. Math. Soc.* **10** 125

Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (Cambridge: CUP) ch 16

Zener C 1932 *Proc. R. Soc.* A **137** 696