A new class of analytic solutions of the two-state problem

1986 J. Phys. A: Math. Gen. 19 3579

(http://iopscience.iop.org/0305-4470/19/17/022)

J. Phys. A: Math. Gen. 19 (1986) 3579-3597. Printed in Great Britain

A new class of analytic solutions of the two-state problem

C E Carroll and F T Hioe

Department of Physics, St John Fisher College, Rochester, NY 14618, USA

Received 7 November 1985

Abstract. A new class of solutions of the time-dependent Schrödinger equation is found for the two-state problem often encountered in quantum optics, magnetic resonance and atomic collisions. We use the Riemann-Papperitz differential equation to find exact solutions in terms of hypergeometric functions. We consider only cases in which the final occupation probabilities are elementary functions of the parameters of the model.

1. Introduction

Solutions of the time-dependent Schrödinger equation are important in quantum dynamics. In the case of only two quantum states, many analytic solutions of the time-dependent Schrödinger equation have been found [1-15] and applied to various physical problems. The early work of Rosen and Zener [1] on the double Stern-Gerlach experiment [16] treats an interesting simple case by using hypergeometric functions and this calculation has been much generalised [2-6]. In this paper, the Riemann-Papperitz differential equation is used to find further solutions in terms of hypergeometric functions. These calculations can be applied to the two-state models used in quantum optics [17], magnetic resonance [18] and atomic collisions [19].

Since there are only two quantum states, the Schrödinger equation has the form

$$i\hbar\frac{d}{dt}\begin{pmatrix}A_1\\A_2\end{pmatrix}=\begin{pmatrix}H_{11} & H_{12}\\H_{21} & H_{22}\end{pmatrix}\begin{pmatrix}A_1\\A_2\end{pmatrix}\qquad(1)$$

where t is the time, A_1 and A_2 are the complex components of the wavefunction and $H_{11},\ldots,H_{22}$ are matrix elements of the Hamiltonian operator. In general, all these components and matrix elements depend on t. The occupation probabilities of the two states are the absolute squares of A_1 and A_2. Rosen and Zener [1] used a simple transformation to make diagonal elements of the Hamiltonian matrix equal to zero. This transformation does not change the relation between the two occupation probabilities and the two components of the wavefunction. After use of this transformation, the Hamiltonian matrix contains only two arbitrary functions of t; it is characterised by the magnitude and phase of one of the off-diagonal elements.

When the two-state model is applied to quantum optics or magnetic resonance, the applied oscillating electric or magnetic field is treated as a classical external field appearing in the equations of motion for the two-state atom or molecule. The three Bloch equations [20] can be used as these equations of motion. We shall ignore the damping terms in the Bloch equations and pay attention to time dependence of the external oscillating field. The undamped Bloch equations contain two arbitrary functions of t, namely the amplitude and detuning of the applied oscillating field. These undamped Bloch equations are equivalent to the Schrödinger equation for the two-state system [21]. But we must emphasise that the undamped Bloch equations have the properties here claimed for them only if we invoke the rotating-wave approximation [17, 20, 21] and make the transformation to the rotating frame of reference [18]. The errors resulting from this approximation have been studied in detail [22]; they are often negligible and they vanish if the optical two-state system is driven by circularly polarised light propagating along an external magnetic field or if the magnetic two-state system is driven by a gyrating magnetic field. In (1) or the Bloch equations, high-frequency terms are eliminated by the rotating-wave approximation and the transformation to the rotating frame. Since this approximation and transformation do not change the form of (1), we shall not consider them further.

In the simplest form of the two-state problem, the applied oscillating field has constant amplitude and constant detuning. The solution of the Schrödinger equation for this case, obtained by Rabi [15], involves only elementary functions. A simple generalisation of this solution has been published [6]. The new class of solutions obtained in this paper can be regarded as a further generalisation of the Rabi solution.

The two-state model has often been applied to avoided crossing of two energy levels in a diatomic molecule or in an atomic collision. This application, which is mentioned by Rosen and Zener [1], led Landau [7] and Zener [8] to formulate and solve a particular form of the time-dependent two-state problem. For its analytic solution by means of confluent hypergeometric functions, see Zener [8] and Wannier [9]. Related two-state problems have been treated by Nikitin [10], Demkov [11], Kaplan [12], Crothers [13] and Lee and George [14]. A generalisation of the Landau-Zener model to three states has recently been treated [23]. In this paper, we do not consider analytic solutions of this sort and do not attempt to list all the cases of the two-state problem that can be solved analytically. The following results are all obtained by the use of hypergeometric functions.

The two-state problem, in its general form, contains two arbitrary functions of t, corresponding to the arbitrary amplitude and detuning of the applied oscillating field. The solution of this general problem presumably cannot be written in explicit form. We shall find two classes of two-state models with useful solutions in terms of hypergeometric functions. The two classes of solutions correspond to the presence and absence of complex singular points in the Riemann-Papperitz differential equation. In either case, we obtain a solution containing one arbitrary function of t and two parameters that can be adjusted to vary the other function of t. When applying these two solutions to the two-state model driven by an oscillating electric or magnetic field, we may interpret the arbitrary function of t as the amplitude of the applied field and the function containing adjustable parameters as the detuning of the applied field; an alternative interpretation is mentioned below. Integration of the arbitrary amplitude over all times t gives the dimensionless area [24] of the pulse applied to the two-state system. We consider only pulses with non-negative amplitude and finite area. Furthermore, we assume that the two-state system starts out in one of its states, say the ground state, at the beginning of the experiment; we interpret this beginning as the limit as $t \to -\infty$. The final occupation probabilities of the two states are the limits of the two occupation probabilities as $t \to +\infty$. We consider only cases in which the final occupation probabilities are elementary functions of the parameters characterising the applied pulse. This restriction, and the restriction to finite area, lead to the two classes of solutions in terms of hypergeometric functions. Complex singular points in the Riemann-Papperitz equation lead to the new class of solutions. If there are no complex singular points, we are led to the old class of solutions, which is described in earlier papers that use hypergeometric functions [1-6]. Some further details about the old class of solutions are given below. Also, some special cases that belong to both classes are described below.

An alternative approach to the two-state model driven by an applied oscillating field is to assume constant detuning and use the adjustable parameters to vary the pulse shape, meaning the time dependence of the amplitude. This approach is used by Bambini and Berman [2] and we can choose our arbitrary function so that our solution agrees with theirs (see also the calculations of Bambini and Lindberg [3]). The assumption of constant detuning seems unnecessarily restrictive. We expect uses for our solutions of the two-state problem, with time-dependent amplitude and detuning, to appear in various places.

In these solutions, the pulse amplitude is an arbitrary function of t. We shall treat explicitly only functions that appear in an ordinary table of indefinite integrals. This restriction leads to quite explicit formulae for the detuning as a function of t, while giving us a great variety of time-dependent pulses.

Before presenting our results as explicit formulae, we write out the undamped Bloch equations and the corresponding Schrödinger equation in § 2. The relevant properties of hypergeometric functions are described in § 3. The two classes of solutions are specified precisely in § 4 and the final occupation probabilities are given. The solutions of the Schrödinger equation are written explicitly in appendix 2. The overlap of the two classes and the solution of Bambini and Berman are treated in § 5. In § 6, seven specific forms of the time-dependent pulse amplitude are used, making our results quite explicit.

2. Equations of motion

The Schrödinger equation (1) will be transformed into a simpler form in this section, following Rosen and Zener [1]. The simpler form will be related to the undamped Bloch equations and separated into two uncoupled second-order differential equations.

We assume that the Hamiltonian operator is Hermitian. This implies that the 2×2 matrix appearing in (1) is Hermitian, so that H_{11} and H_{22} are real functions of t. The transformation that makes the diagonal matrix elements vanish is

$$a_1 = A_1 \exp\left(\mathrm{i}\int^t H_{11}\,\mathrm{d}t\right)$$

and

$$a_2 = A_2 \exp\left(\mathrm{i}\int^t H_{22}\,\mathrm{d}t\right).$$

Here, we have set $\hbar = 1$ and introduced a_1 and a_2, the two components of the new wavefunction. The time-dependent occupation probabilities for the two states are $|a_1|^2 = |A_1|^2$ and $|a_2|^2 = |A_2|^2$. The transformed Schrödinger equation is

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2}\Omega(t)\,\mathrm{e}^{-\mathrm{i}B} \\ -\frac{1}{2}\Omega(t)\,\mathrm{e}^{\mathrm{i}B} & 0 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \tag{2}$$

where

$$\Omega(t)\,\mathrm{e}^{\mathrm{i}B} = -2H_{21}\exp\left(\mathrm{i}\int^t (H_{22}-H_{11})\,\mathrm{d}t\right)$$

and

$$\Omega(t)\,\mathrm{e}^{-\mathrm{i}B} = -2H_{12}\exp\left(-\mathrm{i}\int^{t}(H_{22}-H_{11})\,\mathrm{d}t\right).$$

We assume that $\Omega(t)$, which is proportional to the amplitude of the applied oscillating field, is a non-negative function of t. Thus, we do not consider the 0π pulse [25], which involves sudden changes in the phase of the electric field.

The time-dependent detuning is $\mathrm{d}B/\mathrm{d}t$. Both $\Omega(t)$ and $\mathrm{d}B/\mathrm{d}t$ appear in

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 & -\mathrm{d}B/\mathrm{d}t & 0 \\ \mathrm{d}B/\mathrm{d}t & 0 & \Omega(t) \\ 0 & -\Omega(t) & 0 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} \tag{3}$$

the undamped Bloch equations. Here, u, v, w are the three components of the pseudopolarisation in quantum optics or of the magnetisation in magnetic resonance. They are the components in the rotating frame [18], because we have used the rotating-wave approximation and the associated transformation. The difference between the two occupation probabilities is

$$w = |a_2|^2 - |a_1|^2 \tag{4}$$

and the other components of the pseudopolarisation or magnetisation are

$$u = a_1 a_2^* \mathrm{e}^{\mathrm{i}B} + \mathrm{cc} \qquad v = -\mathrm{i}a_1 a_2^*\,\mathrm{e}^{\mathrm{i}B} + \mathrm{cc}. \tag{5}$$

One can use these transformation formulae to verify that (2) and (3) are equivalent forms of the equation of motion.

In the application to a two-level atom driven by a laser beam, $\Omega(t)$ is the so-called Rabi frequency. It is equal to $2dE$, where d is the transition dipole moment and E is the amplitude of the optical frequency electric field; recall that $\hbar = 1$. We write

$$\Omega(t) = \mathrm{d}A/\mathrm{d}t \tag{6}$$

where A is the dimensionless pulse area [24] up to time t. The total area of the pulse is

$$\alpha = A(+\infty) - A(-\infty) = \int_{-\infty}^{\infty}\Omega(t)\,\mathrm{d}t. \tag{7}$$

If $\mathrm{d}B/\mathrm{d}t$ vanishes identically, then A is the tipping angle of the pseudopolarisation or magnetisation and one can write the solution of (3) in terms of $\sin A$ and $\cos A$. In general, a solution of (3) must take account of effects of both $\mathrm{d}A/\mathrm{d}t$ and $\mathrm{d}B/\mathrm{d}t$. The symmetry operation that interchanges $\mathrm{d}A/\mathrm{d}t$ and $\mathrm{d}B/\mathrm{d}t$ will not be used in this paper. We assume that (7), the total area, is finite; no such condition is applied to $\mathrm{d}B/\mathrm{d}t$.

A change of independent variable, which introduces an arbitrary function, will greatly increase the generality of our solutions. Let z be the new independent variable. It is real when t is real and $\mathrm{d}z/\mathrm{d}t$ is non-negative when t is real. Using (6), we rewrite (2) as

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2}(\mathrm{d}A/\mathrm{d}z)\,\mathrm{e}^{-\mathrm{i}B} \\ -\frac{1}{2}(\mathrm{d}A/\mathrm{d}z)\,\mathrm{e}^{\mathrm{i}B} & 0 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}. \tag{8}$$

We shall choose the functions $A(z)$ and $B(z)$ so that a_1 and a_2 can be written in terms of hypergeometric functions. The relation between z and t will not be specified until we come to the constant-detuning solution of Bambini and Berman and the specific examples in § 6. Elimination of a_2 and a_1 gives

$$\frac{d^2a_1}{dz^2}+\left[\frac{d}{dz}\left(iB-\ln\frac{dA}{dz}\right)\right]\frac{da_1}{dz}+\frac{1}{4}\left(\frac{dA}{dz}\right)^2 a_1=0 \tag{9a}$$

and

$$\frac{d^2a_2}{dz^2}+\left[\frac{d}{dz}\left(-iB-\ln\frac{dA}{dz}\right)\right]\frac{da_2}{dz}+\frac{1}{4}\left(\frac{dA}{dz}\right)^2 a_2=0. \tag{9b}$$

Let $(dA/dz)^2$ and dB/dz be rational functions of z. This condition and some other conditions will allow solution of (9), by methods outlined in the following section.

3. Hypergeometric functions

The Riemann–Papperitz differential equation is shown in this section. We shall use this equation, whose solutions can all be written in terms of hypergeometric functions, and some of the relations between hypergeometric functions and gamma functions. The gamma functions are needed as a step towards the expression of the final occupation probabilities as elementary functions.

The hypergeometric function, $F(a, b; c; x)$, satisfies

$$x(1-x)\,d^2F/dx^2+[c-(a+b+1)x]\,dF/dx-abF=0 \tag{10}$$

the differential equation given by Gauss [26, p 207ff]. An important contribution to the subject was published by Riemann [27] in 1857, and the relevant differential equation

$$\begin{aligned}\frac{d^2y}{dz^2}&+\left(\frac{1-\alpha-\alpha'}{z-a}+\frac{1-\beta-\beta'}{z-b}+\frac{1-\gamma-\gamma'}{z-c}\right)\frac{dy}{dz}\\&+\frac{1}{(z-a)(z-b)(z-c)}\left(\frac{\alpha\alpha'(a-b)(a-c)}{z-a}\right.\\&\left.+\frac{\beta\beta'(b-c)(b-a)}{z-b}+\frac{\gamma\gamma'(c-a)(c-b)}{z-c}\right)y=0\end{aligned} \tag{11}$$

was later written explicitly by Papperitz [28]. The three singular points of this equation are a, b and c; they must be distinct. The corresponding exponents are α, α', β, β', γ and γ'. All nine of these parameters are complex, in general, but one must have $\alpha+\alpha'+\beta+\beta'+\gamma+\gamma'=1$. The general solution of (11) can be written in terms of hypergeometric functions, but (11) suggests more uses of hypergeometric functions than (10) does.

We shall require (9a) and (9b) to have the form of (11). The numerous complex parameters in (11) will lead to three adjustable parameters in (6) and dB/dt, the amplitude and detuning functions. We assume that $(dA/dz)^2$ is a rational function. Then (9) shows that zeros of this function are singular points of the differential equations. On the other hand, study of (11) shows that $(dA/dz)^2$ cannot vanish at a singular point. Hence, $(dA/dz)^{-2}$ must be a polynomial in z. Comparison of (9) and (11) shows that it is a polynomial of degree four, unless one of the singular points is at infinity. Indeed, a, b, c need not all be finite and it is convenient to make one of them infinite. No solutions of the two-state problem are lost by doing this, because the relation between z and t is arbitrary. Assuming that one of the singular points is at infinity, $(\mathrm{d}A/\mathrm{d}z)^{-2}$ is a polynomial of degree two, three or four; its only zeros are the two finite singular points.

Since $\mathrm{d}A/\mathrm{d}t$ and z are real when t is real, $(\mathrm{d}A/\mathrm{d}z)^2$ must be real when z is real; similarly, $\mathrm{d}B/\mathrm{d}z$ is real when z is real. Either a, b, c are real constants or two of them are complex conjugates and the third is real. Although the point at infinity is both real and complex, it is nominally real in this paragraph and we shall call the two possibilities the cases of real and complex singular points. They are treated separately in the following section.

The initial condition for (2) is that one of the two states is occupied with unit probability at early times. We assume that $|a_1|\to 1$ and $a_2\to 0$ as $t\to -\infty$. We have mentioned our requirement that the final occupation probabilities be given by simple formulae. This requirement and the initial condition amount to a requirement that each hypergeometric function can be evaluated in terms of gamma functions, or set equal to unity, in the two limits $t\to \pm\infty$. The alternative possibility is that the hypergeometric functions reduce to elementary functions for all t, but this alternative is unlikely to lead to new solutions of (2).

The function $F(a, b; c; x)$ is defined by a power series, and its value at $x=0$ is unity. The Gaussian formula [26, p 147]

$$F(a, b; c; 1)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \tag{12}$$

is valid whenever the series converges at $x=1$. The other evaluations [29] of $F(a, b; c; x)$ in terms of gamma functions are valid when $x=-1$ or $\frac{1}{2}$ or $-\frac{1}{3}$ or $\ldots$, provided that a, b, c satisfy certain conditions. We consider use of these formulae in appendix 1. None of them is actually useful, given our initial conditions and our requirement that (7) is finite. Since $x=0$ and $x=1$, which are singular points of (10), correspond to two of the singular points of (11), we are saying that $z(t)$ must move from one singular point of (11) to another, or back to the same singular point, as t increases from $-\infty$ to $+\infty$.

If the two finite singular points of (9) are not real, we may use a linear transformation of the variable called z to put them at $\pm\mathrm{i}$. The form of (11) is unchanged by a linear transformation. Using the condition that (7) is finite, we are led to

$$\mathrm{d}A/\mathrm{d}z=(\text{constant})/(z^2+1).$$

If the possibility considered in appendix 1 is not used, z increases from $-\infty$ to $+\infty$ as t increases from $-\infty$ to $+\infty$.

If the two finite singular points of (9) are real, we may assume that $z(t)$ remains finite as $t\to\pm\infty$. Transformations such as $z\to az/(z-a)$ can be used to make $z(t)$ finite without altering the form of (11). Furthermore, we may use a linear transformation to put the three singular points at 0, 1 and ∞. Since the possibilities considered in appendix 1 are not usable, z must increase from 0 to 1 as t increases from $-\infty$ to $+\infty$. The condition that (7) is finite then gives

$$\mathrm{d}A/\mathrm{d}z=(\text{constant})[z(1-z)]^{-1/2}.$$

In this section, we have combined our two assumptions with properties of the hypergeometric function and started to find specific forms for $\mathrm{d}A/\mathrm{d}z$ and $\mathrm{d}B/\mathrm{d}z$, the functions that appear in (9). To justify our use of formula (12) only, more recent formulae [29] are considered in appendix 1.

4. Solution for final occupation probabilities

The requirements of finite area and of simple formulae for the final occupation probabilities imply that there are two classes of solutions of (2), (3) and (8) in terms of hypergeometric functions. The two classes correspond to real and complex singular points in (9) and (11). The amplitude and detuning functions, $\Omega(t)$ and $\mathrm{d}B/\mathrm{d}t$, and the resulting final occupation probabilities are written out in this section. Explicit solutions of (8) are given in appendix 2. The cases that belong to both classes and the constant-detuning solution of Bambini and Berman [2] will be shown in § 5.

The new class of solutions is obtained by putting the singular points of (9) and (11) at $\pm\mathrm{i}$ and ∞; $z(t)$ moves along the real axis from $-\infty$ to $+\infty$ as t increases. The old class of solutions is obtained by putting the singular points of (9) and (11) at 0, 1 and ∞; $z(t)$ moves along the real axis from 0 to 1 as t increases. As t increases from $-\infty$ to $+\infty$, $z(t)$ moves from a singular point back to the same singular point or from one singular point to another. The alternative is another way of stating the distinction between the old and new classes of solution.

The final occupation probabilities are the limits of $|a_1|^2$ and $|a_2|^2$ as $t\to+\infty$, and their difference is the limit of w, according to (4). The limits of u and v as $t\to+\infty$ fail to exist in many cases, because $B(z)$ does not approach a limit; see (5). If these limits of u and v do exist, they are given in appendix 2. Our previous papers [5, 6] did not give limits of u and v.

4.1. Complex singular points

The new class of solutions is obtained by keeping the finite singular points of (9) and (11) off the real axis. Let

$$\Omega(t)=\mathrm{d}A/\mathrm{d}t=(\alpha/\pi)(z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t) \tag{13a}$$

and

$$B(z)=(\beta/\pi)\tan^{-1}(z)+(\gamma/2\pi)\ln(z^2+1). \tag{13b}$$

Here, α satisfies (7); β and γ are the arbitrary parameters in

$$\mathrm{d}B/\mathrm{d}t=\pi^{-1}(\beta+\gamma z)(z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t) \tag{13c}$$

the detuning function. The parameters of the pulse, α, β and γ, should not be confused with the parameters of Riemann and Papperitz, nor with the parameters α and β of Bambini and Berman. The generalisation [6] of the Rabi solution [15] is obtained by setting $\gamma=0$, which kills the singularity at $z=\infty$ and allows the solution of (8) in terms of elementary functions. The other simplified case, obtained by setting $\beta=0$, is considered in § 5. In general, we find that

$$|a_1|^2\to[2\cosh(\gamma)\cos(2\pi r)\cos(2\pi s)-\cos^2(2\pi r)-\cos^2(2\pi s)]/\sinh^2(\gamma) \tag{14a}$$

and

$$|a_2|^2\to[\sinh^2(\gamma)-2\cosh(\gamma)\cos(2\pi r)\cos(2\pi s)+\cos^2(2\pi r)+\cos^2(2\pi s)]/\sinh^2(\gamma) \tag{14b}$$

as $t \to +\infty$. The difference of these absolute squares is w and

$$w \to [\sinh^2(\gamma) - 4\cosh(\gamma)\cos(2\pi r)\cos(2\pi s) + 2\cos^2(2\pi r) + 2\cos^2(2\pi s)]/\sinh^2(\gamma) \tag{14c}$$

as $t \to +\infty$. In (14) and appendix 2, we use the abbreviations

$$r = (4\pi)^{-1}[\alpha^2 + (\beta + \mathrm{i}\gamma)^2]^{1/2} \qquad s = (4\pi)^{-1}[\alpha^2 + (\beta - \mathrm{i}\gamma)^2]^{1/2}. \tag{15}$$

The square roots are complex, in general.

4.2. *Real singular points*

The old class of solutions is obtained by putting the finite singular points of (9) and (11) on the real axis. Let

$$\Omega(t) = \mathrm{d}A/\mathrm{d}t = (\alpha/\pi)[z(1-z)]^{-1/2}(\mathrm{d}z/\mathrm{d}t) \tag{16a}$$

and

$$B(z) = (\gamma/\pi)\ln(z) - [(\beta+\gamma)/\pi]\ln(1-z). \tag{16b}$$

Here, α satisfies (7); β and γ are the arbitrary parameters in

$$\frac{\mathrm{d}B}{\mathrm{d}t} = \frac{1}{\pi}\left(\frac{\gamma}{z} + \frac{\beta+\gamma}{1-z}\right)\frac{\mathrm{d}z}{\mathrm{d}t}. \tag{16c}$$

The limits of the occupation probabilities as $t \to +\infty$ are

$$|a_1|^2 \to [\cosh(\beta+2\gamma) + \cos(\alpha^2-\beta^2)^{1/2}]/[2\cosh(\gamma)\cosh(\beta+\gamma)] \tag{17a}$$

and

$$|a_2|^2 \to [\cosh(\beta) - \cos(\alpha^2-\beta^2)^{1/2}]/[2\cosh(\gamma)\cosh(\beta+\gamma)]. \tag{17b}$$

Here, the square root can be purely imaginary and an imaginary square root leads to vanishing transition probability when $\alpha = 0$. The difference between these two limits is the limit of w as $t \to +\infty$:

$$w \to -\operatorname{sech}(\gamma)\operatorname{sech}(\beta+\gamma)[\sinh(\gamma)\sinh(\beta+\gamma) + \cos(\alpha^2-\beta^2)^{1/2}]. \tag{17c}$$

If $\beta\ (\beta+2\gamma) = 0$, one of the final occupation probabilities (17a) or (17b) can vanish; see discussions given by Robinson [30] and Hioe [4]. If $\beta + 2\gamma = 0$, we have a simplified case considered in § 5.

In this section, explicit solutions of (8), which are given in appendix 2, have been used to find the final occupation probabilities given by (14) and (17).

5. Two special cases

In this section, we show the solutions of the two-state problem that belong to both classes and look at the case of constant detuning. The two classes of solutions are not disjoint and a simple calculation will show how they overlap. In the latter part of this section, we assume that $\mathrm{d}B/\mathrm{d}t$ is constant, in order to show how the solution of Bambini and Berman [2] is related to the present work.

If $\beta=0$ or $\gamma=0$, the new class of solutions of the two-state problem reduces to previously known solutions. We have mentioned that, if $\gamma=0$, the generalisation [6] of Rabi's solution [15] is obtained. On the other hand, let $\beta=0$ in (13). This gives solutions that are also obtained by setting $\beta+2\gamma=0$ in (16). If $\beta=0$, (13b) becomes

$$B(z)=(\gamma/2\pi)\ln(z^2+1).$$

Here, and in (13a), let $\gamma\to-2\gamma$ and $z\to(z-\frac{1}{2})\,[z(1-z)]^{-1/2}$. This gives (16$a$) and

$$B(z)=(\gamma/\pi)\ln[4z(1-z)]$$

which differs from the desired special case of (16b) by a constant. The constant could be removed by changing the phase relation between $a_1(z)$ and $a_2(z)$. Differentiation of this formula gives

$$\frac{\mathrm{d}B}{\mathrm{d}t}=\frac{1}{\pi}\left(\frac{\gamma}{z}-\frac{\gamma}{1-z}\right)\frac{\mathrm{d}z}{\mathrm{d}t}$$

which is the desired form of (16c). It seems obvious that we can set $\beta+2\gamma=0$ in (16) and transform those equations into a special case of (13). These transformations show which solutions of (8) belong to both old and new classes.

More explicit solutions of the two-state problem will now be obtained by fixing the relation between z and t. We start with the case in which the detuning is

$$\mathrm{d}B/\mathrm{d}t=\Delta$$

a constant. The simple case of $\Delta=0$, which was mentioned in § 2, will not be treated here. Integration gives

$$t=B(z)/\Delta.$$

Use of (13b) would give a lower bound or an upper bound for t; this means that the new class of solutions cannot be used here. But (16b) can be used here, if we assume that γ, Δ and $\beta+\gamma$ have the same sign. We find

$$t=(\gamma/\pi\Delta)\ln[z(1-z)^{-1-\beta/\gamma}].$$

This variable ranges over all real values and is an increasing function of z. The Rabi frequency is

$$\Omega(t)=\frac{(\alpha\Delta/\gamma)[z(1-z)]^{1/2}}{1+(\beta/\gamma)z}.$$

These two equations have the same form as equation (28) of Bambini and Berman. See figure 1 in their paper for plots of $\Omega(t)$. Unfortunately, it seems impractical to eliminate z and write the function $\Omega(t)$ more explicity, except when $\beta=0$, $\beta=\gamma$ or $\beta=-\gamma/2$. The pulse shapes shown in table 1 are much more explicit than this.

6. Simple choices for pulse-amplitude function

For both old and new classes of solutions of the two-state problem, the formal results are given in § 4 and appendix 2. The relation between z and t can be chosen to give an arbitrary pulse-amplitude function $\Omega(t)$. Seven simple forms for $\Omega(t)$ are used in table 1, where the detuning functions, $\mathrm{d}B/\mathrm{d}t$, are listed. In each detuning function, the abitrary parameters β and γ appear; they can be used to vary the form of the function as well as its magnitude. The functions $z(t)$ are given, for each case, in table 2.

Table 1. Explicit formulae for the detuning functions obtained from seven simple pulse-amplitude functions. The detuning function, $\mathrm{d}B/\mathrm{d}t$, depends on the choice of singular points in the Riemann–Papperitz equation, and on our parameters β and γ.

Amplitude function $\Omega(t)$	Complex singular points, equations (13) and (14)	Real singular points, equations (16) and (17)
$\dfrac{\alpha}{\tau}\operatorname{sech}\left(\dfrac{\tau}{\tau}\right)$	$\dfrac{\beta+\gamma\sinh(\pi t/\tau)}{\tau\cosh(\pi t/\tau)}$	$\dfrac{1}{\tau}\left[\beta+2\gamma+\beta\tanh\left(\dfrac{\pi t}{\tau}\right)\right]$
$\dfrac{\alpha}{\pi^{1/2}\tau}\exp\left(-\dfrac{t^2}{\tau^2}\right)$	$\dfrac{\exp(-t^2/\tau^2)}{\pi^{1/2}\tau}\times\{\beta+\gamma\tan[\frac{1}{2}\pi\,\mathrm{erf}(t/\tau)]\}$	$\dfrac{\exp(-t^2/\tau^2)}{\pi^{1/2}\cos[\frac{1}{2}\pi\,\mathrm{erf}(t/\tau)]}\times\{\beta+2\gamma+\beta\sin[\frac{1}{2}\pi\,\mathrm{erf}(t/\tau)]\}$
$\dfrac{\alpha\tau}{\pi(t^2+\tau^2)}$	$\dfrac{\beta\tau+\gamma t}{\pi(t^2+\tau^2)}$	$\dfrac{(\beta+2\gamma)(t^2+\tau^2)^{1/2}+\beta t}{\pi(t^2+\tau^2)}$
$\dfrac{\alpha}{2\tau}$ for $\lvert t\rvert<t$; 0 for $\lvert t\rvert\geqslant\tau$	$[\beta+\gamma\tan(\frac{1}{2}\pi t/\tau)]/2\tau$ for $\lvert t\rvert<\tau$	$\dfrac{\beta+2\gamma+\beta\sin(\frac{1}{2}\pi t/\tau)}{2\tau\cos(\frac{1}{2}\pi t/\tau)}$ for $\lvert t\rvert<\tau$
$\dfrac{\alpha}{2\tau}\exp\left(-\dfrac{\lvert t\rvert}{\tau}\right)$	$\dfrac{\exp(-\lvert t/\tau\rvert)}{2\tau}\times\left\{\beta+\gamma(\operatorname{sgn} t)\cot\left[\frac{1}{2}\pi\exp\left(-\dfrac{\lvert t\rvert}{t}\right)\right]\right\}$	$\dfrac{\exp(-\lvert t/\tau\rvert)}{2\tau\sin[\frac{1}{2}\pi\exp(-\lvert t/\tau\rvert)]}\times\left\{\beta+2\gamma+\beta(\operatorname{sgn} t)\cos\left[\frac{1}{2}\pi\exp\left(-\dfrac{\lvert t\rvert}{\tau}\right)\right]\right\}$
$\dfrac{\alpha}{\tau}\exp\left(\dfrac{t}{\tau}\right)$ for $t<0$; 0 for $t\geqslant0$	$\dfrac{\exp(t/\tau)}{\tau}\times\{\beta-\gamma\cot[\pi\exp(t/\tau)]\}$ for $t<0$	$\dfrac{\exp(t/\tau)}{\tau\sin[\pi\exp(t/\tau)]}\times\{\beta+2\gamma-\beta\cos[\pi\exp(t/\tau)]\}$ for $t<0$
0 for $t\leqslant0$; $\dfrac{\alpha}{\tau}\exp\left(-\dfrac{t}{\tau}\right)$ for $t>0$	$\dfrac{\exp(-t/\tau)}{\tau}\times\{\beta+\gamma\cot[\pi\exp(-t/\tau)]\}$ for $t>0$	$\dfrac{\exp(-t/\tau)}{\tau\sin[\pi\exp(-t/\tau)]}\times\{\beta+2\gamma+\beta\cos[\pi\exp(t/\tau)]\}$ for $t>0$

Table 2. Relations between z and t corresponding to the seven simple pulse-amplitude functions.

Amplitude function $\Omega(t)$	Complex singular points $z(t)$	Real singular points $z(t)$
$\frac{\alpha}{\tau}\operatorname{sech}\left(\frac{\pi t}{\tau}\right)$	$\sinh(\pi t/\tau)$	$\frac{1}{2}[1+\tanh(\pi t/\tau)]$
$\frac{\alpha}{\pi^{1/2}\tau}\exp\left(-\frac{t^2}{\tau^2}\right)$	$\tan[\frac{1}{2}\pi\operatorname{erf}(t/\tau)]$	$\frac{1}{2}\{1+\sin[\frac{1}{2}\pi\operatorname{erf}(t/\tau)]\}$
$\frac{\alpha\tau}{\pi(t^2+\tau^2)}$	t/τ	$\frac{1}{2}[1+t/(t^2+\tau^2)^{1/2}]$
$\frac{\alpha}{2\tau}$ for $\lvert t\rvert<\tau$ 0 for $\lvert t\rvert\geqslant\tau$	$\tan(\frac{1}{2}\pi t/\tau)$ for $\lvert t\rvert<\tau$	$\frac{1}{2}[1+\sin(\frac{1}{2}\pi t/\tau)]$ for $\lvert t\rvert<\tau$
$\frac{\alpha}{2\tau}\exp\left(-\frac{\lvert t\rvert}{\tau}\right)$	$(\operatorname{sgn} t)\cot[\frac{1}{2}\pi\exp(-\lvert t/\tau\rvert)]$	$\frac{1}{2}\{1+(\operatorname{sgn} t)\cos[\frac{1}{2}\pi\exp(-\lvert t/\tau\rvert)]\}$
$\frac{\alpha}{\tau}\exp\left(\frac{t}{\tau}\right)$ for $t<0$ 0 for $t\geqslant 0$	$-\cot[\pi\exp(t/\tau)]$ for $t<0$	$\frac{1}{2}\{1-\cos[\pi\exp(t/\tau)]\}$ for $t<0$
0 for $t\leqslant 0$ $\frac{\alpha}{\tau}\exp\left(-\frac{t}{\tau}\right)$ for $t>0$	$\cot[\pi\exp(-t/\tau)]$ for $t>0$	$\frac{1}{2}\{1+\cos[\pi\exp(-t/\tau)]\}$ for $t>0$

Rosen and Zener [1] set the pulse-amplitude function equal to a multiple of $\operatorname{sech}(\pi t/\tau)$, where τ is the time constant. Use of this function gives us the first line in table 1. The change of variable used by Rosen and Zener appears as one entry in table 2. The positive constant τ appears in every entry in our tables. The positive constant α, defined by (7), appears in every function $\Omega(t)$; it is the dimensionless area [24].

The hyperbolic-secant pulse shape received much attention in previous work [1, 2, 4, 17] on the two-state problem. We use this pulse-amplitude function with real or complex singular points and obtain the two detuning functions shown in figure 1. The growth of the occupation probability of state 2 is shown in figure 2 for the same two cases. These occupation probabilities depend on α, the dimensionless area of the pulse. The shapes of the curves in figures 1 and 2 could be changed somewhat by changing β and γ, the detuning parameters. For example, using complex singular points and setting $\gamma=0$ gives a simple case, with even detuning function, that was treated in our previous paper [6]. Using real singular points and setting $\beta=0$ gives the model treated by Rosen and Zener. Furthermore, an odd detuning function proportional to $\tanh(\pi t/\tau)$ is obtained from both real and complex singular points; this function, which is shown in our previous paper [6], represents the overlap of new and old classes of solutions.

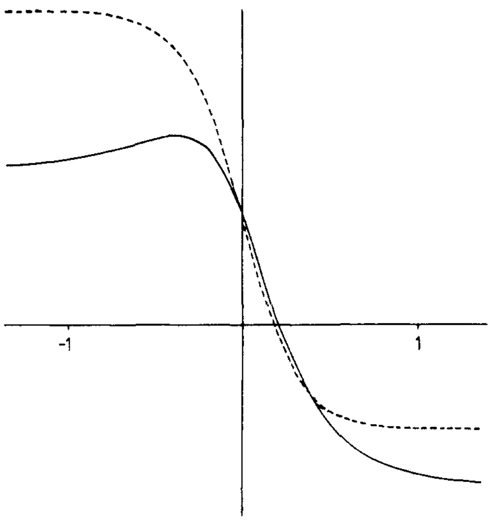

Figure 1. Two detuning functions that can accompany the hyperbolic-secant pulse-amplitude function used by Rosen and Zener. Here $\tau=1$. Full curve: complex singular points, $\beta=2.0$ and $\gamma=-3.0$; broken curve: real singular points, $\beta=-4.0$ and $\gamma=3.0$.

Many other pulse-amplitude functions $\Omega(t)$ can be devised and found in a table of indefinite integrals. The indefinite integrals are needed to solve (13a) and (16a) for $z(t)$. The functions $z(t)$ are used to find explicit detuning functions, such as those shown in table 1. There is no need to use an even function $\Omega(t)$. But we used only even functions, and only real singular points, in our earlier list of examples [6].

A Gaussian pulse-amplitude function leads to trigonometric functions of $\frac{1}{2}\pi \operatorname{erf}(t/\tau)$. Since the behaviour of these trigonometric functions as $t\to\pm\infty$ is not quite obvious, two of the detuning functions are plotted in figure 3. A detuning function

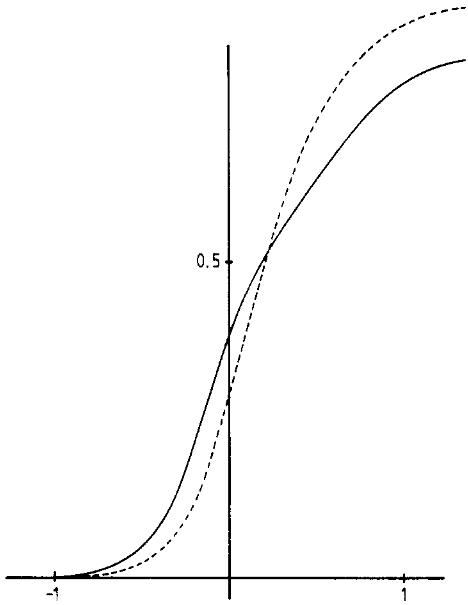

Figure 2. Time-dependent occupation probabilities corresponding to the hyperbolic-secant pulse-amplitude function with $\alpha = 5.0$ and $\tau = 1$. We plot $|a_2|^2$, the occupation probability of state 2. The full and broken curves are calculated for the two detuning functions shown in figure 1.

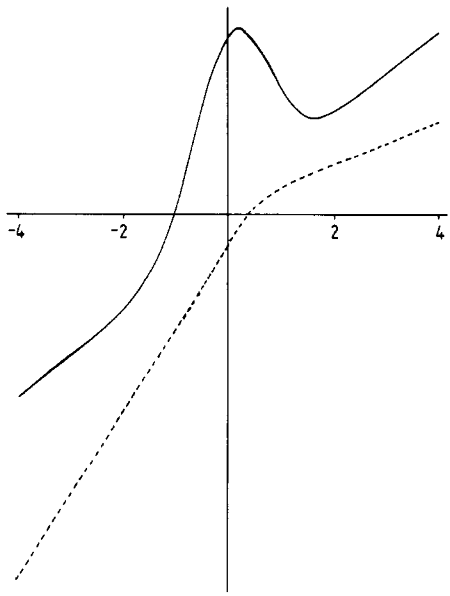

Figure 3. Two detuning functions that can accompany the Gaussian pulse-amplitude function with $\tau = 1$. Full curve: complex singular points $\beta = 18.0$ and $\gamma = 4.0$; broken curve: real singular points, $\beta = 5.0$ and $\gamma = -4.0$.

proportional to $\exp(-t^2/\tau^2)\tan[\frac{1}{2}\pi\,\mathrm{erf}(t/\tau)]$ is obtained from both real and complex singular points. Again, variations in the parameters β and γ would give detuning functions somewhat different from those shown. It would hardly be practical to plot graphs showing all the different detuning functions generated by the seven pulse-amplitude functions listed in table 1.

7. Conclusion

The time-dependent Schrödinger equation for the two-state problem can be solved by use of hypergeometric functions and the Riemann–Papperitz differential equation can be used to apply the hypergeometric functions effectively. We have reduced the number of possibilities by requiring (7), the dimensionless pulse area, to be finite, and by considering only cases in which the transition probability can be written in terms of trigonometric and hyperbolic functions. This leads to two classes of solutions, one of which is new, and an infinite variety of pulse shapes. The numerous simple analytic formulae resulting from this approach should be useful in studies of magnetic resonance and of the effect of collisions or laser beams on atoms and molecules.

Acknowledgment

This work was partially supported by the Division of Chemical Sciences, US Department of Energy under grant number DE-FG02-84-ER13243.

Appendix 1. Other formulae for sum of hypergeometric series?

The assumptions that (7) is finite and that the final occupation probabilities have a simple analytic form are used in this paper to reject many solutions that could be written in terms of hypergeometric functions. The independent variable in (11), the Riemann–Papperitz equation, is z, a non-decreasing function of t, the time. As t increases from $-\infty$ to $+\infty$, $z(t)$ must run from a singular point to a singular point, unless it is feasible to evaluate solutions at a regular point of (11). This question of feasibility is considered in this appendix.

If two of the singular points of (11) are finite and complex, we may assume that they are at $\pm\mathrm{i}$. If $\mathrm{d}A/\mathrm{d}z$ is proportional to $(z^2+1)^{-1/2}$, we cannot expect (7) to be finite. We make $\mathrm{d}A/\mathrm{d}z$ proportional to $(z^2+1)^{-1}$ and this leads to pulse shapes similar to (13). Then, we use hypergeometric functions with argument proportional to $(z-\mathrm{i})/(z+\mathrm{i})$ and seek to evalute them in terms of gamma functions at points on the real z axis. In fact, they can be so evaluated only at $z=0$ and $z=\infty$. We shall use the Gaussian formula (12) and Kummer's formula [31] for

$$F(a, b; 1+a-b; -1). \tag{A1.1}$$

This leads to

$$\Omega(t)=\mathrm{d}A/\mathrm{d}t=(2\alpha/\pi)(z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t) \tag{A1.2}$$

and

$$\mathrm{d}B/\mathrm{d}t=(2\beta z/\pi)(z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t) \tag{A1.3}$$

where α satisfies (7) and β is an arbitrary parameter. Since (A1.1) contains fewer arbitrary parameters than (12), (A1.3) contains only one arbitrary parameter. As t increases from $-\infty$ to $+\infty$, z increases from $-\infty$ to 0 or from 0 to $+\infty$. Detailed computations, which are feasible, appear to lead to another new class of solutions of the two-state problem.

However, (A1.2) and (A1.3) can be derived from (16) by a change of variable, which implies that these solutions belong to the old class of solutions. The derivation from (16) depends on whether the positive or negative half of the real z axis represents real values of t, the time. To treat the first of these two cases, we set $\gamma=0$ in (16c) and obtain $\mathrm{d}B/\mathrm{d}t=(\beta/\pi)(1-z)^{-1}(\mathrm{d}z/\mathrm{d}t)$. Now replace z by $z^2/(z^2+1)$. Then (16a) becomes $\Omega(t)=(2\alpha/\pi)\ (\operatorname{sgn} z)\ (z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t)$ and (16c) becomes (A1.3). Since z is always positive, we have derived the apparently new solutions from (16). In the other case, $z(t)$ is always negative in (A1.2) and (A1.3). Assuming that $\beta+\gamma=0$, (16c) becomes $\mathrm{d}B/\mathrm{d}t=-\beta(\pi z)^{-1}(\mathrm{d}z/\mathrm{d}t)$. Now replace z by $(z^2+1)^{-1}$. Then (16a) becomes $\Omega(t)=(2\alpha/\pi)\ (-\operatorname{sgn} z)\ (z^2+1)^{-1}(\mathrm{d}z/\mathrm{d}t)$ and (16c) becomes (A1.3). Since z is always negative, we have derived the apparently new solutions from (16).

The purpose of this appendix is to consider use of various formulae for evaluation of hypergeometric functions in terms of gamma functions. Formula (12) is the earliest and most important of these formulae; see Oberhettinger [29] for a long list. If two singular points are at $\pm\mathrm{i}$, we seek to evaluate the hypergeometric function somewhere on the unit circle and are led to consider use of Kummer's formula for (A1.1). If the finite singular points are at 0 and 1, we seek to evaluate the hypergeometric function at $z=\frac{1}{2}$ (or elsewhere), but no applicable formula can be found in reference [29]. The result is that only (12), the Gaussian formula, is actually used in this paper.

Appendix 2. Explicit solutions

The solutions of (8) will be written here in terms of hypergeometric functions. The limits of these solutions as $t\to+\infty$ are given below and the absolute squares of these limits give (14) and (17). The limits of w appear as (14c) and (17c). The limits of u and v, defined by (5), are given below, but only in those special cases where these limits exist.

The general solutions of (9) and (11) can be written in terms of hypergeometric functions. The four constants appearing in separate general solutions of (9a) and (9b) can easily be adjusted so that $|a_1|\to 1$ and $a_2\to 0$ as $t\to-\infty$. It is essential to adjust these four constants so that (8) is also satisfied.

The following calculations show that a_1 and a_2, the components of the wavefunction, do not oscillate indefinitely as $t\to\pm\infty$. Although (2) may lead one to expect this result, it is quite different from the behaviour of wavefunctions in the Landau-Zener model [8, 9]. More precisely, we find that the phase of a_1 is bounded as $t\to-\infty$. This allows us to require $a_1\to 1$, $a_2\to 0$ as $t\to-\infty$. Furthermore, we find that a_1 and a_2 approach definite limits as $t\to+\infty$. We can calculate the limits of u and v if and only if $B(z)$, given by (13b) or (16b), is bounded as $t\to+\infty$.

A2.1. Complex singular points

Here, z increases from $-\infty$ to $+\infty$ as t increases from $-\infty$ to $+\infty$ and we use (13). Set $a=\mathrm{i}$ and $b=-\mathrm{i}$ in (11) and take the limit as $c\to\infty$. It is convenient, but not necessary, to refer to the list [32] of 24 solutions of (11), rather than Kummer's list [31] of 24 solutions of (10). Equation (13a) requires us to set $\gamma=0$ in (11), but not in (13b); this simplifies the first two of the 24 solutions. Moreover, we find $\gamma'=1\pm\mathrm{i}\gamma/\pi$; the upper sign is used for (9a). We have to solve quadratic equations to find the remaining parameters in (11); the resulting square roots appear in (15). The first two of the 24 solutions of (11) are independent and will be used. We shall see that

$$\begin{aligned}a_1=\Gamma\left(-\frac{\mathrm{i}\gamma}{\pi}\right)\Bigg\{&\Gamma(2r)\left(\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)^{-(\beta+\mathrm{i}\gamma)/(4\pi)-r}\\&\times F\left(-\frac{\mathrm{i}\gamma}{2\pi}-r+s,-\frac{\mathrm{i}\gamma}{2\pi}-r-s;1-2r;\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)\\&\times\left[\Gamma\left(-\frac{\mathrm{i}\gamma}{2\pi}+r+s\right)\Gamma\left(-\frac{\mathrm{i}\gamma}{2\pi}+r-s\right)\right]^{-1}\\&+\left[\Gamma(-2r)\left(\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)^{-(\beta+\mathrm{i}\gamma)/(4\pi)+r}\right.\\&\left.\times F\left(-\frac{\mathrm{i}\gamma}{2\pi}+r+s,-\frac{\mathrm{i}\gamma}{2\pi}+r-s;1+2r;\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)\right]\\&\times\left[\Gamma\left(-\frac{\mathrm{i}\gamma}{2\pi}-r+s\right)\Gamma\left(-\frac{\mathrm{i}\gamma}{2\pi}-r-s\right)\right]^{-1}\Bigg\}\end{aligned}$$

and

$$\begin{aligned}a_2=-\frac{\alpha}{4\pi}\exp\left(\frac{\gamma-\mathrm{i}\beta}{2}+\frac{\mathrm{i}\gamma}{\pi}\ln 2\right)\Gamma\left(1-\frac{\mathrm{i}\gamma}{\pi}\right)&\\\times\Bigg\{\Bigg[&\Gamma(2r)\left(\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)^{(\beta+\mathrm{i}\gamma)/(4\pi)-r}\\&\times F\left(\frac{\mathrm{i}\gamma}{2\pi}-r+s,\frac{\mathrm{i}\gamma}{2\pi}-r-s;1-2r;\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)\Bigg]\\&\times\left[\Gamma\left(1-\frac{\mathrm{i}\gamma}{2\pi}+r+s\right)\Gamma\left(1-\frac{\mathrm{i}\gamma}{2\pi}+r-s\right)\right]^{-1}\\&+\left[\Gamma(-2r)\left(\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)^{(\beta+\mathrm{i}\gamma)/(4\pi)+r}\right.\\&\left.\times F\left(\frac{\mathrm{i}\gamma}{2\pi}+r+s,\frac{\mathrm{i}\gamma}{2\pi}+r-s;1+2r;\frac{z-\mathrm{i}}{z+\mathrm{i}}\right)\right]\\&\times\left[\Gamma\left(1-\frac{\mathrm{i}\gamma}{2\pi}-r+s\right)\Gamma\left(1-\frac{\mathrm{i}\gamma}{2\pi}-r-s\right)\right]^{-1}\Bigg\}\end{aligned}$$

where the logarithm of $(z-\mathrm{i})/(z+\mathrm{i})$ increases from 0 to $2\pi\mathrm{i}$ as t and z increase from $-\infty$ to $+\infty$. When z is large and negative, these formulae give

$$a_1=1+\ldots$$

and

$$a_2=\frac{\alpha}{4(\mathrm{i}\gamma-\pi)}\exp\left(\frac{\gamma-\mathrm{i}\beta}{2}+\frac{\mathrm{i}\gamma}{\pi}\ln 2\right)\left(\frac{2\mathrm{i}}{z+\mathrm{i}}\right)^{1-\mathrm{i}\gamma/\pi}+\ldots.$$

Terms in z^{-2} and $z^{-2\pm i\gamma/\pi}$ are not shown explicitly here. It is necessary to verify that a_1 contains no term in $z^{-1-i\gamma/\pi}$. This calculation shows that (8) is satisfied.

As $t \to +\infty$ and $z \to +\infty$,

$$a_1 \to \exp(-\tfrac{1}{2}i\beta)\,\mathrm{cosech}(\gamma)[\exp(\tfrac{1}{2}\gamma)\cos(2\pi s) - \exp(-\tfrac{1}{2}\gamma)\cos(2\pi r)]$$

and

$$\begin{aligned} a_2 \to \tfrac{1}{2}i\alpha\,\exp\left(\frac{i\gamma}{\pi}\ln 2\right)\left[\Gamma\left(1-\frac{i\gamma}{\pi}\right)\right]^2 & \\ \times\left[\Gamma\left(1-\frac{i\gamma}{2\pi}+r+s\right)\Gamma\left(1-\frac{i\gamma}{2\pi}+r-s\right)\right. & \\ \left.\times\,\Gamma\left(1-\frac{i\gamma}{2\pi}-r+s\right)\Gamma\left(1-\frac{i\gamma}{2\pi}-r-s\right)\right]^{-1}. & \end{aligned}$$

These formulae are derived from (12) and they give (14). As $z \to +\infty$, $B(z)$ is bounded only if $\gamma = 0$. Setting $\gamma = 0$ gives the generalised Rabi solution [6], for which

$$u \to \alpha\beta(\alpha^2+\beta^2)^{-1}[1-\cos(\alpha^2+\beta^2)^{1/2}]$$

$$v \to -\alpha(\alpha^2+\beta^2)^{-1/2}\sin(\alpha^2+\beta^2)^{1/2}$$

and

$$w \to -(\alpha^2+\beta^2)^{-1}[\beta^2+\alpha^2\cos(\alpha^2+\beta^2)^{1/2}]$$

as $t \to +\infty$.

A2.2. Real singular points

Here, z increases from 0 to 1 as t increases from $-\infty$ to $+\infty$ and we use (16). Set $a=0$ and $b=1$ in (11) and take the limit as $c \to \infty$. Then, (16*a*) gives $\alpha' = \beta' = 0$. This result puts (11) into the form of (10). The hypergeometric series is one solution of (10). An independent solution is given by Gauss [26, p 207ff], by Kummer [31] and by standard references [29, 32].

We shall see that

$$a_1 = F[R - i\beta/(2\pi), -R - i\beta/(2\pi); \tfrac{1}{2} + i\gamma/\pi; z]$$

and

$$a_2 = \frac{\alpha}{(2\gamma - i\pi)} z^{[1/2+(i\gamma/\pi)]} F\left(\frac{1}{2} + R + \frac{i(\beta+2\gamma)}{2\pi}, \frac{1}{2} - R + \frac{i(\beta+2\gamma)}{2\pi}; \frac{3}{2} + \frac{i\gamma}{\pi}; z\right)$$

where

$$R = (2\pi)^{-1}(\alpha^2 - \beta^2)^{1/2}.$$

Expansion in ascending powers of z gives

$$a_1 = 1 + \ldots$$

and

$$a_2 = \frac{\alpha}{(2\gamma - i\pi)} z^{1/2+(i\gamma/\pi)} + \ldots.$$

It is easy to see that the expansion of a_1 contains no term in $z^{1/2-(i\gamma/\pi)}$. This calculation shows that (8) is satisfied.

As $t \to +\infty$ and $z \to 1^-$,

$$a_1 \to \frac{\Gamma(\frac{1}{2}+i\gamma/\pi)\Gamma[\frac{1}{2}+i(\beta+\gamma)/\pi]}{\Gamma[\frac{1}{2}+R+i(\beta+2\gamma)/(2\pi)]\Gamma[\frac{1}{2}-R+i(\beta+2\gamma)/(2\pi)]}$$

and

$$a_2 \to \frac{i\alpha\Gamma(\frac{1}{2}+i\gamma/\pi)\Gamma[\frac{1}{2}-i(\beta+\gamma)/\pi]}{2\pi\Gamma[1+R-i\beta/(2\pi)]\Gamma[1-R-i\beta/(2\pi)]}.$$

These formulae are derived from (12) and they give (17). As $z \to 1^-$, $B(z)$ is bounded only if $\beta+\gamma=0$. If $\beta+\gamma=0$,

$$u+iv \to \frac{-i\pi\alpha\,\mathrm{sech}(\beta)}{\Gamma[\frac{1}{2}+R-i\beta/(2\pi)]\Gamma[\frac{1}{2}-R-i\beta/(2\pi)]\Gamma[1+R+i\beta/(2\pi)]\Gamma[1-R+i\beta/(2\pi)]}$$

as $t \to +\infty$. This calculation was omitted from earlier papers [4-6].

References

[1] Rosen N and Zener C 1932 *Phys. Rev.* **40** 502-7
[2] Bambini A and Berman P R 1981 *Phys. Rev.* A **23** 2496-501
[3] Bambini A and Lindberg M 1984 *Phys. Rev.* A **30** 794-802
[4] Hioe F T 1984 *Phys. Rev.* A **30** 2100-3
[5] Hioe F T and Carroll C E 1985 *J. Opt. Soc. Am.* B **2** 497-502
[6] Hioe F T and Carroll C E 1985 *Phys. Rev.* A **32** 1541-9
[7] Landau L 1932 *Phys. Z. Sowj.* **2** 46-51
[8] Zener C 1932 *Proc. R. Soc.* A **137** 696-702
[9] Wannier G H 1965 *Physics* **1** 251-3
[10] Nikitin E E 1962 *Opt. Spektrosk.* **13** 761-5 (Engl. transl. *Opt. Spectrosc.* **13** 431-3); 1962 *Disc Faraday Soc.* **33** 14-21
[11] Demkov Yu N 1963 *Zh. Eksp. Teor. Fiz.* **45** 195-201 (*Sov. Phys.-JETP* **18** 138-42)
[12] Kaplan A E 1973 *Zh. Eskp. Teor. Fiz.* **65** 1416-30 (*Sov. Phys.-JETP* **38** 705-11); 1975 *Zh. Eksp. Teor. Fiz.* **68** 823-33 (*Sov. Phys.-JETP* **41** 409-13)
[13] Crothers D S F 1978 *J. Phys. B: At. Mol. Phys.* **11** 1025-37
[14] Lee H-W and George T F 1984 *Phys. Rev.* A **29** 2509-17
[15] Rabi I I 1937 *Phys. Rev.* **51** 652-4
[16] Phipps T E and Stern O 1931 *Z. Phys.* **73** 185-91
[17] Allen L and Eberly J H 1975 *Optical Resonance and Two-Level Atoms* (New York: Wiley)
[18] Slichter C P 1980 *Principles of Magnetic Resonance* (Berlin: Springer) ch 2
[19] Nikitin E E and Zülicke L 1978 *Selected Topics of the Theory of Chemical Elementary Processes* (Berlin: Springer) p 135ff
[20] Bloch F 1946 *Phys. Rev.* **70** 460-74
[21] Feynman R P, Vernon F L and Hellwarth R W 1957 *J. Appl. Phys.* **28** 49-52
[22] Bloch F and Siegert A 1940 *Phys. Rev.* **57** 522-7
Stevenson A F 1940 *Phys. Rev.* **58** 1061-7
Shirley J H 1965 *Phys. Rev.* **138** B979-87
[23] Carroll C E and Hioe F T 1986 *J. Phys. A: Math. Gen.* **19** 1151-61; 1985 *J. Opt. Soc. Am.* B **2** 1355-60
[24] McCall S L and Hahn E L 1969 *Phys. Rev.* **183** 457-85
[25] Rothenberg J E, Grischkowsky D and Balant A C 1984 *Phys. Rev. Lett.* **53** 552-5
[26] Gauss C F 1866 *Werke* vol 3 (Göttingen: Königlichen Gesellschaft der Wissenschaften) (reprint 1981 (Hildesheim: G Olms Verlag))

[27] Riemann G F B 1892 *Bernhard Riemann's Gesammelte Mathematische Werke und Wissenschaftlicher Nachlass* (Leipzig: B G Teubner)
[28] Papperitz E 1885 *Math. Ann.* **25** 212-21
[29] Oberhettinger F 1964 *Handbook of Mathematical Functions* ed M Abramowitz and I Stegun (Washington, DC: National Bureau of Standards) pp 555-66
[30] Robinson E J 1981 *Phys. Rev.* A **24** 2239-41
[31] Kummer E E 1836 *J. Reine Ange. Math.* **15** 39-83, 127-72
[32] Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (Cambridge: Cambridge University Press)
Gradshteyn I S and Ryzhik I M 1963 *Tablitsy Integralov, Summ, Ryadov i Proizvedeniy* (Moscow: Gosudarstvennoe Izdatel'stvo Fiziko-Matematicheskoy Literatury) (Engl. transl. (New York: Academic))