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On pulse-induced transition amplitudes in a two-state quantum system without level crossings

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Abstract

An exact dynamical parametrization of pulse-induced transition amplitudes in a Rosen–Zener- or Nikitin-type two-level system is constructed. The three dynamical parameters are closely related to the shape of the interaction pulse and are convenient to calculate. The Milne equation with a complex coefficient function is essential for these calculations. Its complex solution is non-oscillatory and makes the computation of transition probabilities efficient. The paper reviews the quantum calculations for the rectangular pulse, which has well-defined duration and strength. By comparing transition matrix elements from a rectangular pulse with those of a general symmetric pulse, we introduce effective strength and effective duration for a general pulse. It is also possible to define an equivalent rectangular pulse, with respect to the transition probabilities, for each general pulse.

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1. Introduction

A fundamental problem in quantum mechanics is to analyse time evolutions and transitions between a limited number of states. In particular, the two-state system is analysed in much detail [1]. Only in rare cases can this problem be solved analytically. Some simplifying models of the general problem have been constructed to explain various mechanisms responsible for the transitions. For example, the Landau–Zener model [2] focuses on the crossing mechanism of a pair of energy levels while the Nikitin or Rosen–Zener model [3] focuses on non-crossing mechanisms.

Although the Nikitin model originates in the context of inelastic semiclassical collisions, it is generic to a large class of problems including the more recent topics of pulsed laser field-induced coherent population transfer [4, 5]. Particularly for laser-induced transitions it is of interest to have a general grasp of the transition dependence of pulse shapes in terms of

duration, integrated pulse area, etc [6, 7]. Also there are very few analytically solvable cases here (see, e.g., [4, 8]).

The prime purpose of this work is to derive a general dynamical parametrization of transition amplitudes in terms of well-defined parameters which are closely related to the shape of a time-symmetric pulse interaction.

The fact that a linear system of first-order differential equations describing time evolution of atomic-state amplitudes can always be transformed into a system of decoupled second-order equations having the form of the parametric harmonic oscillator (or time-independent Schrödinger) equation, one for each atomic-state amplitude, allows us to apply the recent pulse-dynamical amplitude-phase method [9]. Here the amplitude part of the decomposition of the atomic state is described by the well-known Milne equation [10]. One obstacle related to this approach in the present context is the complex-valued character of the parameters that appear in the final equations. The complex Milne solution behaviour is therefore central to our problem.

The paper is organized in the following way. Section 2 introduces the time-dependent two-state model and clarifies the relations between the transition amplitudes due to the symmetry of the pulse. An example with a rectangular-pulse interaction is analysed in detail. Section 3 reformulates the problem as a decoupled complex second-order differential equation. Certain symmetry solutions are discussed. In section 4 they help us to show that certain well-behaved solutions exist for the Milne equation, associated with the decoupled second-order equation. The particular Milne solution satisfies a conserved energy equation before and after the pulse interaction such that it oscillates between two complex conjugate turning points. Based on this ‘coherent’ Milne solution we derive the original transition matrix elements in section 5. Section 6 discusses quantum-equivalent pulses and the main conclusions are in section 7. A supporting appendix contains some detailed derivations.

2. The quantum state amplitudes

In this paper we analyse a coupled two-state quantum system, where the amplitudes satisfy (in reduced units and scaled time) an equation of the matrix form

$$\dot{\mathbf{a}} = -i\mathbf{H}(t)\mathbf{a} \quad (1)$$

with

$$\mathbf{a} = \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} \quad \mathbf{H}(t) = \begin{pmatrix} -1 & \Omega(t) \\ \Omega(t) & 1 \end{pmatrix} \quad (2)$$

where $\Omega(-t) = \Omega(t)$ is a symmetric pulse function satisfying $\Omega(t) \rightarrow 0$, as $t \rightarrow \pm\infty$. In atom–laser dynamics each diagonal element corresponds to the atom–field detuning and $\Omega(t)$ corresponds to the time-dependent Rabi frequency. The resonant situation when the detuning (diagonal elements in $\mathbf{H}(t)$) is zero is not specifically studied in this work.

We define a fundamental solution matrix $\mathbf{U}(t)$ of state amplitudes from the asymptotic conditions:

$$\mathbf{U}(t) = \begin{pmatrix} \exp(it) & 0 \\ 0 & \exp(-it) \end{pmatrix} \quad \text{as } t \rightarrow -\infty. \quad (3)$$

and

$$\mathbf{U}(t) = \begin{pmatrix} \exp(it) & 0 \\ 0 & \exp(-it) \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{as } t \rightarrow \infty \quad (4)$$

where $\mathbf{U}(t)$ and \mathbf{A} are unitary. In addition we note that

$$\det \mathbf{U}(t) = \det \mathbf{A} = 1. \quad (5)$$

This can easily be seen by noting that the time derivative of the determinant is proportional to $\text{trace}(\mathbf{H})$, which is zero in the present case. Hence the determinant of $\mathbf{U}(t)$ is constant.

The rectangulars of the absolute values of the matrix elements A_{ij} define the transition probabilities in the system. The internal structure (the parametrization) of these matrix elements is important for the development of the theory in later sections.

Due to time symmetry (note that $\mathbf{H}(-t) = \mathbf{H}(t) = \mathbf{H}^*(t)$), we observe that $\mathbf{U}^*(t)$ and $\mathbf{U}(-t)$ satisfy the same equation, but with different boundary conditions. In particular,

$$\mathbf{U}(-t) = \begin{pmatrix} \exp(-it) & 0 \\ 0 & \exp(it) \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{as } t \rightarrow -\infty. \quad (6)$$

To make the boundary conditions agree with those of $\mathbf{U}^*(t)$, we multiply $\mathbf{U}(-t)$ from the right by the matrix \mathbf{A}^\dagger . As a result

$$\mathbf{A}^* = \mathbf{A}^\dagger \quad (7)$$

i.e. the unitarity constraints $A_{11} = A_{22}^*$, $A_{12} = -A_{21}^*$ are sharpened to

$$A_{22} = A_{11}^* \quad (8)$$

$$A_{12} = A_{21} = -A_{12}^*. \quad (9)$$

We note that the off-diagonal elements are equal and imaginary.

Example 1 (Rectangular-pulse transitions). We take the profile $\Omega(t) = \beta$, $-T \leq t \leq T$, and zero elsewhere. The asymptotic forms for the fundamental solutions are defined by the boundary conditions above. We would like to find all amplitudes for the rectangular pulse in this example. This is done by fitting the asymptotic regions to a general solution inside the pulse.

The components are coupled inside the pulse, so we put an ansatz for the first component only:

$$a_1(t) = B_+ \exp(i\gamma t) + B_- \exp(-i\gamma t) \quad \gamma = \sqrt{1 + \beta^2}. \quad (10)$$

This is based on a second differentiation, where the components decouple and satisfy the same second-order equation. The derivative of $a_1(t)$ is

$$\dot{a}_1(t) = i\gamma B_+ \exp(i\gamma t) - i\gamma B_- \exp(-i\gamma t). \quad (11)$$

The component $a_2(t)$ is obtained by inserting both the above expressions into the first of the coupled equations:

$$a_2(t) = \frac{(1 - \gamma)}{\beta} B_+ \exp(i\gamma t) + \frac{(1 + \gamma)}{\beta} B_- \exp(-i\gamma t). \quad (12)$$

The two unknown coefficients B_\pm are determined from continuity at $t = -T$, for each independent solution vector. The result is

$$B_+^{(1)} = \frac{(\gamma + 1)}{2\gamma} e^{-i(1-\gamma)T} \quad B_-^{(1)} = \frac{(\gamma - 1)}{2\gamma} e^{-i(1+\gamma)T} \quad (13)$$

and

$$B_+^{(2)} = -\frac{\beta}{2\gamma} e^{i(1+\gamma)T} \quad B_-^{(2)} = \frac{\beta}{2\gamma} e^{i(1-\gamma)T}. \quad (14)$$

Inserting the coefficients into $a_1(t)$ and $a_2(t)$ and fitting to the asymptotic expressions at $t = T$, all amplitudes A_{ij} are finally found:

$$A_{11} = A_{22}^* = \left(\cos(2\gamma T) + i \frac{1}{\sqrt{1 + \beta^2}} \sin(2\gamma T) \right) e^{-2iT} \quad (15)$$

$$A_{12} = A_{21} = -i \frac{\beta}{\sqrt{1 + \beta^2}} \sin(2\gamma T). \quad (16)$$

Strictly speaking, the area of the field pulse is $2\beta T$. It is thus clear that the dynamic phases in the transition amplitudes correspond to another, combined (or dressed) area $2\gamma T$. The possible maximal transition probability, determined by $|A_{12}|^2 (= |A_{21}|^2)$ for $\sin(2\gamma T) = \pm 1$, is seen to depend only on the strength β of the pulse. The pulse duration $2T$ alone is not present in $|A_{12}|^2$ and $|A_{11}|^2$.

3. Analysis of the second-order equations and transitions

A particular transformation of the first-order quantum mechanical equations (1) can be achieved by a second differentiation, obtaining

$$\ddot{\mathbf{a}} + (\mathbf{H}^2(t) + i\dot{\mathbf{H}}(t))\mathbf{a} = \mathbf{0}. \quad (17)$$

This equation is of the standard coupled parametric-oscillator type and provides interesting applications for amplitude-phase analysis (see, e.g., [11]) and refined standard semiclassical approximations [12, 13].

The second-order coupled equations based on representation (2) are formally equivalent to coordinate-coupled parametric oscillators $\ddot{\mathbf{a}} + \mathbf{K}(t)\mathbf{a} = \mathbf{0}$ with a complex coefficient matrix

$$\mathbf{K}(t) = \begin{pmatrix} 1 + (\Omega(t))^2 & i\dot{\Omega}(t) \\ i\dot{\Omega}(t) & 1 + (\Omega(t))^2 \end{pmatrix}. \quad (18)$$

We apply a real, time-independent Hadamard transform to new state amplitudes:

$$\mathbf{x} = \mathbf{T}\mathbf{a} \quad \mathbf{x} = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} \quad (19)$$

with

$$\mathbf{T} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (20)$$

The transformation leads to a significant formal simplification of the second-order equations later. The first-order equations (1) now read

$$\dot{\mathbf{x}} = -i\mathbf{H}_x(t)\mathbf{x} \quad (21)$$

with

$$\mathbf{H}_x(t) = \begin{pmatrix} \Omega(t) & -1 \\ -1 & -\Omega(t) \end{pmatrix}. \quad (22)$$

By a second differentiation the equation simplifies to a diagonal problem

$$\ddot{\mathbf{x}} + \mathbf{K}_x(t)\mathbf{x} = \mathbf{0} \quad (23)$$

where the coefficient matrix $\mathbf{K}_x(t)$ is

$$\mathbf{K}_x(t) = \begin{pmatrix} 1 + (\Omega(t))^2 + i\dot{\Omega}(t) & 0 \\ 0 & 1 + (\Omega(t))^2 - i\dot{\Omega}(t) \end{pmatrix}. \quad (24)$$

Equations (23) correspond to two decoupled complex parametric oscillators. Due to the unitarity relations (9) we actually need only $x_1(t)$ to finally obtain all the matrix elements A_{ij} . Let us define the principal equation

$$\ddot{x}_1 + \omega^2(t)x_1 = 0 \quad (25)$$

with

$$\omega^2(t) = 1 + (\Omega(t))^2 + i\dot{\Omega}(t). \tag{26}$$

Combining (3), (4) and (19) we can specify the two independent solutions to (25) by the asymptotic conditions

$$g_1(t) = \exp(it) \quad \text{as } t \rightarrow -\infty \tag{27}$$

$$g_1(t) = A_{11} \exp(it) + A_{21} \exp(-it) \quad \text{as } t \rightarrow \infty \tag{28}$$

and

$$g_2(t) = \exp(-it) \quad \text{as } t \rightarrow -\infty \tag{29}$$

$$g_2(t) = A_{12} \exp(it) + A_{22} \exp(-it) \quad \text{as } t \rightarrow \infty. \tag{30}$$

Example 2 (Symmetry solutions for the rectangular pulse). We define $\Omega(t) = \beta, -T \leq t \leq T$, and zero elsewhere. We construct the symmetric basis from the inner region and make an ansatz only for the x_1 component. The coupling of x_1 and x_2 through the first-order equations then provides the corresponding symmetry solution for x_2 . Hence, the symmetric solution for x_1 is

$$C_1(t) = \cos(\gamma t) / \sqrt{\gamma} \quad t < T \quad \gamma = \sqrt{1 + \beta^2} \tag{31}$$

and the anti-symmetric solution is

$$S_1(t) = \sin(\gamma t) / \sqrt{\gamma} \quad t < T \tag{32}$$

with Wronskian $\dot{S}_1(t)C_1(t) - S_1(t)\dot{C}_1(t) = 1$ for the present normalization. The corresponding x_2 components are

$$C_2(t) = \beta \cos(\gamma t) / \sqrt{\gamma} + i\sqrt{\gamma} \sin(\gamma t) \quad t < T \tag{33}$$

and

$$S_2(t) = -i\sqrt{\gamma} \cos(\gamma t) + \beta \sin(\gamma t) / \sqrt{\gamma} \quad t < T. \tag{34}$$

We note that the symmetry basis here does not satisfy the same Wronskian constant. Instead we have $\dot{S}_2(t)C_2(t) - S_2(t)\dot{C}_2(t) = -1$.

Proceeding with both symmetry solutions to the right boundary $t = T$, we fit them to the asymptotic forms

$$x_1(t) = D_+ e^{it} + D_- e^{-it} \quad T < t \tag{35}$$

and

$$x_2(t) = D_+ e^{it} - D_- e^{-it} \quad T < t. \tag{36}$$

In either case we determine D_{\pm} and find in the asymptotic region $t > T$. We get for the symmetric solutions

$$D_{\pm} = \frac{1}{2\sqrt{\gamma}} ([1 \pm \beta] \cos \gamma T \pm i\gamma \sin \gamma T) e^{\mp iT} \tag{37}$$

and for the anti-symmetric solutions

$$D_{\pm} = \frac{1}{2\sqrt{\gamma}} ([1 \pm \beta] \sin \gamma T \mp i\gamma \cos \gamma T) e^{\mp iT}. \tag{38}$$

This result will be used with reference to the existence of certain symmetric so-called Milne solutions pertinent to the second-order oscillator equation.

4. Complex parametric pulses

In this section we discuss the principles that generalize the result of [9] to complex symmetric parametric pulses of the harmonic oscillator. The oscillator subject to the relevant parametric pulse in our problem (see equation (25)) can be written as

$$\ddot{x} + \omega^2(t)x = 0, \quad \omega^2(t) \rightarrow 1 \quad \text{as } t \rightarrow \pm\infty \quad (39)$$

where we assume (see equation (26))

$$[\omega^2(-t)]^* = \omega^2(t) \quad (40)$$

which is known as \mathcal{PT} -symmetry (see, e.g., [14] and references therein).

We stay in the framework of the classical parametric oscillator and review the results obtained for a purely real symmetric parametric pulse. The resulting transition matrix for the fundamental propagating oscillations $[\exp(it), \exp(-it)]$ due to a *real symmetric* pulse was found in the form

$$\mathbf{P} = \begin{pmatrix} (\cos \delta + iE_M \sin \delta) e^{-i\tau} & i\sqrt{E_M^2 - 1} \sin \delta \\ -i\sqrt{E_M^2 - 1} \sin \delta & (\cos \delta - iE_M \sin \delta) e^{i\tau} \end{pmatrix} \quad (41)$$

where the three dynamical parameters E_M , δ and τ are defined in terms of a symmetric and positive solution of the Milne equation (see [9])

$$\ddot{\rho} + \omega^2(t)\rho = \frac{1}{\rho^3}. \quad (42)$$

By direct substitution into (42) it can be shown that a correct asymptotic form for the Milne solution is given by

$$\rho(t) \rightarrow q(t) = \sqrt{E_M - \sqrt{E_M^2 - 1} \cos(2t - \tau)} \quad t \rightarrow +\infty \quad (43)$$

and a corresponding expression for $t \rightarrow -\infty$ is obtained from the symmetry $\rho(-t) = \rho(t)$. Two of the dynamical parameters appear here: E_M is identified as the conserved ‘energy’ of the Milne oscillator as $t \rightarrow +\infty$ (see figure 3), i.e.

$$E_M = \frac{1}{2}\dot{q}^2 + \frac{1}{2}q^2 + \frac{1}{2}q^{-2} \quad (44)$$

and $t = \tau/2$ determines the event of reaching the inner one of the turning points

$$q_{\pm} = \sqrt{E_M \pm \sqrt{E_M^2 - 1}} \quad (45)$$

in that oscillator. With an appropriate choice of angular modulus and comparisons with analytic pulse models, τ was identified as the effective duration of the pulse.

The final parameter, the dynamic phase shift, is given by

$$\delta = 2 \lim_{t \rightarrow +\infty} \left(\int_0^t \rho^{-2}(t') dt' - \int_{\tau/2}^t q^{-2}(t') dt' \right) \pmod{2\pi}. \quad (46)$$

The complex Milne oscillator. Due to the complex parameter $\omega^2(t)$, the Milne solution is expected to become complex valued and oscillating in the asymptotic regions $t \rightarrow \pm\infty$. This does not mean that the Milne energy E_M is complex in general. A study of the turning point expressions (45) for positive E_M reveals that turning points become complex conjugates as $0 < E_M < 1$. For a general complex-valued Milne oscillator the coordinate q traces out a closed loop in the complex plane and there are no turning points (defined by $\dot{q} = 0$). Real and imaginary parts of q do not have coherent (in phase) oscillations along a line as for the real energy case.

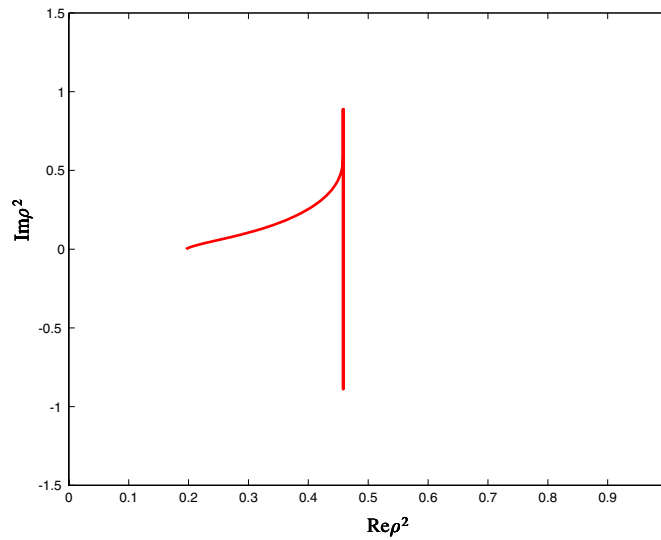


Figure 1. The Milne solution approaches the coherent asymptotic oscillator (with complex conjugate turning points). The pulse is $\Omega(t) = \beta \cos^2(\pi t/(2T))$ with $T = 1$ and $\beta = 5$.

To find a coherent solution we need specific initial conditions. It turns out that the stationary ‘classical’ conditions (see a discussion in [15]) develop the Milne solution into the coherent complex Milne oscillator, i.e.

$$\rho(0) = \omega(0)^{-1/2} \quad \dot{\rho}(0) = 0. \quad (47)$$

For a symmetric pulse, $\rho(0)$ is seen to be real. We assume that the coherent oscillation exists with these initial conditions for a significant class of pulses of interest. In the appendix we clarify the relation between the Milne solution and any fundamental basis of the parametric oscillator equation and we explicitly verify the existence of Milne oscillations with complex turning points for the rectangular pulse.

It is easy to show that the initial conditions (47) are compatible with a symmetric Milne solution $\rho(t)$, which satisfies

$$\rho(-t) = \rho^*(t). \quad (48)$$

Obviously we start at a real turning (or stationary) point of $\rho(t)$ in the inner pulse region and assume that the complex oscillation possesses turning points also in the asymptotic regions.

The asymptotic oscillatory form of the Milne solution is formally the same as in (43) and we may still keep the parameter τ real. If at $t = \tau/2$ the asymptotic Milne solution for $0 < E_M < 1$ is located at the upper (complex) turning point, we have

$$\rho(t) \rightarrow q(t) = \sqrt{E_M + i\sqrt{1 - E_M^2} \cos(2t - \tau)} \quad t \rightarrow +\infty. \quad (49)$$

The squared asymptotic amplitude function $q^2(t)$ is directly decomposed into its real and imaginary parts, whereby the real part (E_M) is constant and the imaginary part oscillates between $\pm\sqrt{1 - E_M^2}$. This is a straight line segment crossing the real axis at E_M in the complex q^2 -plane (compare illustrations in figure 1 and figure 2).

Example 3 (The rectangular-pulse Milne solution I—the indirect derivation). We can construct the Milne solution from the symmetry solutions in example 2. In the appendix the basic theory

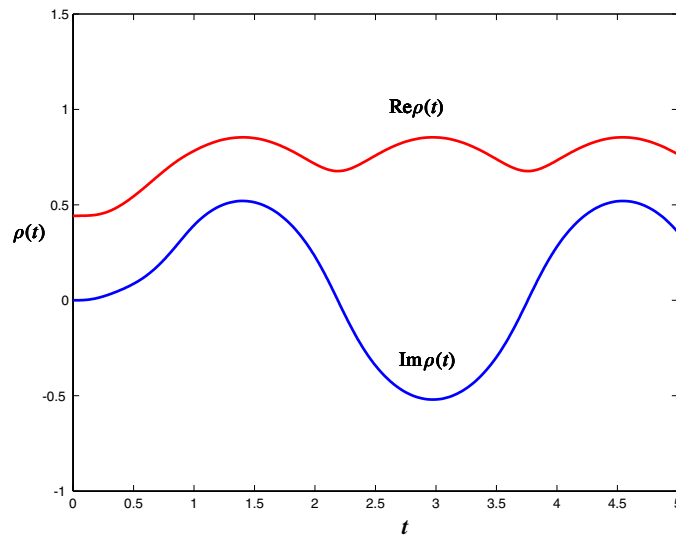


Figure 2. A different view of the Milne solution in figure 1 as a function of time.

for expressing Milne solutions in terms of fundamental solutions of the complex parametric oscillator is outlined. With basic solutions $C_1(t)$ and $S_1(t)$ satisfying a unit Wronskian relation, the Milne solution is obtained as

$$\rho_1(t) = \sqrt{C_1^2(t) + S_1^2(t)}. \quad (50)$$

With basic solutions $C_2(t)$ and $S_2(t)$ having a Wronskian equal to -1 , the Milne solution is obtained as

$$\rho_2(t) = \sqrt{-C_1^2(t) - S_1^2(t)}. \quad (51)$$

For the inner region we thus find

$$\rho_1 = \rho_2 = \frac{1}{\sqrt{\gamma}} = (1 + \beta^2)^{-1/4} \quad 0 \leq t \leq T \quad (52)$$

and for the external region we obtain after some algebra

$$\rho_1(t) = \rho_2^*(t) = \sqrt{\frac{1}{\gamma} + i\frac{\beta}{\gamma} \sin 2(t - T)} \quad t \geq T. \quad (53)$$

We note that the phase shift $2\gamma T$ does not contribute to these expressions and that $2T$ is the range of the rectangular pulse. Finally, the Milne energy is found from (53) (see figure 3), i.e.

$$E_M = \gamma^{-1} = (1 + \beta^2)^{-1/2}. \quad (54)$$

We now use the results of example 3 to define the relevant pulse duration parameter for more general pulse shapes. In particular, we note that the asymptotic oscillation described by (53) starts *between* the turning points rather than *at* a turning point (see the discussion of equation (49)).

The reference form for the asymptotic Milne solution is thus taken as

$$\rho(t) \rightarrow q(t) = \sqrt{E_M + i\sqrt{1 - E_M^2} \sin(2t - \tau_0)} \quad t \rightarrow +\infty \quad (55)$$

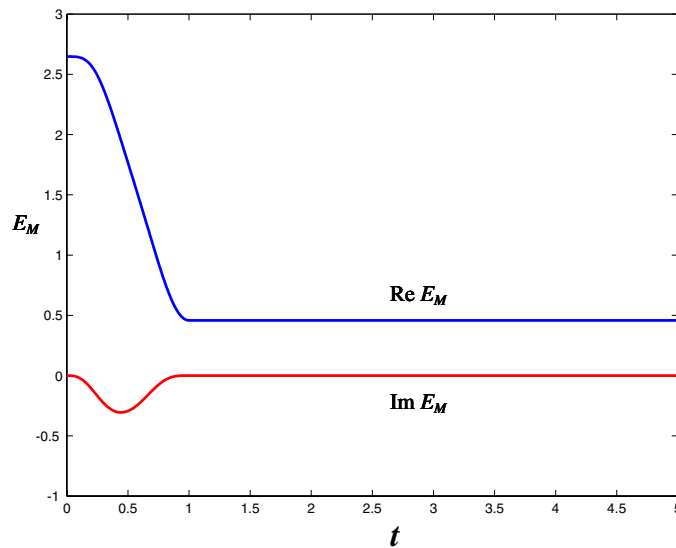


Figure 3. Expression (44) for E_M approaches the constant real value 0.46. Note that E_M is a constant of motion only in the *asymptotic* region.

where $\tau_0/2$ is the real passage prior to the fitting time $t = T$. τ_0 also corresponds to the duration of the pulse in this theory. For negative times this expression has to be complex symmetric: the replacement $\tau_0 \rightarrow -\tau_0$, together with $t \rightarrow -t$, gives $q(-t) = q^*(t)$.

From numerical calculations of $\rho(t)$ and $\dot{\rho}(t)$ we conclude that we can now also compute numerical values of a real E_M and a real τ_0 .

Example 4 (The rectangular-pulse Milne solution II—the direct derivation). Here we directly work with Milne’s equation (42). We determine the constant amplitude ρ in the ‘inner’ region and fit it with the reference form (55) for the outer region.

In the inner region we have $\Omega(t) = \beta$, which is constant, with the consequence that $\omega = \sqrt{1 + \beta^2}$. The ‘stationary’ amplitude function solving the Milne equation becomes

$$\rho = (1 + \beta^2)^{-1/4} \quad (56)$$

which is also constant. This real value has to be fitted to the complex coherent oscillation typical of the asymptotic oscillations with a Milne energy $0 < E_M < 1$. Using formula (55) we derive the pulse duration τ_0 from the matching time ($t = T$) from the relation

$$T = \tau_0/2. \quad (57)$$

The Milne energy is determined also from formula (55) (since ρ is assumed continuous), which gives (same as in example 3)

$$E_M = (1 + \beta^2)^{-1/2}. \quad (58)$$

A concluding note. Consistency with the definition of the Milne energy in the ‘outer region’ requires here (the rectangular-pulse case) a discontinuity of the Milne solution at the instant of the ‘fitting’, so that the asymptotic oscillation starts with

$$\dot{q}(T) = i \sqrt{\frac{1 - E_M^2}{E_M}} \quad t = T. \quad (59)$$

For a continuous pulse, as in figure 1, the derivative of the Milne solution is also continuous.

5. Derivation of transition amplitudes

We now explicitly rederive the transition matrix for the complex symmetric case, following closely the arguments in [9]. We recall that the parametric oscillator (25) has two independent solutions specified by

$$g_1(t) = \exp(it) \quad \text{as } t \rightarrow -\infty \quad (60)$$

$$g_1(t) = A_{11} \exp(it) + A_{21} \exp(-it) \quad \text{as } t \rightarrow \infty \quad (61)$$

and

$$g_2(t) = \exp(-it) \quad \text{as } t \rightarrow -\infty \quad (62)$$

$$g_2(t) = A_{12} \exp(it) + A_{22} \exp(-it) \quad \text{as } t \rightarrow \infty. \quad (63)$$

The matrix elements A_{ij} are labelled according to section 2 and are analysed by the amplitude-phase theory in the present section. As defined here, A_{ij} are formally equivalent to P_{ij} appearing in the classical parametric oscillator in [9].

The amplitude-phase ansatz $x = \rho \exp(i\theta)$ (see [9]), using the symmetric coherent Milne solution $\rho(t)$, suggests the symmetric/anti-symmetric cos/sin fundamental solutions of the form

$$C(t) = \rho(t) \cos\left(\int_0^t \rho^{-2}(t') dt'\right) \quad S(t) = \rho(t) \sin\left(\int_0^t \rho^{-2}(t') dt'\right). \quad (64)$$

Both these solutions satisfy the parametric harmonic oscillator equation (39). The complex symmetries of these (complex odd/even) solutions are

$$C(-t) = C^*(t) \quad S(-t) = -S^*(t). \quad (65)$$

The analysis of the asymptotic region $t \rightarrow +\infty$ in [9] is modified slightly. Here we assume a finite range $2T$ of the symmetric pulse. The asymptotic analysis yields

$$C(t) \rightarrow q(t) \cos(\phi(t) + \delta') \quad S(t) \rightarrow q(t) \sin(\phi(t) + \delta') \quad t \rightarrow +\infty \quad (66)$$

with

$$\phi(t) = \tan^{-1}\left(E_M \tan(t - \tau_0/2) + i\sqrt{1 - E_M^2}\right) \quad (67)$$

$$\delta' = \int_0^T \rho^{-2}(t) dt - \phi(T). \quad (68)$$

A further trigonometric analysis reveals

$$q(t) \cos \phi(t) = \cos(t - \tau_0/2)/\sqrt{E_M} \quad (69)$$

$$q(t) \sin \phi(t) = i\sqrt{\frac{1 - E_M^2}{E_M}} \cos(t - \tau_0/2) + \sqrt{E_M} \sin(t - \tau_0/2). \quad (70)$$

The fully symmetric solutions then become

$$\lim_{t \rightarrow \infty} (C(t), S(t)) = (\cos(t - \tau_0/2), \sin(t - \tau_0/2)) \begin{pmatrix} \frac{1}{\sqrt{E_M}} & i\sqrt{\frac{1 - E_M^2}{E_M}} \\ 0 & \sqrt{E_M} \end{pmatrix} \begin{pmatrix} \cos \delta' & \sin \delta' \\ -\sin \delta' & \cos \delta' \end{pmatrix}. \quad (71)$$

Symmetry provides the asymptotic analysis as $t \rightarrow -\infty$, i.e.

$$\lim_{t \rightarrow -\infty} (C(t), S(t)) = (\cos(t + \tau_0/2), \sin(t + \tau_0/2)) \begin{pmatrix} \frac{1}{\sqrt{E_M}} & i\sqrt{\frac{1-E_M^2}{E_M}} \\ 0 & \sqrt{E_M} \end{pmatrix} \begin{pmatrix} \cos \delta'^* & -\sin \delta'^* \\ \sin \delta'^* & \cos \delta'^* \end{pmatrix}. \quad (72)$$

The ‘ τ_0 -dressed’ forward and backward connections are now defined as matrices:

$$\mathbf{T}_+ = \frac{1}{\sqrt{E_M}} \begin{pmatrix} \cos \delta' - i\sqrt{1-E_M^2} \sin \delta' & \sin \delta' + i\sqrt{1-E_M^2} \cos \delta' \\ -E_M \sin \delta' & E_M \cos \delta' \end{pmatrix} \quad (73)$$

$$\mathbf{T}_- = \frac{1}{\sqrt{E_M}} \begin{pmatrix} \cos \delta'^* + i\sqrt{1-E_M^2} \sin \delta'^* & -\sin \delta'^* + i\sqrt{1-E_M^2} \cos \delta'^* \\ E_M \sin \delta'^* & E_M \cos \delta'^* \end{pmatrix}. \quad (74)$$

These are unit matrices with simple relations to their inverses. They combine to a τ_0 -dressed overall transition (using trigonometry):

$$\mathbf{M}_{\tau_0} = \mathbf{T}_+ \mathbf{T}_-^{-1} = \begin{pmatrix} \cos \delta - i\sqrt{1-E_M^2} \sin \delta & E_M \sin \delta \\ -E_M \sin \delta & \cos \delta + i\sqrt{1-E_M^2} \sin \delta \end{pmatrix}. \quad (75)$$

We have used a redefined real phase $\delta = \delta' + \delta'^*$ here. The pulse-induced transitions for undressed cos/sin oscillations are then given by the matrix elements of \mathbf{M} , where

$$\mathbf{M} = \begin{pmatrix} \cos(\tau_0/2) & -\sin(\tau_0/2) \\ \sin(\tau_0/2) & \cos(\tau_0/2) \end{pmatrix} \mathbf{M}_{\tau_0} \begin{pmatrix} \cos(\tau_0/2) & -\sin(\tau_0/2) \\ \sin(\tau_0/2) & \cos(\tau_0/2) \end{pmatrix}. \quad (76)$$

The corresponding transition matrix for propagating complex solutions ($\exp(it)$, $\exp(-it)$), according to [9] and the note following equation (63), is expressed as

$$\mathbf{A} = \begin{pmatrix} \exp(-i\tau_0/2) & 0 \\ 0 & \exp(i\tau_0/2) \end{pmatrix} \mathbf{A}_{\tau_0} \begin{pmatrix} \exp(-i\tau_0/2) & 0 \\ 0 & \exp(i\tau_0/2) \end{pmatrix} \quad (77)$$

$$\mathbf{A}_{\tau_0} = \mathbf{C}^{-1} \mathbf{M}_{\tau_0} \mathbf{C} \quad (78)$$

with

$$\mathbf{C} = \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \quad (79)$$

In explicit form we have

$$\mathbf{A} = \begin{pmatrix} (\cos \delta + iE_M \sin \delta) e^{-i\tau_0} & -i\sqrt{1-E_M^2} \sin \delta \\ -i\sqrt{1-E_M^2} \sin \delta & (\cos \delta - iE_M \sin \delta) e^{i\tau_0} \end{pmatrix}. \quad (80)$$

Note. For a vanishing pulse, we have $E_M \rightarrow 1$ and $\delta \rightarrow \tau_0$. The transition matrix becomes a unit matrix. As the complex pulse increases the real Milne energy decreases. In the strong pulse limit $E_M \rightarrow 0$ and we recover unit amplitude modulations depending only on δ which corresponds to the area of ω in the pulse region. The formula is similar but different from that of the real pulse.

In figure 4 we illustrate the behaviour of the dynamical model parameters E_m , τ_0 and δ , as functions of the strength β of a pulse model $\Omega(t) = \beta \cos^2(\pi t/(2T))$. The important point with the construction of this theory is to find a simple dependence of dynamical parameters on the pulse parameters (see also [9]).

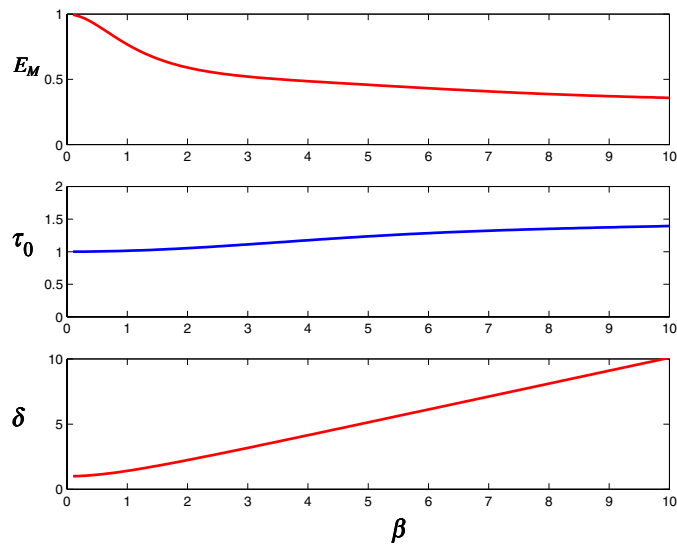


Figure 4. The dynamical parameters δ , τ_0 and E_M as functions of the pulse strength β . The pulse is $\Omega(t) = \beta \cos^2(\pi t/(2T))$ and has a finite range $T = 1$.

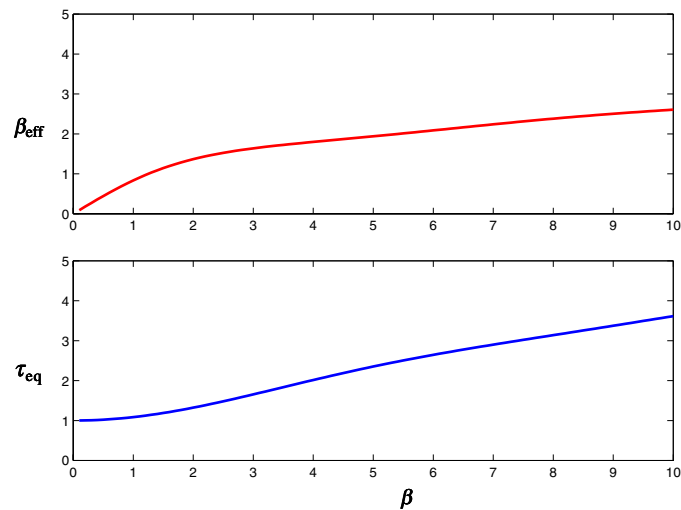


Figure 5. The behaviour of the effective parameters for the \cos^2 -pulse model (top) with fixed range $T = 1$.

6. Equivalent rectangular pulses

In the present section we analyse the dynamics in terms of the new shape parameters and we point out that for each interaction pulse there is an equivalent effective rectangular pulse as regards the transition probabilities in a two-level system. The three new parameters E_M , τ_0 and δ exactly describe the quantal results, and are by construction closely connected to the

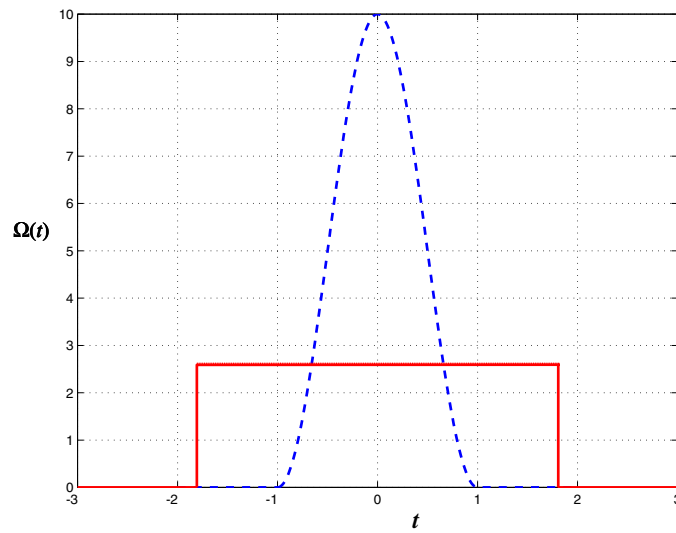


Figure 6. The original \cos^2 -pulse with $\beta = 10$ and $T = 1$ is compared to the equivalent rectangular pulse with $\beta_{\text{eff}} = 2.61$ and $\tau_{\text{eq}} = 3.61$.

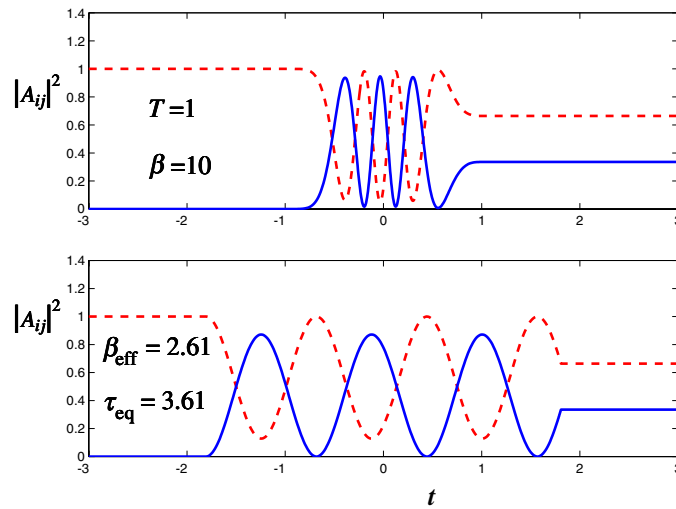


Figure 7. Intermediate dynamics for the \cos^2 -pulse model (top) with $\beta = 10$ and $T = 1$, and the equivalent rectangular pulse (bottom) with $\beta_{\text{eff}} = 2.61$ and $\tau_{\text{eq}} = 3.61$.

properties $(2T, \beta)$ of a rectangular pulse. We recall that

$$E_M = \frac{1}{\sqrt{1 + \beta^2}} \quad (\text{rectangular pulse}) \quad (81)$$

$$\tau_0 = 2T \quad (\text{rectangular pulse}). \quad (82)$$

With the connection to the rectangular pulse they account for three aspects of a more general interaction pulse. From E_M we can define an ‘effective rectangular-pulse strength’ β_{eff} :

$$\beta_{\text{eff}} = \frac{\sqrt{1 - E_M^2}}{E_M} \quad (\text{any pulse}). \quad (83)$$

Similarly, τ_0 becomes the ‘effective rectangular-pulse duration’ and δ , the dynamical phase shift, becomes the ‘effective (dressed) rectangular-pulse area’ (see section 2). However, since only two parameters can be independent, there must exist some relation between them. For the rectangular pulse model we have the explicit relation:

$$\delta = \frac{\tau_0}{E_M} \quad (\text{rectangular pulse}). \quad (84)$$

Such a simple relation does not exist for the ‘effective rectangular-pulse’ parameters of an arbitrary pulse. As a consequence, our effective parameters are so far three independent aspects of the interaction pulse. On the other hand, the actual quantal measurement situation requires only the absolute squares of the transition amplitudes (see equations (61), (63) and (80)), so the ‘effective’ pulse duration is formally redundant. However, if we are to analyse interference effects the pulse duration will be important. With standard definitions of probabilities, we are thus left with δ and β_{eff} as the relevant exact pulse characteristics. In this situation we can also introduce an ‘equivalent rectangular-pulse duration’ (rather than ‘effective’) through the above relation, i.e.

$$\tau_{\text{eq}} = \delta E_M = \frac{\delta}{\sqrt{1 + \beta_{\text{eff}}^2}} \quad (\text{any pulse}). \quad (85)$$

For two-level systems with a pulse interaction we then have with τ_{eq} and β_{eff} a quantally equivalent rectangular pulse which provides exactly the same transition probabilities. We illustrate this idea and compare in figures 5–7 a \cos^2 -shaped pulse

$$\Omega(t) = \beta \cos^2(\pi t/(2T)) \quad (86)$$

and an equivalent rectangular pulse

$$\Omega(t) = \beta_{\text{eff}} \quad -\tau_{\text{eq}}/2 \leq t \leq \tau_{\text{eq}}/2. \quad (87)$$

In figure 5 we observe the monotonic behaviour of τ_{eq} and β_{eff} as functions of the strength parameter β of the \cos^2 -pulse with a fixed $T = 1$. A particular pair of equivalent pulses is shown in figure 6. Both pulses lead to the same transition probabilities, as can be seen from the detailed population dynamics in figure 7.

7. Conclusions

The analysis of the two-state quantum transitions introduces the two quantities E_M and δ in this theory. The phase shift δ is again an accumulated dynamical phase due to the interaction. The Milne energy E_M gives a measure of the strength of the pulse in the sense explained in the preceding section. The effective duration τ_0 of the pulse is no longer explicit, but for illustrative purposes an equivalent rectangular-pulse duration τ_{eq} and a quantum mechanically equivalent interaction pulse can be defined.

The coherent oscillation of the underlying Milne solution, with complex conjugate turning points, is a limiting condition for the applicability of the present theory. Precise conditions for the existence of such oscillations are still lacking.

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Appendix. Connection between Milne solutions and parametric harmonic oscillator solutions

A general solution of Milne's equation can be expressed in terms of any pair of basis solutions for the parametric oscillator. This fact is related to the nonlinear superposition principle for the so-called Ermakov systems (see [15–17]).

Assume a formal amplitude-phase basis and an arbitrary basis of the parametric oscillator in column-vector notation

$$\mathbf{f}(t) = \begin{pmatrix} \rho(t) \cos \int_0^t \rho^{-2}(t') dt' \\ \rho(t) \sin \int_0^t \rho^{-2}(t') dt' \end{pmatrix} \quad \mathbf{g}(t) = \begin{pmatrix} g_1(t) \\ g_2(t) \end{pmatrix}. \quad (\text{A.1})$$

The lower limit of the phase integral in $\mathbf{f}(t)$ is arbitrarily put to $t = 0$ here. As long as $\rho(t)$ satisfies Milne's equation, $\mathbf{f}(t)$ and $\mathbf{g}(t)$ are two bases of the oscillator equation. They can be expressed in terms of each other. Let \mathbf{B} be a 2×2 matrix such that

$$\mathbf{f}(t) = \mathbf{B}\mathbf{g}(t). \quad (\text{A.2})$$

Defining the notation

$$\mathbf{F}(t) = (\mathbf{f}(t), \dot{\mathbf{f}}(t)) \quad \mathbf{G}(t) = (\mathbf{g}(t), \dot{\mathbf{g}}(t)) \quad (\text{A.3})$$

we have

$$\mathbf{F}(t) = \mathbf{B}\mathbf{G}(t). \quad (\text{A.4})$$

Given the basis $\mathbf{g}(t)$, \mathbf{B} is fully determined from the initial conditions $(\rho_0, \dot{\rho}_0)$ of $\rho(t)$ through the relation

$$\mathbf{B} = \mathbf{F}(0)\mathbf{G}^{-1}(0) \quad (\text{A.5})$$

where

$$\mathbf{F}(0) = \begin{pmatrix} \rho_0 & \dot{\rho}_0 \\ 0 & \rho_0^{-1} \end{pmatrix}. \quad (\text{A.6})$$

Different initial conditions $(\rho_0, \dot{\rho}_0)$ result in a different amplitude-phase basis, which however possesses the same Wronskian constant.

Finally $\rho^2(t)$ is solved from (A.2) by taking the scalar product (*not* the complex scalar product), i.e.

$$\rho^2(t) = \mathbf{f}^T(t)\mathbf{f}(t) = \mathbf{g}^T(t)\mathbf{B}^T\mathbf{B}\mathbf{g}(t). \quad (\text{A.7})$$

This leads to

$$\rho^2(t) = \eta g_1^2(t) + \lambda g_2^2(t) + 2\sqrt{\eta\lambda - (\det \mathbf{G})^{-2}} g_1(t)g_2(t) \quad (\text{A.8})$$

where the two new parameters are

$$\eta = B_{11}^2 + B_{21}^2 = ((\rho_0 \dot{g}_2(0) - \dot{\rho}_0 g_2(0))^2 + g_2^2(0)\rho_0^{-2}) / \det \mathbf{G}^2 \quad (\text{A.9})$$

$$\lambda = B_{22}^2 + B_{12}^2 = ((\rho_0 \dot{g}_1(0) - \dot{\rho}_0 g_1(0))^2 + g_1^2(0)\rho_0^{-2}) / \det \mathbf{G}^2. \quad (\text{A.10})$$

It is interesting to recognize so-called Ermakov–Lewis invariants satisfied by the basis solutions $g_1(t)$, $g_2(t)$ (see [11] and original references [18, 19])

$$\mathcal{L}_j = \frac{1}{2}((\rho_0 \dot{g}_j(0) - \dot{\rho}_0 g_j(0))^2 + g_j^2(0)\rho_0^{-2}). \quad (\text{A.11})$$

In terms of these we find the alternative expressions:

$$\eta = 2\mathcal{L}_1 / \det \mathbf{G}^2 \quad \lambda = 2\mathcal{L}_2 / \det \mathbf{G}^2. \quad (\text{A.12})$$

This results in a formal relation between any Milne solution specified by initial conditions and any non-singular basis for the corresponding oscillator equation:

$$\rho^2(t) = \frac{2}{\det \mathbf{G}^2} \left(\mathcal{L}_1 g_1^2(t) + \mathcal{L}_2 g_2^2(t) + \sqrt{4\mathcal{L}_1 \mathcal{L}_2 - \det \mathbf{G}^2} g_1(t) g_2(t) \right). \quad (\text{A.13})$$

This equation includes two Lewis invariants rather than one [15]. Moreover, this relation is valid for complex parameter functions $\omega^2(t)$. For the present purposes we treat the version in (A.8) as our basic result for ρ^2 .

Some specific examples. For stationary initial conditions ($\dot{\rho}_0 = 0$) and a standard real basis ($g_1(0), g_2(0) = (1, 0)$ and ($\dot{g}_1(0), \dot{g}_2(0) = (0, 1)$), we have from (A.9) and (A.10) the explicit expressions

$$\eta = \rho_0^2 \quad \lambda = \rho_0^{-2} \quad \text{with} \quad \det \mathbf{G} = 1. \quad (\text{A.14})$$

For a standard complex basis ($g_1(0), g_2(0) = (1, 1)$ and ($\dot{g}_1(0), \dot{g}_2(0) = (i, -i)$), we find instead

$$\eta = \frac{1}{4} (\rho_0^2 - \rho_0^{-2}) \quad \lambda = \frac{1}{4} (\rho_0^2 - \rho_0^{-2}) \quad \text{with} \quad \det \mathbf{G} = -2i. \quad (\text{A.15})$$

The Milne solution (A.8) is still the same function of time, as can be verified from these two examples.

Example 5 (The rectangular-pulse amplitude function). Symmetry solutions for the rectangular pulse are obtained in example 2. In the pulse region, $x_1(t)$ and $x_2(t)$ satisfy the same second-order differential equation. However, the first-order differential equations constrain the basis for $x_2(t)$ to be some linear combination of the basis for $x_1(t)$. We show in this example how a stationary Milne solution develops in the different components $x_1(t)$ and $x_2(t)$. With the specific basis for $x_1(t)$

$$g_1(t) = C_1(t) = \cos(\gamma t)/\sqrt{\gamma} \quad g_2(t) = S_1(t) = \sin(\gamma t)/\sqrt{\gamma} \quad t < T \quad (\text{A.16})$$

the stationary Milne solution at $t = 0$ is described by

$$\eta = \gamma \rho_0^2 \quad \lambda = \gamma^{-1} \rho_0^{-2} \quad \det \mathbf{G} = 1. \quad (\text{A.17})$$

Inserting into (A.8) we get

$$\rho_1^2(t) = \rho_0^2 \cos^2(\gamma t) + \gamma^{-2} \rho_0^{-2} \sin^2(\gamma t) \quad t < T. \quad (\text{A.18})$$

For this to be truly constant inside the pulse we choose the initial value

$$\rho_0 = 1/\sqrt{\gamma}. \quad (\text{A.19})$$

Then we have

$$\rho_1^2(t) = g_1^2(t) + g_2^2(t) = \frac{1}{\gamma} (\cos^2(\gamma t) + \sin^2(\gamma t)) = 1/\gamma \quad t < T. \quad (\text{A.20})$$

With the different basis for $x_2(t)$,

$$g_1(t) = C_2(t) = \beta \cos(\gamma t)/\sqrt{\gamma} + i\sqrt{\gamma} \sin(\gamma t) \quad t < T \quad (\text{A.21})$$

$$g_2(t) = S_2(t) = -i\sqrt{\gamma} \cos(\gamma t) + \beta \sin(\gamma t)/\sqrt{\gamma} \quad t < T \quad (\text{A.22})$$

the stationary Milne solution at $t = 0$ is described by

$$\eta = \beta^2 \gamma \rho_0^2 - \gamma \rho_0^{-2} \quad \lambda = -\gamma^3 \rho_0^2 + \beta^2 \gamma^{-1} \rho_0^{-2} \quad \det \mathbf{G} = -1. \quad (\text{A.23})$$

Choosing the same initial condition (A.19) these expressions simplify to $\eta = \lambda = -1$ and the corresponding Milne solution satisfies

$$\rho_2^2(t) = -g_1^2(t) - g_2^2(t). \quad (\text{A.24})$$

Inserting the basis functions we again get the constant behaviour (A.19)–(A.20) in the pulse region.

References

- [1] Landau L D and Lifshitz E M 1965 *Quantum Mechanics: Nonrelativistic Theory* (New York: Pergamon)
- Merzbacher E 1970 *Quantum Mechanics* (New York: Wiley)
- [2] Landau L D 1965 *Collected Papers of L D Landau* (Oxford: Pergamon)
- Zener C 1932 *Proc. R. Soc. A* **137** 696
- [3] Nikitin E E 1968 *Chem. Phys. Lett.* **2** 402
- Rosen N and Zener C 1932 *Phys. Rev.* **40** 502
- [4] Shore B W 1990 *The Theory of Coherent Atomic Excitation* vols 1, 2 (New York: Wiley)
- [5] Bergmann K, Theuer H and Shore B W 1998 *Rev. Mod. Phys.* **70** 1003
- [6] Berman P R, Lixin Yan, Keng-Hwee Chiam and Ruwang Sung 1998 *Phys. Rev. A* **57** 79
- [7] Nesbitt B S, Crothers D S F, O'Rourke S F C and Berman P R 1997 *Phys. Rev. A* **56** 1670
- [8] Boyd J K 2000 *J. Math. Phys.* **41** 4330
- [9] Thylwe K-E and Korsch H J 2001 *J. Phys. A: Math. Gen.* **34** 3497
- [10] Milne W E 1930 *Phys. Rev.* **35** 863
- [11] Thylwe K-E and Korsch H J 1998 *J. Phys. A: Math. Gen.* **31** L279
- [12] Fulling S A 1978 *J. Math. Phys.* **20** 1202
- [13] Boiron M, Lombardi M and Wiesenfeld L 1997 *J. Phys. A: Math. Gen.* **30** 3907
- [14] Ahmed Z 2001 *Phys. Lett. A* **286** 231
- [15] Matzkin A 2000 *Phys. Rev. A* **63** 012103
- [16] Reinisch G 1997 *Phys. Rev. A* **56** 3409
- [17] Haas F and Goedert J 1999 *J. Phys. A: Math. Gen.* **32** 2835
- [18] Ermakov V P 1880 *Univ. Izv. Kiev Serie III* **9** 1
- [19] Lewis H R 1968 *J. Math. Phys.* **9** 1976
- Lewis H R and Riesenfeldt W B 1969 *J. Math. Phys.* **10** 1458
- Lewis H R and Leach P G L 1982 *J. Math. Phys.* **23** 237