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Abstract

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Analytic solution of the two-state problem

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An exact solution of the time-dependent Schrödinger equation is obtained for a simple model with only two quantum states. The calculated transition probability involves only exponential and hyperbolic functions.

Analytic solutions of the time-dependent Schrödinger equation are sometimes useful in dynamical studies. For the case of only two quantum states, many analytic solutions[1-3] have been found in the course of various studies of atomic collisions, magnetic resonance, and quantum optics. Here, we call attention to a simple analytic solution that appears to be new; it should be useful in various areas of physics. The time-dependent Hamiltonian has a simple form, and the wave functions can be written in terms of confluent hypergeometric functions. A natural choice of the initial and final times will be used to avoid explicit computation of these functions, with the results that the S matrix can be written in terms of Γ functions and the transition probability involves only exponential and hyperbolic functions.

The Schrödinger equation for the two-state problem may be written as

$$i\frac{d}{dt}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}\Delta(t) & -\frac{1}{2}\Omega^*(t) \\ -\frac{1}{2}\Omega(t) & \frac{1}{2}\Delta(t) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, \tag{1}$$

where a_1 and a_2 are time-dependent probability amplitudes for states 1 and 2, t is the time, and $\hbar=1$. The 2×2 Hamiltonian matrix contains only two arbitrary functions of t, because we have chosen a phase factor so that the trace vanishes at all times. $\Delta(t)$ can be regarded as the detuning of an applied oscillating force having amplitude proportional to $\Omega(t)$, which is often called the Rabi frequency. However, the oscillation frequency calculated by Rabi,[2] for the case of constant Δ and Ω, is $(|\Omega|^2+\Delta^2)^{1/2}$.

In the simple model treated here,

$$\Omega(t)=\frac{2\alpha}{z^{1/2}}\frac{dz}{dt}, \quad \Delta(t)=\left[\pm 1+\frac{\beta}{z}\right]\frac{dz}{dt}. \tag{2}$$

Here, $z(t)$ is real and α may be complex; $z(t)$ is an arbitrary monotonic function. The arbitrary parameters are α, β, and the ambiguous sign. Two independent solutions of (1) can be written in terms of confluent hypergeometric functions,[4] and they can be used to satisfy initial conditions applied at any particular values of t and z. To simplify the application of initial conditions and the resulting final occupation probabilities, we assume that the initial and final times correspond to $z\to 0$ and $z\to +\infty$, or vice versa. Note that $|\Omega(t)|$ is vanishingly small compared to $|\Delta(t)|$ in these two limits, unless $\beta=0$. We can choose $z(t)$ so that $\Omega(t)$ vanishes at the initial and final times, which are the beginning and end of a pulse applied to the two-state system. We shall obtain definite limits for the two occupation probabilities as $z\to 0$ and as $z\to +\infty$, even if $\beta=0$. These limits depend on α and β, not on the choice of $z(t)$. One of them is the transition probability calculated below.

We should mention that the detuning function obtained from (2) changes sign if $\pm\beta<0$, whereas $\Omega(t)$ has a fixed sign or is complex. The area theorem of McCall and Hahn[5] leads us to mention that

$$\int_{-\infty}^{+\infty}|\Omega(t)|dt=+\infty \tag{3}$$

holds for this model. This integral is dimensionless, and is finite if we arrange for $z(t)$ to vary through a finite range. However, the simplifying assumption in the preceding paragraph requires an infinite range.

Examples of pulse shapes applied to two-state systems can be derived from (2). In our first example, $z(t)=\frac{1}{2}ct^2$, where c is a positive constant. This means that t varies from $-\infty$ to 0 or from 0 to $+\infty$. We find that $\Omega(t)=2^{3/2}\alpha c^{1/2}$ is a constant, and

$$\Delta(t)=\pm ct+2\beta/t$$

is a simple function. If $\beta=0$, this example is rather similar to the Landau-Zener model,[1] in which $\Omega(t)$ is constant and $\Delta(t)$ is proportional to t. The difference is that t varies from $-\infty$ to $+\infty$ in the Landau-Zener model, so that $\Omega(t)/\Delta(t)$ vanishes at the beginning and end of the process. Our calculations do not apply to this model, but Wannier[6] uses one of the confluent hypergeometric functions to give a concise derivation of the final occupation probabilities.

In a second example, $\Delta(t)$ is a nonzero constant, which we call Δ_0. The calculation of $\Omega(t)$ is taken from a recent paper,[7] which treats a three-state generalization of the present model. We assume that t varies from $-\infty$ to $+\infty$. This requires $\pm\beta>0$. We find

$$\Omega(t)=\frac{\pm\Delta_0\alpha}{|\beta|^{1/2}}\left[\frac{z}{|\beta|}\right]^{1/2}\left[\frac{z}{|\beta|}+1\right]^{-1},$$

where $z(t)$ is given implicitly by

$$\pm z-\beta+\beta\ln(z/|\beta|)=\Delta_0 t\ .$$

The pulse shape shown in Fig. 1 is applicable to all these cases of constant detuning.

For both examples, and for any other example derived from (2), the transition probability can be found by explicit solution of (1). In the first place, suppose that $z(t)$ increases from 0 to $+\infty$ during the process considered, and that the two-state system is certainly in state 1 at the initial time ($z=0$). The appropriate solution of (1) and (2) is

$$a_1=z^{(1/2)i\beta}\exp(\pm\tfrac{1}{2}iz)F(\mp i|\alpha|^2;\tfrac{1}{2}+i\beta\ ;\mp iz)$$

and

$$a_2=\frac{\alpha}{\beta-\frac{1}{2}i}z^{(1/2)(1+i\beta)}\exp(\pm\tfrac{1}{2}iz)$$
$$\times F(1\mp i|\alpha|^2;\tfrac{3}{2}+i\beta\ ;\mp iz)\ ,$$

where

$$F(A;B;x)=1+\frac{A}{B}\frac{x}{1!}+\frac{A(A+1)}{B(B+1)}\frac{x^2}{2!}+\cdots$$

is Kummer's series.[8] The behavior of a_1 and a_2 as $z\to+\infty$ is found from the asymptotic expansion[4]

$$F(A;B;x)\sim\frac{\Gamma(B)}{\Gamma(A)}e^x x^{A-B}\left[1+\frac{\text{const}}{x}\right]$$
$$+\frac{\Gamma(B)}{\Gamma(B-A)}(-x)^{-A}\left[1+\frac{\text{const}}{x}\right],$$

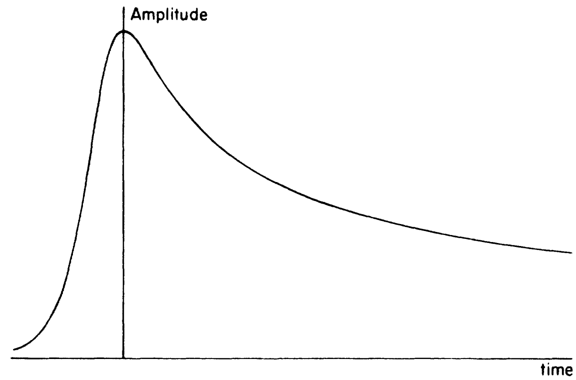

FIG. 1. Amplitude of applied oscillating force, for the case of constant detuning. Time increases to the right or the left, as desired. The long tail on the right is consistent with (3).

and the final occupation probabilities are

$$\lim_{z\to+\infty}|a_1|^2=\frac{\exp(-\pi|\alpha|^2)\cosh(\pi|\alpha|^2\pm\pi\beta)}{\cosh(\pi\beta)}$$

and

$$\lim_{z\to+\infty}|a_2|^2=\frac{\exp(-\pi|\alpha|^2\mp\pi\beta)\sinh(\pi|\alpha|^2)}{\cosh(\pi\beta)}\ . \tag{4}$$

The transition probability is this last limit. It is an increasing function of $|\alpha|$ and a decreasing function of $\pm\beta$. For fixed $|\alpha|$ and $|\beta|$, the transition probability is therefore largest when $\pm\beta$ is negative; this means that a change of the sign of $\Delta(t)$ favors transitions.

The transition probabilities for other cases need not be computed separately. The probability of transitions from state 2 to state 1 is given by (4), and the transition probabilities for the case of $z(t)$ decreasing from $+\infty$ to 0 are also given by (4). All these transition probabilities are equal, because the S matrix is a unitary 2×2 matrix.

A simple analytic solution of the two-state problem has been presented here, and it could have applications in many areas of physics.

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