

Simulation of quantum systems with the coupled channel method

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We describe a computational method for simulating time-dependent quantum mechanical systems interacting with external fields. In this method, the Schrödinger equation is solved by expanding the wave function in the basis set of the unperturbed Hamiltonian. The expansion yields a set of coupled ordinary differential equations for the expansion coefficients. This coupled channel method can be applied to many time-dependent problems. We apply the coupled channel method to a particle in a box interacting with a laser pulse. We show that if only two states are involved, the method leads naturally to the solutions for Rabi flopping, and that the system exhibits Rabi flopping behavior even with realistic, nonmonochromatic laser pulses. We also discuss instances where simulations could improve the understanding or address misconceptions of beginning students in quantum mechanics. © 2008 American Association of Physics Teachers.

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I. INTRODUCTION

Like any subject in physics, quantum mechanics has its fair share of conceptual difficulties to beginning students. These difficulties often manifest themselves as alternative conceptions (or misconceptions) in the students' understanding.^{1,2} There are little direct visual aids or intuitive experience when learning quantum mechanics, as there are for classical mechanics.³ In addition, there are fewer exactly solvable problems in quantum mechanics, especially time-dependent problems, that would help students gain a better understanding.

Computer simulations can help to address the misconceptions by visualizations.⁴ The simulations broaden the scope of the type of problems that can be studied and may be viewed as virtual experiments with adjustable parameters.

In this paper we describe the coupled channel method for the simulation of quantum systems. The method is introduced in Sec. II where the time-dependent Schrödinger equation is reduced to a set of coupled ordinary differential equations. We apply the method in Sec. III mainly to a particle in a box interacting with a laser field. We calculate the excitation probabilities as well as the particle density as a function of time. In Sec. IV we show how the coupled channel method for a two-state system leads naturally to Rabi flopping. We conclude in Sec. V with suggestions of student projects for further exploration.

II. THE COUPLED CHANNEL METHOD

The coupled channel method is commonly used in atomic physics.^{5,6} The coupled channel method attempts to solve the time-dependent Schrödinger equation by expanding the wave function in the basis set of the unperturbed Hamiltonian. The result consists of a set of coupled ordinary differential equations for the expansion coefficients. The coupled channel method can be applied to many time-dependent problems and can use any higher order numerical solutions developed for ordinary differential equations. It represents an alternative approach to solving the time-dependent Schrödinger equation, such as by a direct discretization of time and space.⁷⁻⁹

In the following we consider a quantum system with an external field. We assume that the external field is turned on at $t=0$ and turned off at $t=\tau$.

Let H_0 be the unperturbed Hamiltonian of the isolated system in one dimension. The unperturbed Hamiltonian is assumed to be solvable with known eigenfunctions u_n and eigenenergies E_n . The eigenfunctions u_n are orthonormal and satisfy

$$H_0 u_n(x) = E_n u_n(x) \quad (1a)$$

$$\int u_m^*(x) u_n(x) dx = \delta_{mn}. \quad (1b)$$

The u_n forms a complete basis set¹⁰ for all n , that is, any function can be expanded in terms of u_n .

With the external field turned on, the full Hamiltonian H of the system consists of the unperturbed H_0 plus the interaction $V(x, t)$. Let $\psi(x, t)$ be the wave function of the perturbed system. Then ψ evolves in time according to

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \quad (2)$$

with $H=H_0+V$. To solve for ψ , we expand it in the complete basis set u_n as

$$\psi(x, t) = \sum_n a_n(t) u_n(x) \exp(-iE_n t/\hbar), \quad (3)$$

where $a_n(t)$ are the expansion coefficients or the amplitudes in the interaction picture because of the explicit inclusion of the time factor $\exp(-iE_n t/\hbar)$. The task of solving for the wave function ψ is turned into the task of finding the coefficients a_n . All observables can be obtained once $a_n(t)$ are known. For example, the probability of finding the system in state n is given by

$$P_n(t) = |a_n(t)|^2, \quad (4)$$

with $\sum_n |a_n(t)|^2 = 1$.

To determine the coefficients $a_n(t)$, we substitute the wave function $\psi(x, t)$ of Eq. (3) into Eq. (2). We take the time derivative on the left-hand side of Eq. (2) and use the fact that $H_0 u_n = E_n u_n$ on the right-hand side to obtain

$$\begin{aligned} \sum_n \left(E_n a_n(t) + i\hbar \frac{da_n(t)}{dt} \right) u_n(x) e^{-iE_n t/\hbar} \\ = \sum_n (E_n + V) a_n(t) u_n(x) e^{-iE_n t/\hbar}. \end{aligned} \quad (5)$$

The terms involving $E_n a_n(t)$ on both sides of Eq. (5) cancel, leading to

$$i\hbar \sum_n \frac{da_n(t)}{dt} u_n(x) e^{-iE_n t/\hbar} = \sum_n a_n(t) V u_n(x) e^{-iE_n t/\hbar}. \quad (6)$$

With the help of Eq. (1b), the left-hand side of Eq. (6) may be collapsed to a single term by projection onto the state m . The result is

$$\frac{da_m(t)}{dt} = -\frac{i}{\hbar} \sum_n a_n(t) V_{mn}(t) \exp(i\omega_{mn}t). \quad (7)$$

The transition matrix element V_{mn} is given by¹⁰

$$V_{mn}(t) = \int u_m^*(x) V(x, t) u_n(x) dx, \quad (8)$$

where the transition frequency $\omega_{mn} = (E_m - E_n)/\hbar$. Note that $V_{mn}(t)$ is independent of x and is a function of time only.

Equation (7) is the desired result of the coupled channel method. The amplitude of one channel (state) depends on all the other channels. Equation (7) is exact, provided the sum includes all the channels. But in practice, we can include only a finite number of channels, say $n=1$ to N . Usually, the larger the N , the better the approximation. With the sum truncated to N terms, Eq. (7) forms a closed system of N coupled ordinary differential equations. It may be solved numerically with well-known techniques such as the Runge-Kutta method.^{7-9,11}

If the system is in the ground state $n=1$ at $t=0$, the N amplitudes can be computed from Eq. (7) subject to the initial condition

$$a_n(0) = \begin{cases} 1 & \text{if } n = 1, \\ 0 & \text{if } n \neq 1. \end{cases} \quad (9)$$

Although the initial values of $a_n(0)$ in Eq. (9) are real, the amplitudes at later times, $a_n(t)$, will generally be complex. If the chosen programming language has support for complex arithmetic, we can work directly with Eq. (7). Occasions arise when real arithmetic is desired, either due to lack of native support for complex numbers, or reasons such as efficiency. In this case, real versions of Eq. (7) can be obtained by separating the real R_n and imaginary I_n parts of a_n as

$$a_n(t) = R_n(t) + iI_n(t). \quad (10)$$

We substitute Eq. (10) into Eq. (7), equate the real and imaginary parts on both sides, and obtain two equations involving only real numbers, as

$$\frac{dR_m(t)}{dt} = \frac{1}{\hbar} \sum_n (R_n(t) \sin(\omega_{mn}t) + I_n(t) \cos(\omega_{mn}t)) V_{mn}(t), \quad (11a)$$

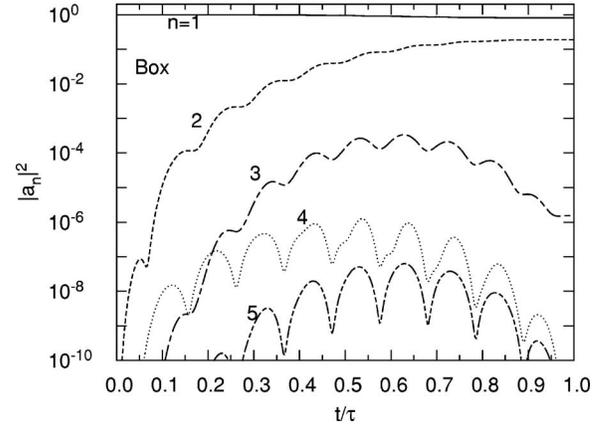


Fig. 1. Excitation probabilities of a particle in a box in a laser field as a function of time. The box width is 2 \AA . The laser center frequency is resonant with the transition between the ground state $n=1$ and the first excited state $n=2$. The laser duration is $\tau=40$ and the field amplitude is $F_0=1/8$.

$$\frac{dI_m(t)}{dt} = \frac{1}{\hbar} \sum_n (I_n(t) \sin(\omega_{mn}t) - R_n(t) \cos(\omega_{mn}t)) V_{mn}(t). \quad (11b)$$

We have assumed that V_{mn} is real, which is generally true. The results in this paper are calculated with real numbers by integrating the $2N$ differential equations of Eq. (11).

III. PARTICLE IN A BOX IN A LASER FIELD

As an example, we apply the coupled channel method to an electron in an infinite potential well and interacting with a laser field. The well-known unperturbed eigenfunctions and eigenenergies are $u_n(x) = \sqrt{2/L} \sin(n\pi x/L)$ and $E_n = \pi^2 \hbar^2 n^2 / 2m_e L^2$, where L is the width of the box and m_e is the electron mass.

The laser can be specified as a pulse of electric field $F(t)$.¹² A proper choice for $F(t)$ is

$$F(t) = F_0 \sin^2(\pi t/\tau) \cos(\omega_L t), \quad (0 \leq t \leq \tau). \quad (12)$$

Here F_0 is the field amplitude, τ is the laser duration, and ω_L is the laser center frequency. The function $\sin^2(\pi t/\tau)$ is also known as the envelope function.

The laser-electron interaction is given by

$$V(x, t) = eF(t)(x - L/2), \quad (13)$$

where e is the electron charge. For convenience, the zero-point potential is chosen at $x=L/2$. The matrix element in Eq. (8) is

$$V_{mn}(t) = eF(t) \langle m | x - L/2 | n \rangle = eF(t) (x_{mn} - \delta_{mn} L/2), \quad (14)$$

with

$$x_{mn} = \begin{cases} \frac{L}{2} & \text{if } m = n \\ 0 & \text{if } m \neq n \text{ and } m+n \text{ is even} \\ -\frac{8L}{\pi^2} \frac{mn}{(m^2 - n^2)^2} & \text{if } m \neq n \text{ and } m+n \text{ is odd.} \end{cases} \quad (15)$$

In Fig. 1 we show the results for an electron in a box of

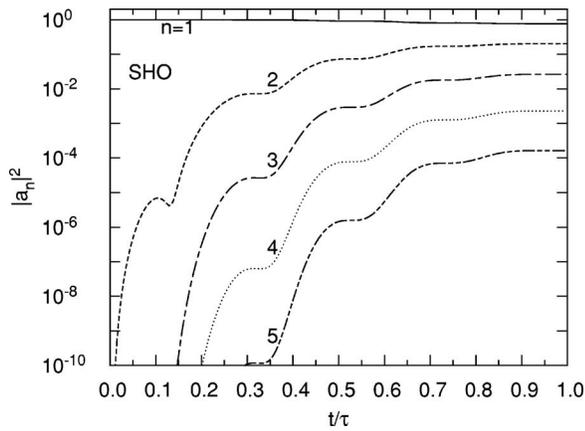


Fig. 2. Excitation probabilities of the simple harmonic oscillator in a laser field as a function of time. The laser center frequency is resonant with the natural frequency of the simple harmonic oscillator. The laser duration is $\tau=20$ and the field amplitude is $F_0=1/8$.

width $L=2 \text{ \AA}$. Numerically, it is easier not to use SI units, but rather to use a natural unit system such as atomic units. We found it convenient to use a similar system, which we call box units. In these units the unit of length is 1 \AA , the unit of mass is the electron mass, and the unit of energy is the ground state energy in a box of 1 \AA (37.5 eV). The unit of time is $1.75 \times 10^{-17} \text{ s}$, and the unit of the electric field is $3.75 \times 10^{11} \text{ V/m}$. Unless otherwise stated, all quantities are in box units.

Five channels $N=5$ were included in the simulation results of Fig. 1. The laser center frequency is chosen to be resonant with the transition between the first two states $n=1$ and $n=2$, $\omega_L=3/4$. Therefore, the primary excitation channel is to the $n=2$ state (see Fig. 1). When the laser is turned on, the excitation probability increases rapidly, followed by a plateau near the end of the laser pulse. The dominance of the $n=2$ excitation remains throughout the duration of the laser, reaching a final value of about 0.2 for this moderately strong laser (amplitude $F_0=1/8$).

For the particle in the box (Fig. 1), the excitation probabilities to nonresonant states ($n=3, 4, 5$), are small but non-zero. The small probabilities are mostly due to the fact the laser pulse has a finite duration and an envelope that broadens the center frequency, causing finite but negligible excitations to nonresonant states. A noticeable anomaly may be seen at the beginning where the probability for the $n=3$ state is below the $n=4$ state but crosses over at $t/\tau \approx 0.2$. By symmetry [see Eq. (15)], the direct transition from $n=1$ to $n=3$ is dipole-forbidden, but is dipole-allowed to $n=4$. This (first order) selection rule is responsible for the initially suppressed excitation to $n=3$. Second (or higher) order processes eventually take over so the $n=3$ state is populated, though still negligible compared to $n=2$. For these resonant transitions the results would not change much if only two states ($n=1, 2$) were included. There are also small-scale oscillations in Fig. 1 that are caused by the more rapid oscillations of the laser itself [the $\cos(\omega_L t)$ term] around the center frequency.

The same procedure was used to compute the results for the simple harmonic oscillator (Fig. 2). The matrix element x_{mn} for the simple harmonic is given by

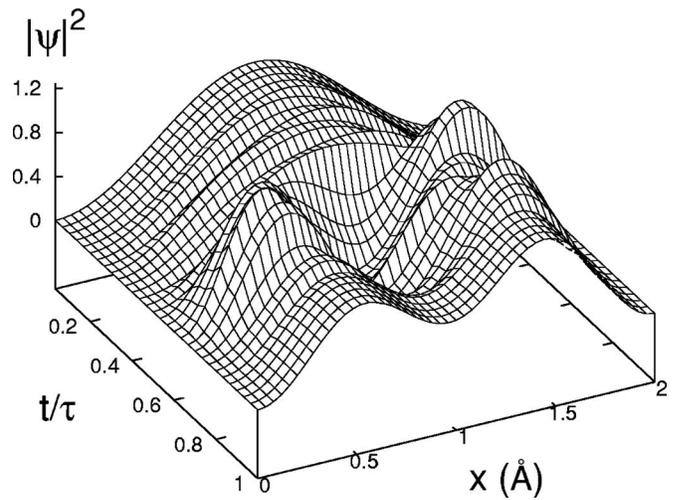


Fig. 3. The particle density, $|\psi(x,t)|^2$, of a particle in a box in a laser field. The parameters are the same as in Fig. 1, except for the laser field amplitude $F_0=5/8$.

$$x_{mn} = \sqrt{\frac{\hbar}{2m_e\omega}} [\sqrt{m}\delta_{m,n+1} + \sqrt{m+1}\delta_{m,n-1}], \quad (16)$$

where ω is the angular frequency of the simple harmonic oscillator. For the resonant transitions considered here, $\omega = \omega_L$. The quantum numbers m, n start from zero, and the zero-point potential is at $x=0$ instead of $L/2$ [see Eq. (13)]. Because the simple harmonic oscillator has equal energy-level spacing, the laser frequency is resonant with all transitions between neighboring states ($m=n \pm 1$). Because the transition matrix elements in Eq. (16) connect the same neighboring states, transitions can proceed from the ground state up the “ladder” to higher states, which cannot happen resonantly for the particle in a box. As a result, the second and higher excited states have much larger probabilities than the particle in the box at the end of the laser pulse. For this reason, the pulse duration for the simple harmonic oscillator was chosen to be shorter ($\tau=20$). Longer pulses would require more (than five) channels to be included.

The temporal-spatial electron density, $|\psi(x,t)|^2$, is shown in Fig. 3 for a stronger laser, $F_0=5/8$. The relatively strong field induces large changes in the electron density, from the initial peak at the center of the box to the valley at the end of the laser pulse.

The twin peaks near the sides are not symmetrical about the center of the box, so we can conclude from Fig. 3 that the average position of the particle $\langle x \rangle$ is not exactly at $L/2$ and is changing with time. A discussion aimed at some misconceptions of beginning students of quantum mechanics might lead to the opposite (but obviously incorrect) conclusion that the $\langle x \rangle$ should be a constant at $L/2$.^{4,13} The results of numerical calculations may be helpful in confronting certain conceptual difficulties in an introductory quantum mechanics course.

IV. RABI FLOPPING

As seen in Sec. III, only the two states resonant with the laser center frequency contribute substantially to the transi-

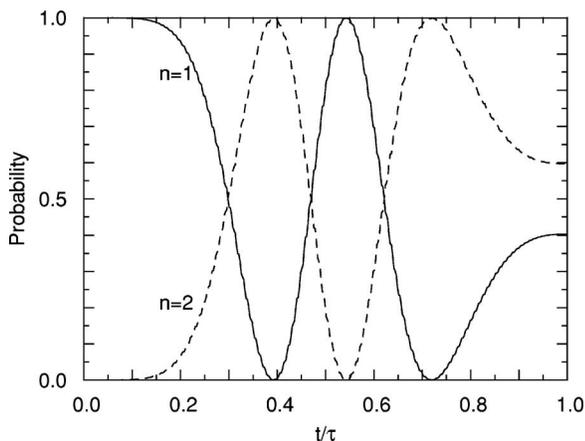


Fig. 4. The two-state Rabi flopping of a particle in a box in a laser field of finite duration. The parameters are the same as in Fig. 1, except for the laser duration $\tau=480$.

tions. The resulting dynamics can be understood in terms of Rabi flopping, an important concept in the behavior of a two-state quantum system.¹⁴

The two-state system is exactly solvable for simple interactions¹⁵ such as the monochromatic lasers discussed in Appendix A. According to Eq. (A6), the probabilities of finding the two states at time t are

$$P_1(t) = |a_1(t)|^2 = \cos^2(\Omega_R t), \quad (17a)$$

$$P_2(t) = |a_2(t)|^2 = \sin^2(\Omega_R t). \quad (17b)$$

Clearly, $P_1(t) + P_2(t) = 1$, as required by Eq. (4). The two states flip-flop back and forth with the Rabi frequency Ω_R given by Eq. (A5). The flopping frequency can be controlled through the interaction strength V_0 in Eq. (A2). Rabi flopping occurs in many situations, such as nuclear magnetic resonance, quantum computing, and optics.^{14,16}

An example of Rabi flopping for a particle in a box is shown in Fig. 4. The calculation is done using Eq. (A3) without the rotating wave approximation (see Appendix A). For the given field amplitude $F_0=1/8$ and box width $L=2$, the Rabi frequency from Eq. (A5) is $2/9\pi^2$. The oscillation period is $9\pi^3/2 \approx 140$. The duration of the laser is chosen to be $\tau=480$, relatively long so Rabi flopping can form.

Due to the initial ramping up of the laser, Rabi flopping does not begin until about $t/\tau \approx 0.1$ (Fig. 4). It goes through about 1.5 full oscillations before the back end of the envelope (around $t/\tau \approx 0.8$) terminates the process. (A dynamic simulation is given in Ref. 17 that displays the Rabi flopping and the particle density.) In a complete cycle the two states are populated and depopulated completely and complementarily. The complete cycles can be well understood from Eq. (17), an idealized situation for infinitely long, monochromatic light. Although no simple analytic solutions for Rabi flopping are known with a realistic laser pulse described by Eq. (12), the numerical solutions are straightforward and the results demonstrate the universal nature of the important phenomenon. The longer the pulse, the greater number of complete oscillations. Closer examination of the curves in Fig. 4 also shows small, periodic steps of probability fluctuations. The origin of the steps is the same as the oscillations seen in Fig. 1: it is due to the faster center frequency of the laser on a smaller time scale.

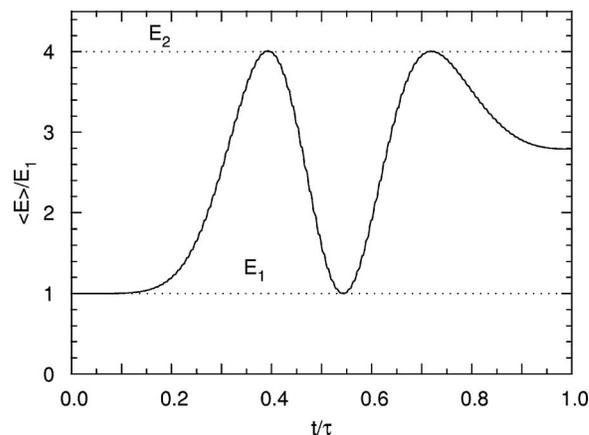


Fig. 5. The energy of the two-state system in Rabi flopping as a function of time. The parameters are the same as in Fig. 1, except for the laser duration $\tau=480$. The lower and the upper dotted lines indicate the energies of the $n=1$ and $n=2$ states, respectively.

The energy of the two-state system corresponding to the same Rabi flopping process is shown in Fig. 5. As expected, the average energy varies between the two states. The average energy can be obtained by $\langle E \rangle = E_1|a_1|^2 + E_2|a_2|^2$, unlike the analogous expression for the average position. The system exchanges energy with the external field by absorbing and emitting virtual photons continuously. This example shows that the transitions take time, and there is no sudden “jump” in the energy, a common misconception of students carried over from introductory modern physics courses where quantum transitions are first introduced.

V. SUMMARY AND DISCUSSION

We have described the coupled channel method for simulating time-dependent quantum systems. In this method the Schrödinger equation is expanded in the basis set of the unperturbed Hamiltonian, reducing it to a set of coupled ordinary differential equations for the expansion coefficients.

When only two states are involved, the coupled channel method leads naturally to analytic solutions for Rabi flopping within the rotating-wave approximation and for monochromatic light. Numerical results obtained with the coupled channel method show that the particle in a box exhibits universal Rabi flopping with nonmonochromatic laser pulses.

There are several types of possible student projects. One might start from Fig. 1 with a simple change of parameters such as the pulse duration or the laser strength, and the laser center frequency, or change the envelope function (to a Gaussian, for example). Other possibilities include changing the initial condition so that the system starts from a coherent state (a mixture of two or more states) to simulate quantum beats, and calculating expectation values such as $d\langle x \rangle / dt$ and $d^2\langle x \rangle / dt^2$, and comparing them to the momentum $\langle p \rangle$ and the force $F(t)$, respectively. For more advanced projects students could calculate the decay time of the initial state for different field strengths F_0 (finding the slope of the $n=1$ curve in Fig. 1), or calculate the excitation probabilities as a function of F_0 and compare with perturbation results.

The coupled channel method may be used for other interacting systems such as the simple harmonic oscillator and atomic hydrogen, as long as the transition matrix elements

can be readily evaluated (in case N is large). It should be possible to explore the simple harmonic oscillator further, such as the effect of quasirevivals in the driven simple harmonic oscillator for longer pulses. The ladderlike transitions, discussed following Fig. 2, can lead to an almost total reversal of the initial configuration: the ground state can be completely depopulated, while the highest channel in the system is fully populated. This behavior of state revival is similar to the quantum revival of an unperturbed system.¹⁸

There is one limitation to the coupled channel method: if continuum states are open and contribute significantly, for example, if ionization occurs, the method needs to be modified, either by discretizing the continuum or by using pseudostates.¹² This limitation is not a problem if the system does not possess continuum states as for the particle in a box, or if the photon energy is not resonant with the continuum states so that their contribution is negligible.

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APPENDIX A: RABI OSCILLATIONS

We assume the two states to be the ground state with energy E_1 and the first excited state with E_2 . To see Rabi flopping most clearly, we assume that the laser field is monochromatic and its center frequency is equal to the transition frequency, $\omega_L = \omega = (E_2 - E_1)/\hbar$, as

$$f(t) = F_0 \cos(\omega t). \quad (\text{A1})$$

This form of the laser field is used only to simplify the derivation of Rabi flopping. In all the numerical calculations, the realistic pulse Eq. (12) is used.

The transition matrix elements can be obtained with the help of Eq. (15) as

$$V_{11} = V_{22} = 0, \quad V_{12} = V_{21} = V_0 \cos(\omega t), \quad (\text{A2})$$

where $V_0 = -16eLF_0/9\pi^2$.

Substitution of Eq. (A2) into Eq. (7) for $N=2$ yields

$$\frac{da_1}{dt} = -\frac{iV_0}{2\hbar} a_2 (1 + \exp(-2i\omega t)), \quad (\text{A3a})$$

$$\frac{da_2}{dt} = -\frac{iV_0}{2\hbar} a_1 (1 + \exp(+2i\omega t)). \quad (\text{A3b})$$

Although Eq. (A3) is readily solvable, a further approximation is useful. Over a time long compared to $1/\omega$, the factors $\exp(\pm 2i\omega t)$ in Eq. (A3) undergo many oscillations, and their average value will be zero so that we can then ignore them in Eq. (A3). This approximation is the well-known rotating wave approximation.¹⁵ The simplified equations are

$$\frac{da_1}{dt} = -\frac{iV_0}{2\hbar} a_2 \quad \text{and} \quad \frac{da_2}{dt} = -\frac{iV_0}{2\hbar} a_1. \quad (\text{A4})$$

Equation (A4) is equivalent to the following second-order differential equations

$$\frac{da_{1,2}^2}{dt^2} + \Omega_R^2 a_{1,2} = 0, \quad (\text{A5})$$

where $\Omega_R = |V_0|/2\hbar$ is the Rabi frequency.

The solution subject to the initial condition $a_1(0)=1$, $a_2(0)=0$ is

$$a_1(t) = \cos(\Omega_R t), \quad a_2(t) = -i \sin(\Omega_R t). \quad (\text{A6})$$

Equation (A6) is the desired result in the rotating wave approximation of a two-state system driven by an external field.

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¹³One common misconception is to write the expectation value $\langle x \rangle = \sum_n |a_n|^2 \langle n|x|n \rangle$. By Eqs. (4) and (15), $\langle x \rangle = (\sum_n |a_n|^2) L/2 = L/2$. This approach is incorrect because $|n \rangle$ is not an eigenfunction of x . Also see Ref. 4.

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