Dynamics of two-level systems

We study the dynamics of two-level systems evolving under the influence of external forces of various kinds. The three cases studied are:

(a) A time independent external potential. This problem can be solved exactly and allows the accuracy of the perturbation solution to any order to be gauged.

(b) A sinusoidal off-diagonal perturbation, treated in the rotating wave approximation. This exactly soluble problem is of interest in connection with magnetic and optical resonance, and allows the phenomenon of “Rabi flopping” to be understood.

(c) A spin driven by a magnetic field precessing on the surface of a cone. This problem can be solved exactly and allows the accuracy of the perturbation and adiabatic approximations to be gauged.

The above topics are dealt with in the following three sections.

1. A time independent external potential

Let $H_0$ be the Hamiltonian of a two-level system whose ground and excited states $|1\rangle$ and $|2\rangle$, have energies $E_1$ and $E_2$, and let $\omega = (E_2 - E_1)/\hbar$ be the Bohr frequency of the transition between the levels. Suppose $H'$ is a time dependent perturbation acting on the system (this will be specialized to a time independent perturbation shortly). The Schrodinger equation for the system is

$$i\hbar \frac{d}{dt} |\psi\rangle = (H_0 + H') |\psi\rangle. \quad (1)$$

On substituting $|\psi\rangle = a_1(t) \exp\left(-\frac{i}{\hbar} E_1 t\right) |1\rangle + a_2(t) \exp\left(-\frac{i}{\hbar} E_2 t\right) |2\rangle$ into (1), one gets the following pair of coupled differential equations for the amplitudes $a_1$ and $a_2$:

$$\dot{a}_1 = -\frac{i}{\hbar} H_{12}^* e^{-i\omega t} a_2, \quad \dot{a}_2 = -\frac{i}{\hbar} H_{21}^* e^{i\omega t} a_1 \quad (2)$$

We have used the notation $H_{12}^* = \langle 1 | H' | 2 \rangle$ and $H_{21}^* = \langle 2 | H' | 1 \rangle$ and also assumed that the diagonal elements of the perturbation vanish i.e. $H_{11} = H_{22} = 0$. Equation (2) is just the Schrodinger equation for the two-level system written in the interaction or “Dirac” representation.

The pair of equations in (2) cannot be solved in closed form for an arbitrary time dependent Hamiltonian $H'$. The technique of time dependent perturbation theory consists of solving these equations iteratively to arbitrary order in the interaction strength $H'$.

**Ex.1.** Obtain a formal iterative solution to Eq.(2), to second order in $H'$, for the initial conditions $a_1(0) = a_{10}$ and $a_2(0) = a_{20}$. From the form of this solution, you should be able to write down the solution to all higher orders.

**Ex.2.** Specialize the solution of Ex.1 to a time independent perturbation $H'$ and verify that $|a_1(t)|^2 + |a_2(t)|^2 = 1$ up to terms of second order in $H'$. Use the parameterization $H_{12}^* = \hbar \kappa e^{-i\phi}$ and
obtain expressions for $a_i(t)$ and $a_\omega(t)$ in terms of the dimensionless real parameters $\nu_0 = 2\kappa/\omega_0$ and $\theta_0 = \omega_0 t/2$ before proceeding. Challenge: verify the normalization up to fourth order in $H'$. The computer algebra program Maple could prove helpful in tackling this challenge and the later ones.

**Ex.3.** Specialize the solution to Ex.2 to the simpler initial conditions $a_i(0) = 1$ and $a_\omega(0) = 0$ and use it to calculate the probability of finding the system in its excited state at time $t$ to second order in $H'$ (challenge: do it up to fourth order in $H'$). Express your answer in terms of the dimensionless quantities $\nu_0$ and $\theta_0$ introduced in Ex.1. This answer can be compared to the exact answer for the problem, to be presented shortly.

**Ex.4.** Suppose, contrary to what was assumed earlier, that $H_{11}$ and $H_{22}$ do not vanish, so that extra terms would occur on the right sides of (2). Following Griffiths (Ch.9), one can reduce the problem to the one considered earlier by the following device. One introduces the new amplitudes

$$b_1 = \exp\left(\frac{i}{\hbar} \int_0^t H_{11}(t')dt'\right)a_1 \quad \text{and} \quad b_2 = \exp\left(\frac{i}{\hbar} \int_0^t H_{22}(t')dt'\right)a_2 \tag{3}$$

and notes that they also obey Eq.(2), but with $H_{21}$ replaced by $e^{i\phi} H_{21}$ and $H_{12}$ by $e^{-i\phi} H_{12}$ where $\phi$ is the time dependent phase

$$\phi = \frac{1}{\hbar} \int_0^t [H_{22}(t') - H_{11}(t')]dt'. \tag{4}$$

Verify this conclusion. Note that for a time independent perturbation, $\phi = \gamma t$ and the sole effect of this added complication is to shift the Bohr frequency from $\omega_0$ to $\omega_0 + \gamma$.

We now develop the exact solution to Eq.(2) for a time independent perturbation. This will be done under the most general circumstances: $H'$ will be allowed to have both diagonal and off-diagonal elements and the initial conditions will be allowed to be arbitrary. The full Hamiltonian for the problem is given by the 2 x 2 matrix

$$H = H_0 + H' = \begin{pmatrix} E_1 + H_{11} & H_{12} \\ H_{21} & E_2 + H_{22} \end{pmatrix}. \tag{5}$$

This Hamiltonian can be diagonalized to obtain its energy eigenvalues and eigenstates. The time development operator can then be constructed and applied to the initial state to generate the final state at time $t$, and thence the required probabilities. The calculations are straightforward, but one could get bogged down in a lot of algebra. We describe here a simple method of getting the time development operator without first having to calculate the eigenstates. This technique, which exploits the Pauli matrices, has utility in other situations aside from the present one.

Before we begin, though, we simplify the Hamiltonian (5) by shifting the zero of energy so that it is midway between the two diagonal elements of the matrix in (5). The Hamiltonian can then be rewritten as
\[ \frac{H}{\hbar} = \begin{pmatrix} \delta & \kappa e^{-i\phi} \\ \kappa e^{i\phi} & -\delta \end{pmatrix} = \kappa \cos \phi \sigma_x + \kappa \sin \phi \sigma_y + \delta \sigma_z \]  \tag{6} 

where \( \delta, \kappa \), and \( \phi \) are real parameters (with units of frequency) characterizing the Hamiltonian and \( \sigma_x, \sigma_y, \sigma_z \) are the usual Pauli matrices. On introducing the vector \( \vec{n} = (\kappa \cos \phi, \kappa \sin \phi, \delta) \), the Hamiltonian can be written as \( H = \vec{n} \cdot \vec{\sigma} \) from which it follows that the time development operator 
\[ U = \exp \left( -\frac{i}{\hbar} H t \right) \] is just the rotation operator for a spin-1/2 particle. We therefore have that 
\[ U = \exp (-i \vec{n} \cdot \vec{\sigma}) = I \cos \theta - i \vec{n} \cdot \vec{\sigma} \sin \theta \]  \tag{7} 

where \( \theta = t \sqrt{\delta^2 + \kappa^2} \). \( \vec{n} \) is the unit vector along the direction of \( \vec{n} \) and \( I \) is the 2 x 2 identity matrix. Applying this unitary matrix to the initial state yields the final state at time \( t \), from which the required transition probabilities can be calculated.

We now specialize our treatment to the case \( \delta = -\omega_0 / 2 \) and the initial conditions \( a_1(0) = 1 \) and \( a_2(0) = 0 \), which correspond to the problem treated in Ex.3. On introducing the dimensionless parameters \( \nu = \tan^{-1} \nu_0 = \tan^{-1} \left( 2\kappa / \omega_0 \right) \) and \( \theta = -\theta_0 \sec \nu = -\frac{1}{2} \omega_0 t \sec \nu \), working out \( U \) explicitly, and applying it to the initial state, we find that the amplitudes at time \( t \) are given by 
\[ a_1(t) = (\cos \theta + i \sin \theta \cos \nu) \] 
and \[ a_2(t) = -i e^{i\theta} \sin \theta \sin \nu \]  \tag{8} 

The probability of finding the system in its excited state at time \( t \) is 
\[ P_2(t) = \left| a_2(t) \right|^2 = \sin^2 \theta \sin^2 \nu \]  \tag{9} 

while the probability of finding it in its ground state is \( P_1(t) = \left| a_1(t) \right|^2 \), which is seen to be equal to \( 1 - P_2(t) \), showing that probability is indeed conserved. The time dependence in \( P_2(t) \) enters through the angle \( \theta \), while the angle \( \nu \) characterizes the strength of the perturbation.

**Ex.5.** To compare the exact solution (9) with the perturbation solution obtained in Ex.3, make a Taylor expansion of (9) about \( \nu_0 \) in powers of \( \nu_0 \) and verify that the lowest two terms in this expansion give you back the second and fourth order perturbation results found in Ex.3. (The use of the "taylor" command in Maple can be very useful in doing this problem).

**Ex.6.** To get a quantitative feeling for how good the perturbation solutions are, compare the second and fourth order solutions against the exact solution for \( \nu_0 = .2, .4 \) and .6, plotting the transition probabilities in the range \( 0 \leq \theta_0 \leq \pi \) in each case.
How can one apply a constant perturbation to a two level system? Suppose, for concreteness, that the system is a spin-1/2 particle that is initially in static magnetic field along the z-axis. This field causes a splitting between the spin up and spin down states along the z-axis, described by the frequency $\omega_0$, which is also the precession frequency about the field direction of any spin state not polarized along the field. Now suppose that a constant magnetic field is turned on along some other direction (say the x-axis). The resultant field will cause a precession about a new direction with an increased frequency, which will manifest itself as a partial nutation in the unperturbed basis. The exact solution (9) captures these effects correctly by the perturbation solution does so only incompletely: on the one hand, it does not account for the saturation of the transition (reflected in the shift from $\nu_0$ to $\nu$) and, on the other, it does not account for the change in the precession frequency from $\omega_0$ to $\omega$.

**Solutions to Exercises.**

**Ex.1.** The solutions for the amplitudes to second order are

$$ a_1(t) = a_{10} + a_{20} \left( -\frac{i}{\hbar} \right) \int_0^t H_{12} e^{-i\omega_0 t'} \right) dt'_{12} + a_{10} \left( -\frac{i}{\hbar} \right)^2 \int_0^t H_{12} e^{-i\omega_0 t'} \int_0^t H_{21} e^{i\omega_0 t'} dt'_{12} ,$$

$$ a_2(t) = a_{20} + a_{10} \left( -\frac{i}{\hbar} \right) \int_0^t H_{21} e^{i\omega_0 t'} dt'_{21} + a_{20} \left( -\frac{i}{\hbar} \right)^2 \int_0^t H_{21} e^{i\omega_0 t'} \int_0^t H_{12} e^{-i\omega_0 t'} dt'_{21} .$$

(10)

The expressions for the amplitudes to arbitrary order can be expressed as

$$ a_1(t) = \sum_{n=0}^{\infty} c(n)(-i)^n F_n(t) \quad \text{and} \quad a_2(t) = \sum_{n=0}^{\infty} c(n+1)(-i)^n F^*_n(t)$$

(11)

where $c(n) = a_{10} \text{ or } a_{20}$ according as $n$ is even or odd and the dimensionless functions $F_n(t)$ are defined via the recursion relation

$$ F_n(t) = \frac{1}{\hbar} \int_0^t H_{12} e^{-i\omega_0 t'} F^*_{n-1}(t') \quad \text{with} \quad F_0(t) = 1 .$$

(12)

**Ex.2** The functions $F_n(t)$ will now be evaluated for a time independent potential $H'$ with matrix element $H_{12} = \kappa e^{-i\phi}$. On introducing the dimensionless time variable $\theta_0 = \omega_0 t / 2$ and the dimensionless strength parameter $\nu_0 = 2\kappa / \omega_0$, the recursion relation (12) can be written as

$$ F_n(\theta_0) = \nu_0 e^{i\phi} \int_0^{\theta_0} dx e^{-2i\alpha} F^*_n(x) \quad \text{with} \quad F_0(\theta_0) = 1$$

(13)

The validity of the normalization condition $|a_1(\theta_0)|^2 + |a_2(\theta_0)|^2 = 1$ is guaranteed up to terms of n-th order in $H'$ if the functions $F_n$ satisfy the following relationships:
0th order: \[ |a_{10}|^2 + |a_{20}|^2 = 1 \]
2nd order: \[ F_2 + F_2^* - |F_1|^2 = 0 \]
4th order: \[ F_4 + F_4^* - F_3 F_1^* - F_3^* F_1 + |F_2|^2 = 0 \] \( (14) \)
6th order: \[ F_6 + F_6^* - F_5 F_1^* - F_5^* F_1 + F_4 F_2^* + F_4^* F_2 - |F_3|^2 = 0 \]
\[ \cdots \cdots \cdots \]

Any relationship in (14), together with the ones above it, guarantees that the normalization is satisfied up to the order indicated next to the relationship. No relationships are given for the odd orders because they are all satisfied trivially as identities.

On doing the integrals in (13), we find that the four lowest functions \( F_n \) are

\[
F_1 = V_0 e^{-i\varphi} \sin \theta_0 e^{-i\theta_0}
\]
\[
F_2 = -\frac{i}{2} V_0^2 \left[ \theta_0 - e^{-i\theta_0} \sin \theta_0 \right]
\]
\[
F_3 = \frac{1}{2} V_0^2 e^{-i\theta_0} \left[ \sin \theta_0 - \theta_0 \cos \theta_0 \right]
\]
\[
F_4 = \frac{i}{8} V_0^4 \left[ e^{-i\theta_0} \left( 3 \sin \theta_0 - 2 \theta_0 \cos \theta_0 \right) - \theta_0 + i\theta_0^2 \right]
\] \( (15) \)

Using these, it is easy to verify that the 2nd and 4th order constraints in (14) are satisfied. The constraints (14) really express the unitarity of the time development operator to each order in the perturbation. This order by order unitarity actually holds for an arbitrary perturbation, whether it is time independent or time dependent.

**Ex.3.** The expressions for the transition probabilities to fourth order in \( H' \) are

\[
P_1(t) = |a_1(t)|^2 = |1 - F_2 + F_4|^2 = 1 - (F_2 + F_2^*) + |F_2|^2 + F_4 + F_4^*
\]
\[
P_2(t) = |a_2(t)|^2 = -iF_1 + iF_3^*|^2 = |F_1|^2 - \left( F_2 F_1^* + F_3 F_1^* \right).
\] \( (16) \)

Note that the probabilities add up to 1, in view of (14). The detailed expression for the transition probability to the upper state is

\[
P_2(t) = V_0^2 \sin^2 \theta_0 + V_0^4 \sin \theta_0 \left( \theta_0 \cos \theta_0 - \sin \theta_0 \right)
\] \( (17) \)

with the first and second terms being the contributions arising from second and fourth order in \( H' \).

**Ex.4.** This involves straightforward substitution and simplification.

**Ex.5.** A Taylor expansion of (9) using Maple shows that
\[ P_2(t) = v_0^2 \sin^2 \theta_0 + v_0^4 \sin \theta_0 (\theta_0 \cos \theta_0 - \sin \theta_0) \\
+ v_0^6 \left[ \sin \theta_0 \left( \sin \theta_0 - \frac{5}{4} \theta_0 \cos \theta_0 \right) + \frac{1}{4} \theta_0^2 \cos 2\theta_0 \right] + O(v_0^8) \] (18)

where the last term is what would have been yielded by a third order perturbation calculation.

**Ex.6.** Upper left is \( v_0 = .1 \), upper right is \( v_0 = .4 \), lower left is \( v_0 = .6 \) and lower right is \( v_0 = .8 \). Dashed curve = 2\(^{nd}\) order, dotted curve = 4\(^{th}\) order and solid curve = exact result.
2. A sinusoidal off-diagonal perturbation (the case of magnetic resonance)

Consider a spin-1/2 particle in a static magnetic field $B_0$ along the z-axis and an oscillating field $B_1 \cos \omega t$ along the x-axis. The magnetic moment of the particle is $\mu = g\vec{S}$, where $g$ is the gyromagnetic ratio and $\vec{S} = \frac{1}{2} \hbar \vec{\sigma}$ is the spin operator of the particle, with $\vec{\sigma}$ being the vector Pauli operator. The Hamiltonian of the particle in these fields is

$$H = -\mu \left( B_0 \hat{z} + B_1 \cos \omega t \hat{x} \right) = -\frac{1}{2} \hbar \left( \omega_\sigma \sigma_z + 2\lambda \cos \omega t \sigma_x \right) = H_0 + H' \quad (19)$$

where $\omega_\sigma = gB_0$ is the Larmor precession frequency in the static field and $\lambda = \frac{1}{2} \frac{g}{2} B_1$ is the frequency of the “Rabi flopping” induced by the oscillating field (the meaning of this term will become clearer later). The two pieces of the Hamiltonian arising from the static and oscillating fields will be denoted $H_0$ and $H'$, respectively.

Let $\left| 0 \right>$ and $\left| 1 \right>$ denote the spin-up and spin-down states of the spin along the z-axis. These states are eigenstates of $\sigma_z$ with eigenvalues +1 and -1, respectively.\(^1\) The action of the other Pauli operators on these states is as follows: $\sigma_+ \left| 0 \right> = \left| 1 \right>, \sigma_- \left| 0 \right> = \left| 0 \right>, \sigma_x \left| 0 \right> = i \left| 1 \right>, \sigma_y \left| 0 \right> = -i \left| 0 \right>$. In the basis provided by these states, the Hamiltonian (19) can be written as the 2 x 2 matrix

$$H = -\frac{\hbar}{2} \begin{pmatrix} \omega_\sigma & 2\lambda \cos \omega t \\ 2\lambda \cos \omega t & -\omega_\sigma \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 & 0 \\ 0 & -\omega_\sigma \end{pmatrix} -\frac{\hbar}{2} \begin{pmatrix} 0 & 2\lambda \cos \omega t \\ 2\lambda \cos \omega t & 0 \end{pmatrix}, \quad (20)$$

where the pieces due to $H_0$ and $H'$ have been separated out at the end. The basic problem we want to solve is this: if the spin is prepared at time 0 in the state $|\psi(0)\rangle = a_0 |0\rangle + a_1 |1\rangle$ and then placed in the above fields, what is its state at time $t$? The state at time $t$ can be written quite generally as $|\psi(t)\rangle = a_0(t) \exp \left( i\omega_\sigma t / 2 \right) |0\rangle + a_1(t) \exp \left( -i\omega_\sigma t / 2 \right) |1\rangle$, with the time dependence due to the static field $H_0$ taken out and the coefficients $a_0$ and $a_1$ being allowed to carry the remainder of the time dependence. On putting this into the Schrodinger equation, one finds that the coefficients $a_0$ and $a_1$ obey the pair of coupled differential equations

$$\dot{a}_0 = i\lambda \cos \omega t e^{-i\omega t}a_1, \quad \dot{a}_1 = i\lambda \cos \omega t e^{i\omega t}a_0. \quad (21)$$

These equations are completely equivalent to the original (time dependent) Schrodinger equation for the problem. We first look at a perturbative solution of (21), following which we turn to its exact solution within the “rotating wave approximation”.

\(^1\)In the quantum computation literature a spin-1/2 particle, or indeed any two-state system, is known as a “qubit” and its basis states are chosen to be eigenstates of the Pauli operator $\sigma_z$. The eigenstate with eigenvalue +1 is denoted $\left| 0 \right>$ while that with eigenvalue -1 is denoted $\left| 1 \right>$. We have adopted this terminology here, which is a little different from what was used in the previous section.
Ex.7. Treat $H_0$ as the unperturbed Hamiltonian and $H'$ as a perturbation and solve (21) to first order in the perturbation for the initial conditions $a_{00} = 1$ and $a_{10} = 0$. Use this solution to calculate the probability of finding the system in its spin down state $|1\rangle$ at time $t$. Do this in the “rotating wave approximation” (RWA), in which the matrix elements of the perturbation are taken to be

$$\langle 0|H'|1\rangle = -\hbar \frac{\lambda}{2} e^{i\alpha} \quad \text{and} \quad \langle 1|H'|0\rangle = -\hbar \frac{\lambda}{2} e^{-i\alpha}.$$  

Note that the RWA Hamiltonian is hermitian, as it must be if it is to conserve probability. Can you see why the RWA is so good? Griffiths, Schiff and many other authors point out that keeping the term neglected in the RWA gives rise to an additional term in the transition probability that is totally negligible, in most practical circumstances, to the term that is actually retained. Another justification for the RWA will be given in an exercise below.

Ans: You should find that $P_1(t) \equiv |a_1(t)|^2 = \left( \frac{\lambda}{\delta} \right)^2 \sin^2 \left( \frac{\delta t}{2} \right)$, where $\delta = \omega - \omega_0$ is the “detuning” i.e. the mismatch between the natural precession frequency and the frequency of the driving field. Note that at exact resonance, $\delta = 0$, the transition probability increases as $t^2$ for all times, which would eventually make it exceed unity; this is obviously absurd and points to the breakdown of perturbation theory at large times. Even off resonance, $\delta \neq 0$, the transition probability could become larger than unity if $\lambda > |\delta|$.

In the RWA (21) reduces to the pair of equations

$$\dot{a}_0 = i \frac{\lambda}{2} e^{i\delta t} a_1, \quad \dot{a}_1 = i \frac{\lambda}{2} e^{-i\delta t} a_0 \quad (22)$$

We now show how to solve (22) exactly by three different methods.

Ex.8. Solve (22) exactly for the initial conditions $a_0(0) = 1$ and $a_1(0) = 0$. To do this, differentiate each equation in (22) and substitute the other equation into it to obtain a pair of uncoupled second order differential equations for the amplitudes, which are readily solved. Use your solution to calculate the probabilities of finding the system in each of its states at time $t$. You should be able to see that the system flip-flops between the states $|0\rangle$ and $|1\rangle$, and you should be able to get an expression for the frequency of this “Rabi flopping”.

Ex.9. The method of the previous exercise can be formulated in a more general way that allows one to solve the problem for arbitrary initial conditions without getting bogged down in a lot of algebra. The idea is to go to a new state $|\psi\rangle = U |\psi\rangle$ related to the old state by a unitary transformation $U$ and to choose $U$ so that $|\psi\rangle$ obeys a Schrodinger equation (SE) with a time independent Hamiltonian $\tilde{H}$. The time evolution of $|\psi\rangle$ can then be worked out by the technique of Sec.1 and one can finally undo the unitary transformation to calculate $|\psi\rangle = U^{-1} |\tilde{\psi}\rangle$. The detailed method of doing this is sketched out in the various parts of this exercise:

(a) Show that $|\tilde{\psi}\rangle$ satisfies the SE $i\hbar \frac{d}{dt} |\tilde{\psi}\rangle = \tilde{H} |\tilde{\psi}\rangle$ with $\tilde{H} = i\hbar \frac{dU}{dt} U^\dagger + UHU^\dagger$. 

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(b) Show that taking \( U = \exp \left( -\frac{i}{\hbar} \sigma \omega t \right) \) makes the transformed Hamiltonian have the form
\[
\bar{H} = \frac{\hbar}{2} \left( \delta \lambda - \sigma \right) = \frac{\hbar}{2} \left( \delta \sigma_z + \lambda \sigma_x \right)
\] (23)

Note that \( U = \exp \left( \frac{i}{\hbar} H_0(\omega) t \right) \), where \( H_0 \) is the unperturbed Hamiltonian but with \( \omega_0 \) replaced by \( \omega \). The geometrical meaning of this transformation will be made clearer later.

(c) Use the technique of Sec.1 to calculate the time development operator \( \exp \left( -\frac{i}{\hbar} \bar{H} t \right) \) and show that it is equal to \( \cos \left( \frac{1}{2} \kappa t \right) I - i \left( \hat{n} \cdot \hat{\sigma} \right) \sin \left( \frac{1}{2} \kappa t \right) \) where \( \kappa = \sqrt{\lambda^2 + \delta^2} \) and \( \hat{n} \) is a unit vector with components \( \left( \frac{\lambda}{\kappa}, 0, \frac{\delta}{\kappa} \right) \).

(d) The initial conditions on \( \psi \) are the same as those on \( \psi \). Thus one can solve for \( \psi(t) \) using the time development operator found in (c) and then apply the inverse operator \( U^{-1} = U^\dagger \) to obtain \( \psi(t) \). Complete the solution for the same initial conditions as in Ex.7 and verify that you obtain the same transition probabilities as before. But you will find it much easier to calculate the transition probabilities for more complex initial conditions using the present approach.

(e) The method followed in this exercise has a transparent geometrical meaning. The transformation \( U \) in (b) effects a transformation to a rotating coordinate system (rotating about the \( z \)-axis at frequency \( \omega \)) that largely cancels out the precession due to the static field (the cancellation is exact at resonance) and makes the oscillating field (or rotating field in the RWA) stand still; in this new frame one has a static magnetic field with comparable \( z \)- and \( x \)-components that causes the state to precess about it; it is this precession (actually a nutation) that gives rise to the Rabi flopping. Keeping this geometrical picture in mind can enable one to solve problems involving Rabi flopping quickly without doing a lot of calculation.

**Ex.10.** We solve the problem yet another way, using the Heisenberg picture. First note that the Hamiltonian (19) can be rewritten as
\[
H = -\frac{1}{2} \hbar \omega_0 \sigma_z - \frac{1}{2} \hbar \lambda \left( \cos \omega t \sigma_x - \sin \omega t \sigma_y \right) - \frac{1}{2} \hbar \lambda \left( \cos \omega t \sigma_x + \sin \omega t \sigma_y \right)
\] (24)

where the second and third terms arise from magnetic fields clockwise and counterclockwise about the \( z \)-axis. Of these, the former rotates in the sense of the particle’s precession while the latter rotates in the opposite sense, and therefore only the former is retained in the RWA. In the Heisenberg picture approach, the spin operator \( \vec{S} \), or its dimensionless equivalent \( \vec{\sigma} \), is regarded as a function of time (note that the components of \( \vec{\sigma} \) are not to be confused with the standard Pauli matrices to which they reduce at time \( t = 0 \) and from which they evolve by means of unitary transformations). Proceed as follows:

(a) Use the Hamiltonian (24) with the last term omitted (which amounts to the RWA) to write down the Heisenberg equations of motion for the operators \( \sigma_x, \sigma_y \) and \( \sigma_z \). Denote the expectation
values of these operators in the initial state of the system as \( P_x, P_y, P_z \); recall that these are just the components of the polarization vector \( \vec{P} \) along which the spin is certain to be found up. Show that \( \vec{P} \) obeys the precession equation

\[
\frac{d\vec{P}}{dt} = \vec{\Omega} \times \vec{P}, \quad \text{where} \quad \vec{\Omega} = (-\lambda \cos \omega t, \lambda \sin \omega t, -\omega_0)
\]

(b) Now make a transformation to a rotating frame in which the new polarization vector components (denoted by primes) are related to the old (unprimed) components by

\[
P'_x = P_x \cos \omega t - P_y \sin \omega t
\]
\[
P'_y = P_x \sin \omega t + P_y \cos \omega t
\]
\[
P'_z = P_z
\]

Show that the new polarization vector obeys the equation

\[
\frac{d\vec{P}'}{dt} = \vec{\Omega}' \times \vec{P}', \quad \text{where} \quad \vec{\Omega}' = (-\lambda, 0, \delta)
\]

which shows that, in the rotating frame, the polarization precesses about a static field in the x-z plane made up of a small residual field along the z-axis and an additional field along the x-axis.

(c) Show that the solution to (25) can be written as

\[
\vec{P}'(t) = \vec{P}'(0) \cos \left( \Omega' t \right) + (1 - \cos \Omega' t) \frac{\vec{\Omega}' \cdot \vec{P}'(0)}{\Omega'^2} \vec{\Omega}' + \frac{\vec{\Omega}' \times \vec{P}'(0)}{\Omega'} \sin \left( \Omega' t \right)
\]

where \( \vec{P}'(0) \) denotes the initial value. If one is told the initial state of the system one can calculate \( \vec{P}(0) \), which is equal to \( \vec{P}'(0) \), from (26). Then one can calculate \( \vec{P}'(t) \) from (27) and hence \( \vec{P}(t) \) by using the inverse of the transformation in (25). From \( \vec{P}(t) \) one can calculate all the system properties of interest. Very often one is simply interested in knowing the probability of finding the system in either of its states at time \( t \). These can be calculated as \( \frac{1}{2} \left( 1 \pm P_z(t) \right) \), with \( P_z(t) \) calculated from (27).

**Sense of precession/nutation.** Some words should be added about the sense of the precession and nutation in the external fields. If the gyromagnetic ratio \( g \) of the particle is positive, both \( \omega_0 \) and \( \lambda \) are positive and the precession about the z-axis and the on-resonance nutation about the x-axis are both in the clockwise sense. If \( g < 0 \) both \( \omega_0 \) and \( \lambda \) are negative and \( \omega \) is to be replaced by \( -\omega \) in all the formulae above, since it is the third term in (24) rather than the second that is to be retained in the RWA. Thus, for \( g < 0 \), the sense of both the precession and on-resonance nutation gets reversed.
Several further problems are suggested below. They illuminate further aspects of magnetic resonance/ Rabi flopping and also illustrate applications of the general ideas discussed above. In doing many of the problems below, it is convenient to measure (angular) frequencies in units of \( \lambda \) and time in units of \( \lambda^{-1} \) where \( \lambda \) is the Rabi flopping frequency at exact resonance. Thus, for example, a detuning of .2 means that \( \delta = .2\lambda \) and a time of \( \pi \) means that \( \lambda t = \pi \). The polarization components \( P_\perp = P_\parallel \) are often referred to as the “inversion”. The inversion is +1 if the particle is in its spin-up state, -1 if it is in its spin-down state, and somewhere in between otherwise.

**Ex.11.** Calculate the precession frequency for protons in a field of 1.5T, which is typical for NMR applications. In most NMR applications \( \lambda \ll \omega_0 \) and \( \omega = \omega_0 \), for which the RWA can be shown to be an excellent approximation. From your calculation, estimate the frequencies at which NMR work is typically done (is it in the optical, radio or infrared part of the spectrum?). What sort of strengths might be used for the oscillating field and how would they compare with that of the static field?

**Ex.12. The Bloch-Siegert shift.** The “counter-rotating” term in the Hamiltonian (19) that is left out in the RWA has only a tiny effect on the particle dynamics. The reason for this is that, in the rotating frame, this term fluctuates very rapidly and averages out to zero over a few cycles of precession. The RWA term, by contrast, is steady and produces a cumulative effect over many precession periods. The main effect of the non-RWA term is to cause a small shift in the precession frequency known as the Bloch-Siegert shift, which can be estimated as follows. Regard the counter-rotating term, i.e. the last term in (24), as a small perturbation to the RWA Hamiltonian. Replacing this term with its absolute magnitude, one can do second order perturbation theory to calculate the shift that it produces in each of the unperturbed levels. Assuming that \( \lambda \ll \omega_0 \), show that this leads to a shift in the precession frequency of order \( \frac{\lambda^2}{\omega_0^2} \).

**Ex.13.** Suppose that \( \delta = .2 \) and that the system initially has inversion +1 i.e. it starts out in its spin-up state, as in Ex.7.

(a) At what time after \( t = 0 \) would the inversions predicted by the first order perturbation calculation of Ex.7 and the exact calculation of Ex.8 differ by 5%? By 10%?

(b) According to the exact calculation, what is the earliest time after \( t = 0 \) at which the minimum inversion would occur, and what would its value be?

(c) At what times would the inversion be zero?

**Ex.14.** Suppose that \( \delta = .2 \) and the system is prepared initially in the state \( \frac{1}{2} |0\rangle + \frac{\sqrt{3}}{2} |1\rangle \).

(a) Calculate the initial polarization vector and inversion.

(b) Calculate the inversion after a quarter and a half of the Rabi period of this motion.

(c) At what times does the inversion achieve its minimum value, and what is this value?

**Ex.15.** Solve for the dynamics of a particle in a magnetic field precessing on the surface of a cone. (Hint: this problem can be solved exactly by a transformation to the rotating frame, as in Exs.9 and 10. The answer is given in Griffiths Problem 9.19 and Sec.10.1.3, where a comparison with the perturbation and adiabatic treatments is also made).
**Solutions to exercises.**

**Ex.8** On carrying out the indicated differentiation and substitution, one finds that \( a_0(t) \) obeys the second order differential equation \( \ddot{a}_0 - i \delta \dot{a}_0 + \frac{\lambda^2}{4} a_0 = 0 \), where \( \delta \) is the detuning introduced in Ex.7. On substituting the trial solution \( a_0 = \alpha_0 e^{i \mu t} \) into this equation we obtain a quadratic equation for \( \mu \) whose two roots are \( \pm \frac{1}{2} \delta \pm \frac{1}{2} \kappa \), where \( \kappa = \sqrt{\delta^2 + \lambda^2} \). This leads to the solutions

\[
a_0(t) = e^{i \delta t/2} \left[ c_1 \cos \left( \frac{1}{2} \kappa t \right) + c_2 \sin \left( \frac{1}{2} \kappa t \right) \right] \quad \text{and} \quad a_1(t) = e^{-i \delta t/2} \left[ d_1 \cos \left( \frac{1}{2} \kappa t \right) + d_2 \sin \left( \frac{1}{2} \kappa t \right) \right],
\]

where the latter solution was obtained by noting that \( a_1(t) \) obeys the same differential equation as \( a_0(t) \) but with \( \delta \) replaced by \( -\delta \). It remains only to fix the constants \( c_1, c_2, d_1, \) and \( d_2 \), which can be done from the initial conditions \( a_0(0) = 1 \) and \( a_1(0) = 0 \) and from the requirement that the solutions satisfy (22). In this way we find that the solutions are

\[
a_0(t) = e^{i \delta t/2} \left[ \cos \left( \frac{1}{2} \kappa t \right) \right] - i \frac{\delta}{\kappa} \sin \left( \frac{1}{2} \kappa t \right) \quad \text{and} \quad a_1(t) = e^{-i \delta t/2} \left( \frac{\lambda}{\kappa} \right) \sin \left( \frac{1}{2} \kappa t \right)
\]

The probabilities of finding the system in its two states at time \( t \) are

\[
P_0(t) = |a_0^2(t)| = \cos^2 \left( \frac{\kappa t}{2} \right) + \frac{\delta^2}{\kappa^2} \sin^2 \left( \frac{\kappa t}{2} \right) \quad \text{and} \quad P_1(t) = |a_1^2(t)| = \left( \frac{\lambda}{\kappa} \right)^2 \sin^2 \left( \frac{\kappa t}{2} \right)
\]

The above formulae show that the system flip-flops between its two states with the Rabi frequency \( \kappa = \sqrt{\delta^2 + \lambda^2} \). If \( \delta = 0 \) (resonance), the Rabi frequency is just \( \lambda \) and the oscillation between the two states is perfect (i.e. the system is found in each of the states with probability 1 at regularly repeating intervals). However, if \( \delta \neq 0 \), the frequency of the Rabi flopping increases and the probability of occupying the other state also drops from unity.

**Ex.13.** (a) The inversion at time \( t \) is \( I(t) = P_0(t) - P_1(t) = 1 - 2P_1(t) \). The expressions for the inversion in the two cases of interest are

First order perturbation theory:

\[
I(t) = 1 - 2 \left( \frac{\lambda}{\delta} \right)^2 \sin^2 \left( \frac{\delta t}{2} \right)
\]

Exact result:

\[
I(t) = 1 - 2 \left( \frac{\lambda}{\kappa} \right)^2 \sin^2 \left( \frac{\kappa t}{2} \right)
\]

If \( \delta = 0.2 \) then \( \kappa = \sqrt{1.04} \) and the above two expressions become
First order perturbation theory:  

\[ I(t) = 1 - 50 \sin^2(1.1t) \]

Exact result:  

\[ I(t) = 1 - 2 \left( \frac{1}{\sqrt{1.04}} \right)^2 \sin^2\left( \frac{\sqrt{1.04}t}{2} \right) \]

I found, using Maple, that the two expressions differ by 5% for \( t = 0.93 \) and by 10% for \( t = 1.055 \). Thus, the perturbation solution starts becoming inaccurate at less than a quarter of the Rabi period.

(b) The inversion reaches its minimum value when the argument of the sine becomes \( \pi / 2 \), i.e. when \( \frac{\sqrt{1.04}}{2}t = \frac{\pi}{2} \) or \( t = 3.08 \). The value of the inversion is then \( 1 - (2/1.04)^2 = -0.9231 \).

(c) The inversion becomes zero when \( 1 - 2 \left( \frac{1}{\sqrt{1.04}} \right)^2 \sin^2\left( \frac{\sqrt{1.04}t}{2} \right) \). The earliest time at which this happens is \( t = 1.58 \) (in units of \( \lambda^{-1} \)).

**Ex.14.** (a) On comparing the given initial state with the general state \( \cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i\phi}|1\rangle \) we see that \( \theta = 2\pi/3 \) and \( \phi = 0 \) is the direction along which this state is polarized. The polarization vector of this state has components \( (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta) \) which work out numerically to \( \bar{P}(0) = \left( \frac{\sqrt{3}}{2}, 0, -\frac{1}{2} \right) \). The initial inversion is the z-component of this vector, or \(-1/2\).

(b) The polarization vector in the rotating frame at any time \( t \) can be worked out using (27) along with \( \bar{\Omega} = (-\lambda, 0, \delta) = (-1, 0, 1/5) \), \( \Omega = \sqrt{\lambda^2 + \delta^2} = \sqrt{1 + 0.2^2} = \sqrt{26}/5 \) and choosing the time suitably. In this way one finds that the inversions are

- At a quarter period \( \Omega' t = \pi / 2 \), \( P_z(t) = -\frac{1}{52} (1 + 5\sqrt{3}) = -0.1857 \)
- At a half period \( \Omega' t = \pi \), \( P_z(t) = \frac{1}{26} (12 - 5\sqrt{3}) = 0.1284 \)

A geometrical method allows us to obtain the first of these answers approximately and the second exactly. For this, note that the polarization vector traces out a cone about the direction of \(-\bar{\Omega}'\), beginning vertically below it and drawing more or less level with it at a quarter of the Rabi period; the inversion would therefore be given by the vertical (or z-)component of the unit vector along the direction of \(-\bar{\Omega}'\), which is \(-\delta / \sqrt{\delta^2 + \lambda^2} = -1/\sqrt{26} = -0.1961\), which is a little lower than the exact answer obtained above. The reason for this lower value is that the projection of the center of the cone on to the Bloch sphere is slightly lower than the two lateral edges of the cone. Next, note that the angle between the initial polarization vector and the axis of the cone on which it moves is

\[ \alpha = \cos^{-1} \left[ -\bar{\Omega}' \cdot \bar{P}(0) / |\bar{\Omega}'| \right] = \cos^{-1} \left[ \left( \frac{\sqrt{3}}{2} + \frac{1}{10} \right) \left( \frac{5}{\sqrt{26}} \right) \right] = 0.3262 \]. We saw that the cone axis is
inclined an angle $\beta = \sin^{-1}(.1961) = .1973$ below the vertical, so after half a Rabi period the polarization vector would have moved from directly below the cone axis to directly above it; in other words, the polarization vector would be at an angle $(-\beta + \alpha)$ to the horizontal and the inversion would be $\sin(-\beta + \alpha) = \sin(-.1973 + .3262) = .1284$, which matches the result we got earlier.

(c) The inversion attains its minimum value at integer multiples of the Rabi period and is then equal to its initial value. It is easy to see this from the fact that the axis of the cone about which the precession takes place lies in the $x$-$z$ plane. This also shows that the maximum inversion occurs at half the Rabi period, and at all later times separated from this by multiples of the Rabi period.