

Quantum Physics 2011/12

Solutions to Tutorial Sheet 4: Time-dependence

1. An easy one to start with! A particle moving in the infinite 1-d square well potential

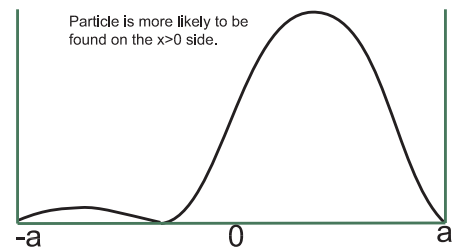
$$V(x) = 0 \quad \text{for } |x| < a, \quad V(x) = \infty \quad \text{for } |x| > a$$

is set up in the initial state ($t = 0$) described by the wavefunction

$$\Psi(x, 0) \equiv \psi(x) = [u_1(x) + u_2(x)] / \sqrt{2}$$

where $u_1(x)$, $u_2(x)$ are the energy eigenfunctions corresponding to the energy eigenvalues E_1 and E_2 respectively. Sketch the probability density at $t = 0$.

The wavefunction has positive interference for $x > 0$, and negative for $x < 0$. It is zero at $\cos(\pi x/2a) - \sin(\pi x/a) = 0$, i.e. $-\pi/6$



What is the wavefunction at time t ?

Recall that the expansion in energy eigenfunctions of a general solution of the TDSE is

$$\Psi(x, t) = \sum_n c_n \exp(-iE_n t/\hbar) u_n(x)$$

where the coefficients c_n are constant in time if the Hamiltonian is time-independent, which is the case here, so that

$$\Psi(x, 0) = \sum_n c_n u_n(x)$$

In the present case, $c_1 = c_2 = 1/\sqrt{2}$ and $c_n = 0, n \geq 3$ and thus

$$\Psi(x, t) = \frac{1}{\sqrt{2}} \exp(-iE_1 t/\hbar) u_1(x) + \frac{1}{\sqrt{2}} \exp(-iE_2 t/\hbar) u_2(x)$$

Calculate the probabilities P_1 and P_2 that at $t = 0$ a measurement of the total energy yields the results E_1 and E_2 respectively. Do P_1 and P_2 change with time?

The probability of getting the result E_n in a measurement of the energy at $t = 0$ is $P(E_n) = |c_n|^2$. Thus

$$P(E_1) = P(E_2) = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}$$

At time t , the corresponding probabilities are:

$$\begin{aligned} |c_1 \exp(-iE_1 t/\hbar)|^2 &= |c_1|^2 = \frac{1}{2} \\ |c_2 \exp(-iE_2 t/\hbar)|^2 &= |c_2|^2 = \frac{1}{2} \end{aligned}$$

so that $P(E_1)$ and $P(E_2)$ are time independent.

Calculate the probabilities $P_+(t)$ and $P_-(t)$ that at time t the particle is in the intervals $0 < x < a$ and $-a < x < 0$ respectively and try to interpret your results.

The probability that, at time t , the particle is in the interval $0 < x < a$ is

$$P_+(t) = \int_0^a |\Psi(x, t)|^2 dx$$

since $|\Psi(x, t)|^2 dx$ is the probability of finding the particle in the infinitesimal interval $x \rightarrow x + dx$.

Now

$$\begin{aligned} |\Psi(x, t)|^2 &= \frac{1}{2} |\exp(-iE_1 t/\hbar) u_1(x) + \exp(-iE_2 t/\hbar) u_2(x)|^2 \\ &= \frac{1}{2} |u_1(x)|^2 + \frac{1}{2} |u_2(x)|^2 + \frac{1}{2} \exp[-i(E_1 - E_2)t/\hbar] u_1(x) u_2^*(x) \\ &\quad + \frac{1}{2} \exp[i(E_1 - E_2)t/\hbar] u_1^*(x) u_2(x) \end{aligned}$$

Defining $\omega \equiv (E_2 - E_1)/\hbar$, and noting that u_1 and u_2 are real, we obtain

$$P_+(t) = \frac{1}{2} \int_0^a |u_1(x)|^2 dx + \frac{1}{2} \int_0^a |u_2(x)|^2 dx + \cos \omega t \int_0^a u_1(x) u_2(x) dx$$

We can write down the values of the first two integrals without explicit evaluation if we observe that both integrands are even functions of x , so that

$$\int_0^a |u_1(x)|^2 dx = \frac{1}{2} \int_{-a}^a |u_1(x)|^2 dx = \frac{1}{2}$$

from the normalisation, with a similar result for u_2 . This tells us that particles in the eigenstates u_1 and u_2 have equal chance of being on either side of zero.

We still have to evaluate

$$\int_0^a u_1(x) u_2(x) dx = \frac{1}{a} \int_0^a \cos\left(\frac{\pi x}{2a}\right) \sin\left(\frac{\pi x}{a}\right) dx$$

on substituting in the explicit form of the lowest two eigenfunctions for the symmetric infinite square well.

Using the trigonometric identity

$$\sin A \cos B \equiv \frac{1}{2} \{ \sin(A + B) + \sin(A - B) \}$$

we obtain

$$\int_0^a u_1(x) u_2(x) dx = \frac{1}{2a} \int_0^a \left\{ \sin\left(\frac{3\pi x}{2a}\right) + \sin\left(\frac{\pi x}{2a}\right) \right\} dx$$

$$\begin{aligned}
&= \frac{1}{2a} \left[-\frac{2a}{3\pi} \cos\left(\frac{3\pi x}{2a}\right) - \frac{2a}{\pi} \cos\left(\frac{\pi x}{2a}\right) \right]_0^a \\
&= \frac{1}{2a} \left[\frac{2a}{3\pi} + \frac{2a}{\pi} \right] \\
&= \frac{4}{3\pi}
\end{aligned}$$

Putting it all together, we find

$ \begin{aligned} P_+(t) &= \frac{1}{2} + \frac{4}{3\pi} \cos \omega t \\ P_-(t) &= 1 - P_+(t) = \frac{1}{2} - \frac{4}{3\pi} \cos \omega t \end{aligned} $

Which implies that over time the probability distribution moves from side to side!

2. A system has just two independent states, $|1\rangle$ and $|2\rangle$, represented by the column matrices

$$|1\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |2\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

With respect to these two states, the Hamiltonian has a time-independent matrix representation

$$\begin{pmatrix} E & V \\ V & E \end{pmatrix}$$

where E and V are both real.

Show that the probability of a transition from the state $|1\rangle$ to the state $|2\rangle$ in the time interval t is given without approximation by

$$p(t) = \sin^2\left(\frac{Vt}{\hbar}\right)$$

[Hint: expand the general state $|\Psi, t\rangle$ in terms of $|1\rangle$ and $|2\rangle$ and substitute in the TDSE. Note that $|1\rangle$ and $|2\rangle$ are not energy eigenstates!]

The states $|1\rangle$ and $|2\rangle$ are NOT energy eigenstates, since the perturbed Hamiltonian is not diagonal! Nevertheless, they form a complete set and we can expand an arbitrary state as follows:

$$|\Psi, t\rangle = \sum_{r=1}^2 c_r(t) |r\rangle$$

which has the matrix representation

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = c_1(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Substituting in the TDSE gives

$$i\hbar \begin{pmatrix} \dot{c}_1(t) \\ \dot{c}_2(t) \end{pmatrix} = \begin{pmatrix} E & V \\ V & E \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

which yields the coupled equations

$$\begin{aligned}
i\hbar \dot{c}_1 &= E c_1 + V c_2 \\
i\hbar \dot{c}_2 &= V c_1 + E c_2
\end{aligned}$$

The neatest way to solve these equations is to take the sum and difference:

$$\begin{aligned} i\hbar (\dot{c}_1 + \dot{c}_2) &= (E + V)(c_1 + c_2) \Rightarrow c_1 + c_2 = A \exp[-i(E + V)t/\hbar] \\ i\hbar (\dot{c}_1 - \dot{c}_2) &= (E - V)(c_1 - c_2) \Rightarrow c_1 - c_2 = B \exp[-i(E - V)t/\hbar] \end{aligned}$$

where A and B are constants of integration.

Alternatively one can find the eigenvalues and eigenvectors of the Hamiltonian $(1, 1)/\sqrt{2}$ and $(1, -1)/\sqrt{2}$ and write down the time evolution of state vector in the usual way.

If the system is in the state $|1\rangle$ at $t = 0$, then $c_1(0) = 1$ and $c_2(0) = 0$. Imposing these initial conditions gives $A = B = 1$, so that

$$c_2(t) = \frac{1}{2} \exp(-iEt/\hbar) \{ \exp(-iVt/\hbar) - \exp(iVt/\hbar) \} = -i \exp(-iEt/\hbar) \sin\left(\frac{Vt}{\hbar}\right)$$

Thus the probability that the system is in state $|2\rangle$ at time t is

$$p(t) = |c_2(t)|^2 = \sin^2\left(\frac{Vt}{\hbar}\right)$$

Compute the transition probability using first-order time-dependent perturbation theory, taking the unperturbed Hamiltonian matrix to be that for which $|1\rangle$ and $|2\rangle$ are energy eigenstates. By comparing with the exact result, deduce the conditions under which you expect the approximation to be good.

We can treat the problem by perturbation theory by writing $\hat{H} = \hat{H}_0 + \hat{V}$, where

$$\hat{H}_0 \rightarrow \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \quad \text{and} \quad \hat{V} \rightarrow \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix}$$

so that $|1\rangle$ and $|2\rangle$ are eigenstates of \hat{H}_0 with eigenvalue $E \equiv E_1 = E_2$.

Time-dependent perturbation theory for the constant perturbation \hat{V} then gives

$$p_{21}(t) = \frac{1}{\hbar^2} \left| \int_0^t V_{21} \exp[i(E_2 - E_1)t'/\hbar] dt' \right|^2 = \frac{V^2}{\hbar^2} \left| \int_0^t dt' \right|^2 = \frac{V^2 t^2}{\hbar^2}$$

This is the leading term in the series expansion of \sin^2 and so agrees with the exact result provided that $V^2 t^2 / \hbar^2 \ll 1$, that is, $Vt \ll \hbar$.

3. * A 1-d harmonic oscillator of charge q is acted upon by a uniform electric field which may be considered to be a perturbation and which has time dependence of the form

$$\mathcal{E}(t) = \frac{A}{\sqrt{\pi} \tau} \exp\left\{-\frac{t^2}{\tau^2}\right\}$$

Assuming that when $t = -\infty$, the oscillator is in its ground state, evaluate the probability that it is in its first excited state at $t = +\infty$ using time-dependent perturbation theory. You may assume that

$$\begin{aligned} \int_{-\infty}^{\infty} \exp(-y^2) dy &= \sqrt{\pi} \\ \langle n+1 | \hat{x} | n \rangle &= \sqrt{\frac{(n+1)\hbar}{2m\omega}} \\ \langle n+i | \hat{x} | n \rangle &= 0 \quad -1 > i > 1 \end{aligned}$$

First-order time-dependent perturbation theory for small $\hat{V}(t)$ gives

$$p_{mk}(\infty) = \frac{1}{\hbar^2} \left| \int_{-\infty}^{\infty} V_{mk}(t) \exp(i\omega_{mk}t) dt \right|^2$$

where

$$V_{mk} = \langle m | \hat{V}(t) | k \rangle$$

In the present case,

$$\hat{V}(t) = -q\mathcal{E}(t)\hat{x}$$

Since \hat{x} is proportional to $(\hat{a} + \hat{a}^\dagger)$, it only connects “nearest-neighbour” states in the energy eigenvalue spectrum. Thus if the initial state is the oscillator ground state, $n = 0$, the only possible final state (at first order) is the $n = 1$ state.

$$V_{10} = \langle 1 | \hat{V}(t) | 0 \rangle = -q\mathcal{E}(t) \langle 1 | \hat{x} | 0 \rangle = -q \left(\frac{\hbar}{2m\omega} \right)^{1/2} \mathcal{E}(t) \quad \text{and} \quad \omega_{10} = \omega$$

Thus

$$p_{10} = \frac{q^2 A^2}{2\pi\tau^2 m \hbar \omega} \left| \int_{-\infty}^{\infty} \exp\{i\omega t - t^2/\tau^2\} dt \right|^2$$

The integral may be evaluated by ‘completing the square’:

$$i\omega t - t^2/\tau^2 = -\left(t/\tau - \frac{1}{2}i\omega\tau\right)^2 - \frac{1}{4}\omega^2\tau^2$$

We now change variables:

$$y \equiv t/\tau - \frac{1}{2}i\omega\tau, \quad dy = dt/\tau$$

and the desired integral becomes a standard Gaussian integral:

$$\int_{-\infty}^{\infty} \exp\{i\omega t - t^2/\tau^2\} dt = \exp(-\frac{1}{4}\omega^2\tau^2) \tau \int_{-\infty}^{\infty} \exp(-y^2) dy = \exp(-\frac{1}{4}\omega^2\tau^2) \tau \sqrt{\pi}$$

Substituting in the expression for the transition probability yields:

$$p_{10} = \frac{q^2 A^2}{2m\hbar\omega} \exp(-\frac{1}{2}\omega^2\tau^2)$$

Discuss the behaviour of the transition probability and the applicability of the perturbation theory result when (a) $\tau \ll \frac{1}{\omega}$, and (b) $\tau \gg \frac{1}{\omega}$.

(a) if $\tau \ll \frac{1}{\omega}$, then $\exp(-\frac{1}{2}\omega^2\tau^2) \simeq 1$ and we have

$$p_{10} \simeq \frac{q^2 A^2}{2m\hbar\omega} = \text{constant}$$

We expect perturbation theory to be good if $p_{10} \ll 1$, that is, if

$$\frac{q^2 A^2}{2m} \ll \hbar\omega$$

Remark: In the limit $\tau \rightarrow 0$, the electric field becomes proportional to a Dirac δ -function:

$$\lim_{\tau \rightarrow 0} \mathcal{E}(t) = A\delta(t)$$

and we obtain the stated result for $\tau \ll \frac{1}{\omega}$. This is the *impulse approximation*.

(b) if $\tau \gg \frac{1}{\omega}$, then $\exp(-\frac{1}{2}\omega^2\tau^2) \rightarrow 0$ and thus the transition probability tends to zero, even in the case $q^2A^2/2m \approx \hbar\omega$. This is the *adiabatic approximation*.

4. The Hamiltonian which describes the interaction of a static spin- $\frac{1}{2}$ particle with an external magnetic field, \underline{B} , is

$$\hat{H} = -\hat{\mu} \cdot \underline{B}$$

When \underline{B} is a static uniform magnetic field in the z -direction, $\underline{B}_0 = (0, 0, B_0)$, the matrix representation of \hat{H}_0 is simply

$$-\frac{1}{2}\gamma B_0 \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with eigenvalues $\mp \frac{1}{2}\gamma B_0 \hbar$ and for this time-independent Hamiltonian, the energy eigenstates are represented by the 2-component column matrices

$$|\uparrow\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\downarrow\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Now consider superimposing on the static field \underline{B}_0 a time-dependent magnetic field of constant magnitude B_1 , rotating in the $x - y$ plane with constant angular frequency ω :

$$\underline{B}_1(t) = (B_1 \cos \omega t, B_1 \sin \omega t, 0)$$

If the Hamiltonian is now written as $\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$, write down a matrix representation of $\hat{V}(t)$.

$$\hat{V}(t) = -\frac{1}{2}\gamma \hbar B_1 (\sigma_x \cos \omega t + \sigma_y \sin \omega t) = -\frac{1}{2}\gamma \hbar B_1 \begin{pmatrix} 0 & \exp(-i\omega t) \\ \exp(i\omega t) & 0 \end{pmatrix}$$

Any spin state can be written

$$|\Psi, t\rangle = c_1(t) \exp(-iE_{\uparrow}t/\hbar) |\uparrow\rangle + c_2(t) \exp(-iE_{\downarrow}t/\hbar) |\downarrow\rangle$$

Obtain, without approximation, the coupled equations for the amplitudes $c_1(t), c_2(t)$.

The full Hamiltonian has the representation

$$\hat{H}(t) = -\frac{1}{2}\gamma \hbar \begin{pmatrix} B_0 & B_1 \exp(-i\omega t) \\ B_1 \exp(i\omega t) & -B_0 \end{pmatrix}$$

The matrix representation of the state vector at time t is

$$|\Psi, t\rangle \rightarrow \begin{pmatrix} c_1(t) \\ 0 \end{pmatrix} \exp(-iE_{\uparrow}t/\hbar) + \begin{pmatrix} 0 \\ c_2(t) \end{pmatrix} \exp(-iE_{\downarrow}t/\hbar)$$

Substituting this into the TDSE

$$i\hbar \frac{\partial}{\partial t} |\Psi, t\rangle = \hat{H}(t) |\Psi, t\rangle$$

gives the coupled first-order equations for the amplitudes:

$$\begin{aligned} i\hbar \dot{c}_1(t) &= -\frac{1}{2}\gamma \hbar B_1 \exp[i(\omega_{\uparrow} - \omega)t] c_2(t) \\ i\hbar \dot{c}_2(t) &= -\frac{1}{2}\gamma \hbar B_1 \exp[i(\omega_{\downarrow} + \omega)t] c_1(t) \end{aligned}$$

where we have used the fact that the unperturbed energy eigenvalues are

$$E_{\uparrow} = -\frac{1}{2}\gamma\hbar B_0 \quad \text{and} \quad E_{\downarrow} = \frac{1}{2}\gamma\hbar B_0$$

and defined

$$\omega_{\uparrow\downarrow} = -\omega_{\downarrow\uparrow} \equiv \frac{(E_{\uparrow} - E_{\downarrow})}{\hbar} = -\gamma B_0$$

* *If initially at $t = 0$ the system is in the spin-down state, show that the probability that at time t , the system is in the spin-up state is given without approximation by*

$$p_1(t) = |c_1(t)|^2 = A \sin^2 \left\{ \frac{1}{2} [(\gamma B_1)^2 + (\omega + \gamma B_0)^2]^{1/2} t \right\}$$

where

$$A = \frac{(\gamma B_1)^2}{\{(\gamma B_1)^2 + (\omega + \gamma B_0)^2\}}$$

What is the corresponding probability, $p_2(t)$, that the system is in the spin-down state? Sketch $p_1(t)$ and $p_2(t)$ as functions of time.

The given initial conditions correspond to $c_1(0) = 0$ and $c_2(0) = 1$.

We can obtain an exact solution to the above coupled equations by first eliminating say $c_2(t)$ between the two equations.

The first equation gives

$$c_2(t) = -\frac{2i}{\gamma B_1} \exp[-i(\omega_{\uparrow\downarrow} - \omega)t] \dot{c}_1(t)$$

Differentiating with respect to t , we find that

$$\dot{c}_2(t) = -\frac{2i}{\gamma B_1} \exp[-i(\omega_{\uparrow\downarrow} - \omega)t] \ddot{c}_1(t) - \frac{2(\omega_{\uparrow\downarrow} - \omega)}{\gamma B_1} \exp[-i(\omega_{\uparrow\downarrow} - \omega)t] \dot{c}_1(t)$$

but from the second of the coupled equations,

$$\dot{c}_2(t) = \frac{i\gamma B_1}{2} \exp[i(\omega_{\downarrow\uparrow} + \omega)t] c_1(t)$$

Equating these expressions for $\dot{c}_2(t)$, noting that $\omega_{\uparrow\downarrow} = -\omega_{\downarrow\uparrow} = -\gamma B_0$, and simplifying gives the following second-order differential equation for $c_1(t)$:

$$\ddot{c}_1 + i\Omega \dot{c}_1 + \left(\frac{1}{2}\gamma B_1\right)^2 c_1 = 0$$

where $\Omega \equiv \omega + \gamma B_0$.

To solve this, try a solution of the form $c_1(t) = A \exp(ipt)$, which yields the auxiliary equation

$$-p^2 - p\Omega + \left(\frac{1}{2}\gamma B_1\right)^2 = 0$$

with roots

$$p = -\frac{1}{2}\Omega \pm \frac{1}{2}\sqrt{\Omega^2 + (\gamma B_1)^2} \equiv -\frac{1}{2}\Omega \pm \frac{1}{2}\Delta$$

where we have defined $\Delta = \sqrt{\Omega^2 + (\gamma B_1)^2}$.

Thus the general solution is

$$c_1(t) = \exp(-\frac{1}{2}i\Omega t) \left[A_1 \cos(\frac{1}{2}\Delta t) + A_2 \sin(\frac{1}{2}\Delta t) \right]$$

The first initial condition $c_1(0) = 0$ fixes the value of A_1 to be zero. Thus

$$c_1(t) = \exp(-\frac{1}{2}i\Omega t) \times A_2 \sin(\frac{1}{2}\Delta t)$$

To determine A_2 , we need to use the second initial condition, $c_2(0) = 1$. From the first of the coupled equations, we have

$$c_2(t) = -\frac{2i}{\gamma B_1} \exp(i\Omega t) \dot{c}_1(t) = -\frac{2iA_2}{\gamma B_1} \exp(\frac{1}{2}i\Omega t) \left[-\frac{i\Omega}{2} \sin(\frac{1}{2}\Delta t) + \frac{\Delta}{2} \cos(\frac{1}{2}\Delta t) \right]$$

Setting $t = 0$ gives

$$c_2(0) = 1 = -\frac{2iA_2}{\gamma B_1} \frac{\Delta}{2}$$

so that

$$A_2 = \frac{i\gamma B_1}{\Delta}$$

Finally, then we have for the probability amplitude

$$c_1(t) = \frac{i\gamma B_1}{\Delta} \exp(-\frac{1}{2}i\Omega t) \sin(\frac{1}{2}\Delta t)$$

so that the probability of finding the system in the spin up state at time t is

$$p_1(t) = |c_1(t)|^2 = \left| \frac{\gamma B_1}{\Delta} \right|^2 \sin^2(\frac{1}{2}\Delta t) = A \sin^2 \left\{ \frac{1}{2} [(\gamma B_1)^2 + (\omega + \gamma B_0)^2]^{1/2} t \right\}$$

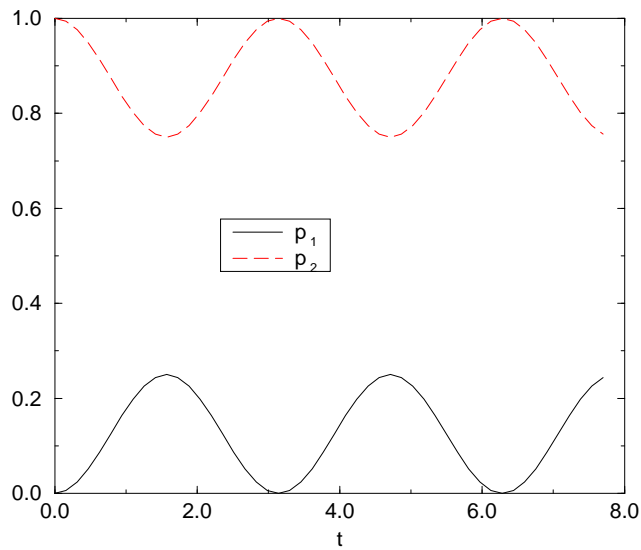
where

$$A = \frac{(\gamma B_1)^2}{\{[(\gamma B_1)^2 + (\omega + \gamma B_0)^2]\}}$$

The probability that the system is in the spin down state at time t is simply

$$p_2(t) = 1 - p_1(t) = 1 - A \sin^2 \left\{ \frac{1}{2} [(\gamma B_1)^2 + (\omega + \gamma B_0)^2]^{1/2} t \right\}$$

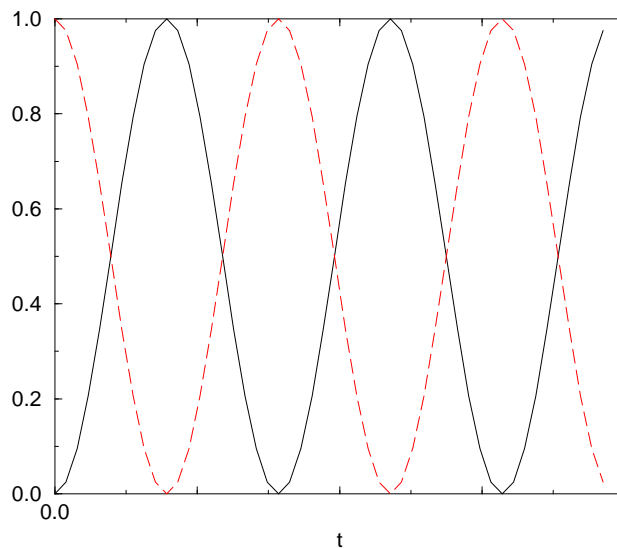
Thus the two probabilities are periodic; $p_1(t)$ oscillates between 0 and its maximum value, A , whilst $p_2(t)$ oscillates between its maximum value of 1 and its minimum value of $(1 - A)$.



Usually in practice, one has $B_1 \ll B_0$, so that the amplitude A is quite small, being of order $(B_1/B_0)^2$. However, something interesting happens if the angular frequency of the rotating field, ω is tuned to the Bohr frequency $\omega_{\uparrow\downarrow}$ of the transition. In this case, $A = 1$ and the probabilities

$$p_1(t) = \sin^2\left(\frac{1}{2}\gamma B_1 t\right), \quad p_2(t) = \cos^2\left(\frac{1}{2}\gamma B_1 t\right)$$

are large, oscillating between 0 and 1, even for $B_1 \ll B_0$. This is a *resonance phenomenon*.



The analysis of this problem forms the basis for high-precision methods for determining magnetic moments of atoms and subatomic particles, and for techniques such as nuclear magnetic resonance (NMR).