On the Rotating Wave Approximation

In these notes we derive the formula for Rabi oscillations without the approximation used in Townsend. Townsend's approximation is more formally known as the *rotating wave approximation*, and it is applied when we have near resonance quantum systems. In such systems, there is a system frequency ω_0 and a driving frequency ω, and whenever we are near resonance (i.e., $\omega \simeq \omega_0$) we neglect terms proportional $e^{i(\omega+\omega_0)t}$ in lieu of the more slowly oscillating $e^{i(\omega-\omega_0)t}$. The claimed interpretation is that the fast oscillating term $e^{i(\omega+\omega_0)t}$ "averages to zero", but a more rigorous way to obtain the same result is to show how such terms are not ultimately relevant in computing the probabilities of the quantum system.

Problem

1. **General Two-state systems**
   Say we have a two-state system defined by the (time-independent) Hamiltonian (in the $|\pm, \mathbf{z}\rangle$ basis)

$$\hat{H} = \begin{pmatrix} E_1 & W_{12} \\ W_{21} & E_2 \end{pmatrix}, \tag{1}$$

   where E_1 and E_2 (with $E_1 \neq E_2$) are real quantities and W_{12} and W_{21} are complex quantities.

   (a) Compute the energy eigenvalues of $\hat{H}$, and show that the energy eigenstates are

$$|\phi_+\rangle = \cos\frac{\theta}{2}|+, \mathbf{z}\rangle + \sin\frac{\theta}{2}e^{i\phi}|-, \mathbf{z}\rangle, \qquad |\phi_-\rangle = \sin\frac{\theta}{2}|+, \mathbf{z}\rangle - \cos\frac{\theta}{2}e^{i\phi}|-, \mathbf{z}\rangle \tag{2}$$

   where

$$\tan\theta = \frac{2|W_{12}|}{E_1 - E_2}, \quad e^{i\phi} = \frac{W_{21}}{|W_{21}|}, \tag{3}$$

   with $\theta \in [0, \pi]$.

   (b) Invert the change of basis matrix implied by Eq.(2) to find the $|\pm, \mathbf{z}\rangle$ states in terms of $|\phi_\pm\rangle$.

   (c) Write the general time dependent state $|\psi(t)\rangle$ as a linear combination of $|\phi_+\rangle$ and $|\phi_-\rangle$ with the appropriate time-dependent coefficients.

   (d) Say our system begins in the state $|\psi(0)\rangle = |-, \mathbf{z}\rangle$. Compute the probability that the system is in the state $|+, \mathbf{z}\rangle$ at time t. (Express the final answer in terms of the parameters of the Hamiltonian)

2. **Rabi Oscillations**
   Say we have a spin-1/2 particle in a magnetic field. The magnetic field can be divided into a constant part $\mathbf{B}_0$ and an oscillatory part $\mathbf{B}_1(t)$. The Hamiltonian of the system is then

$$\hat{H} = -\gamma\, \mathbf{S} \cdot (\mathbf{B}_0 + \mathbf{B}_1(t)), \tag{4}$$

   where γ is the gyromagnetic ratio and $\mathbf{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ is the spin operator vector.

   (a) If the magnetic fields are $\mathbf{B}_0 = -(\omega_0/\gamma)\mathbf{z}$ and $\mathbf{B}_1(t) = -(\omega_1/\gamma)(\cos(\omega t)\,\mathbf{x} + \sin(\omega t)\,\mathbf{y})$, show that the Hamiltonian Eq.(4) becomes

$$\hat{H} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix}. \tag{5}$$

(b) For the state $|\psi(t)\rangle$ written in the $|\pm, \mathbf{z}\rangle$ basis we have

$$|\psi(t)\rangle = c_+(t)|+, \mathbf{z}\rangle + c_-(t)|-, \mathbf{z}\rangle. \tag{6}$$

Use the time dependent Schrödinger equation and Eq.(5) to write two coupled differential equations for $c_+(t)$ and $c_-(t)$.

(c) Define new functions $\alpha_+(t)$ and $\alpha_-(t)$ by setting

$$\alpha_+(t) = e^{i\omega t/2} c_+(t) \quad \alpha_-(t) = e^{-i\omega t/2} c_-(t). \tag{7}$$

This amounts to transforming the system to a frame rotating at the same angular frequency as $\mathbf{B}_1(t)$. Substitute these expressions into the coupled differential equations obtained in part (b). What are the new coupled differential equations for α_+ and α_-?

(d) From the coupled differential equation in (b), reverse construct the "Hamiltonian" for $\alpha_+(t)$ and $\alpha_-(t)$ coefficients. What is the correspondence between this Hamiltonian and Eq.(1)

(e) Say our system begins in the state $|\psi(0)\rangle = |-, \mathbf{z}\rangle$. Using the above correspondence, compute the probability that the system is in the state $|+, \mathbf{z}\rangle$ at time t. (Express the final answer in terms of the parameters of the Hamiltonian)

Solution

1. (a) For 2×2 matrices, we know that the eigenvalues are given by

$$E_\pm = \frac{\mathrm{Tr}\,\hat{H} \pm \sqrt{(\mathrm{Tr}\,\hat{H})^2 - 4 \det \hat{H}}}{2}. \tag{8}$$

We thus find

$$E_\pm = \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4|W_{12}|^2}\right]. \tag{9}$$

To show that Eq.(2) are the eigenkets of the system with eigenvalues Eq.(9), we need to prove the two equalities

$$\begin{pmatrix} E_1 - E_+ & W_{12} \\ W_{21} & E_2 - E_+ \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix} \stackrel{?}{=} 0\,, \qquad \begin{pmatrix} E_1 - E_- & W_{12} \\ W_{21} & E_2 - E_- \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} e^{i\phi} \end{pmatrix} \stackrel{?}{=} 0. \tag{10}$$

We will prove the first equality given that the proof of the second is similar. Toward this proof we assume $E_1 > E_2$, without loss of generality, and thus find

$$\begin{aligned} E_1 - E_+ &= E_1 - \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4|W_{12}|^2}\right] \\ &= \frac{1}{2}\left[E_1 - E_2 + (E_1 - E_2)\sqrt{1 + 4|W_{12}|^2/(E_1 - E_2)^2}\right] \\ &= (E_1 - E_2)\Big[1 + \sqrt{1 + \tan^2\theta}\Big] \\ &= (E_1 - E_2)\Big[1 + \sec\theta\Big] \\ &= -(E_1 - E_2)\frac{\cos^2\frac{\theta}{2}}{\cos\theta}. \end{aligned} \tag{11}$$

Similarly we find

$$E_2 - E_+ = -(E_1 - E_2)\frac{\sin^2\frac{\theta}{2}}{\cos\theta}. \tag{12}$$

And using $W_{21} = |W_{21}|e^{i\phi} = W_{12}^*$ we obtain the following system for the left equality of Eq.(10):

$$
\begin{aligned}
0 &\stackrel{?}{=} -(E_1 - E_2)\frac{\sin^2\frac{\theta}{2}\cos\frac{\theta}{2}}{\cos\theta} + |W_{21}|\sin\frac{\theta}{2} \\
0 &\stackrel{?}{=} \left[|W_{21}|\cos\frac{\theta}{2} - (E_1 - E_2)\frac{\cos^2\frac{\theta}{2}\sin\frac{\theta}{2}}{\cos\theta}\right]e^{i\phi}.
\end{aligned} \tag{13}
$$

Applying trigonometric identities and factoring phases, we then obtain

$$
\begin{aligned}
0 &\stackrel{?}{=} \left[-(E_1 - E_2)\frac{\tan\theta}{2} + |W_{21}|\right]\sin\frac{\theta}{2} \\
0 &\stackrel{?}{=} \left[|W_{21}| - (E_1 - E_2)\frac{\tan\theta}{2}\right]\cos\frac{\theta}{2}e^{i\phi},
\end{aligned} \tag{14}
$$

both of which are valid by Eq.(3).

(b) The change of basis matrix to go from the $|\pm, \mathbf{z}\rangle$ states to the $|\phi_\pm\rangle$ states is (by Eq.(2))

$$
\hat{U}_{\mathbf{z}\to\phi} = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{i\phi} \\ \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix}. \tag{15}
$$

Thus the change of basis matrix to go from the $|\phi_\pm\rangle$ states to the $|\pm, \mathbf{z}\rangle$ states is

$$
\hat{U}_{\phi\to\mathbf{z}} = \hat{U}^\dagger_{\mathbf{z}\to\phi} = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{-i\phi} & -\cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix}, \tag{16}
$$

and we have

$$
|+, \mathbf{z}\rangle = \cos\frac{\theta}{2}|\phi_+\rangle + \sin\frac{\theta}{2}|\phi_-\rangle \tag{17}
$$

$$
|-, \mathbf{z}\rangle = \left(\sin\frac{\theta}{2}|\phi_+\rangle - \cos\frac{\theta}{2}|\phi_-\rangle\right)e^{-i\phi}. \tag{18}
$$

The phase factor in $|-, \mathbf{z}\rangle$ falls out of all physical quantities so we can neglect it, but we keep it here for explicitness.

(c) For a system with Hamiltonian $\hat{H}$ and energy eigenvalues $E_\pm$, an arbitrary state $|\psi\rangle$ is

$$
|\psi(t)\rangle = c_+ e^{-iE_+ t/\hbar}|\phi_+\rangle + c_- e^{-iE_- t/\hbar}|\phi_-\rangle. \tag{19}
$$

(d) Our system begins in a state $|\psi(0)\rangle = |-, \mathbf{z}\rangle$ and thus we have

$$
|\psi(0)\rangle = \left(\sin\frac{\theta}{2}|\phi_+\rangle - \cos\frac{\theta}{2}|\phi_-\rangle\right)e^{-i\phi}. \tag{20}
$$

From Eq.(19) we can infer

$$
c_+ = \sin\frac{\theta}{2}e^{-i\phi}, \qquad c_- = -\cos\frac{\theta}{2}e^{-i\phi}. \tag{21}
$$

The time-dependent state is then

$$
|\psi(t)\rangle = \left(\sin\frac{\theta}{2}e^{-iE_+ t/\hbar}|\phi_+\rangle - \cos\frac{\theta}{2}e^{-iE_- t/\hbar}|\phi_-\rangle\right)e^{-i\phi}. \tag{22}
$$

Therefore, the probability amplitude to be in the state $|+,\mathbf{z}\rangle$ is

$$\begin{aligned}\langle +,\mathbf{z}|\psi(t)\rangle &= \left(\sin\frac{\theta}{2}e^{-iE_+t/\hbar}\langle +,\mathbf{z}|\phi_+\rangle - \cos\frac{\theta}{2}e^{-iE_-t/\hbar}\langle +,\mathbf{z}|\phi_-\rangle\right)e^{-i\phi} \\ &= \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\phi}\left(e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}\right), \qquad (23)\end{aligned}$$

and the probability to transition from $|-,\mathbf{z}\rangle$ to $|+,\mathbf{z}\rangle$ in a time t is

$$\begin{aligned}P_{-,\mathbf{z}\to+,\mathbf{z}}(t) &= |\langle +,\mathbf{z}|\psi(t)\rangle|^2 \qquad (24)\\ &= \frac{1}{2}\sin^2\theta\left[1-\cos\left(\frac{E_+-E_-}{\hbar}t\right)\right] \\ &= \sin^2\theta\sin^2\left(\frac{E_+-E_-}{2\hbar}t\right), \qquad (25)\end{aligned}$$

or with Eq.(3) and Eq.(9) we obtain

$$P_{-,\mathbf{z}\to+,\mathbf{z}}(t) = \frac{4|W_{12}|^2}{4|W_{12}|^2+(E_1-E_2)^2}\sin^2\left[\frac{t}{2\hbar}\sqrt{(E_1-E_2)^2+4|W_{12}|^2}\right]. \qquad (26)$$

2. (a) For the Hamiltonian Eq.(4) and the given magnetic fields we obtain

$$\begin{aligned}\hat{H} &= \left(\hat{S}_x\omega_1\cos(\omega t)+\hat{S}_y\omega_1\sin(\omega t)+\hat{S}_z\omega_0\right) \\ &= \frac{\hbar}{2}\left(\hat{\sigma}_1\omega_1\cos(\omega t)+\hat{\sigma}_2\omega_1\sin(\omega t)+\hat{\sigma}_3\omega_0\right) \\ &= \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \cos(\omega t)-i\sin(\omega t) \\ \cos(\omega t)+i\sin(\omega t) & -\omega_0\end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0\end{pmatrix}. \qquad (27)\end{aligned}$$

(b) For the state $|\psi(t)\rangle = c_+(t)|+,\mathbf{z}\rangle + c_-(t)|-,\mathbf{z}\rangle$, the matrix form of the Schrödinger equation is

$$i\hbar\frac{d}{dt}\begin{pmatrix}c_+(t)\\c_-(t)\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0\end{pmatrix}\begin{pmatrix}c_+(t)\\c_-(t)\end{pmatrix}, \qquad (28)$$

or, written as a system of coupled differential equations,

$$\begin{aligned}i\frac{d}{dt}c_+(t) &= \frac{\omega_0}{2}c_+(t)+\frac{\omega_1}{2}e^{-i\omega t}c_-(t) \qquad (29)\\ i\frac{d}{dt}c_-(t) &= \frac{\omega_1}{2}e^{-i\omega t}c_+(t)-\frac{\omega_0}{2}c_-(t). \qquad (30)\end{aligned}$$

(c) If we define new coefficients $\alpha_+(t)$ and $\alpha_-(t)$ according to

$$c_+(t) = e^{-i\omega t/2}\alpha_+(t)\,, \quad c_-(t) = e^{i\omega t/2}\alpha_-(t), \qquad (31)$$

then the system of differential equations for $\alpha_\pm(t)$ becomes

$$\begin{aligned}i\frac{d}{dt}\alpha_+(t) &= \frac{\omega_0-\omega}{2}\alpha_+(t)+\frac{\omega_1}{2}\alpha_-(t) \qquad (32)\\ i\frac{d}{dt}\alpha_-(t) &= \frac{\omega_1}{2}\alpha_+(t)-\frac{\omega_0-\omega}{2}\alpha_-(t). \qquad (33)\end{aligned}$$

(d) The Schrödinger equation for the coefficients $\alpha_\pm(t)$ is then

$$i\hbar\frac{d}{dt}\begin{pmatrix}\alpha_+(t)\\ \alpha_-(t)\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\omega_0-\omega & \omega_1\\ \omega_1 & -(\omega_0-\omega)\end{pmatrix}\begin{pmatrix}\alpha_+(t)\\ \alpha_-(t)\end{pmatrix} \tag{34}$$

which suggests this "rotating system" is governed by the the time-independent "Hamiltonian"

$$\hat{\tilde{H}} = \frac{\hbar}{2}\begin{pmatrix}\omega_0-\omega & \omega_1\\ \omega_1 & -(\omega_0-\omega)\end{pmatrix}. \tag{35}$$

The correspondence between Eq.(35) and Eq.(1) is established through the transformations

$$\begin{aligned} E_1 &\to \frac{\hbar}{2}(\omega_0-\omega)\\ E_2 &\to -\frac{\hbar}{2}(\omega_0-\omega)\\ W_{21} &\to \frac{\hbar}{2}\omega_1. \end{aligned} \tag{36}$$

(e) If our system is initially in the state $|\psi(0)\rangle = |-,\mathbf{z}\rangle$ and we want to find the probability to be in the state $|+,\mathbf{z}\rangle$ at time t, we compute

$$|\langle +,\mathbf{z}|\psi(t)\rangle|^2 = |c_+(t)|^2 = |\alpha_+(t)|^2, \tag{37}$$

given $c_-(0) = 1$, and $\alpha_-(0) = 1$ by corollary. However, with $\alpha_\pm(t)$ governed by the "Hamiltonian" Eq.(35), this probability is precisely what we computed more generally in Problem 1(d). Thus we find (with the transformations Eq.(36)), Eq.(26) becomes

$$P_{-,\mathbf{z}\to+,\mathbf{z}}(t) = \frac{\omega_1^2}{(\omega-\omega_0)^2+\omega_1^2}\sin^2\left[\frac{t}{2}\sqrt{(\omega-\omega_0)^2+\omega_1^2}\right], \tag{38}$$

which is the Rabi oscillation formula.

Discussion

Through this problem we essentially showed that when we apply a certain time-dependent rotation (given by Eq.(7)) to a spin-1/2 particle in an oscillatory magnetic field, we can effectively rotate away the oscillation frequency of the magnetic field. The resulting Hamiltonian is then time-independent and depends on $\omega-\omega_0$ (and *not* $\omega+\omega_0$) and is amenable to the standard analysis for time-independent quantum systems. In the two problems above, we showed this in reverse: starting with a calculation for the transition probability in a general 2×2 Hamiltonian system, and then showing that the Hamiltonian of a spin-1/2 particle in a time-dependent magnetic field can be made time-independent with the appropriate transformation.