QUANTUM MECHANICS I

PHYS 516

Solutions to Problem Set # 5

1. Crossed E and B fields: A hydrogen atom in the N = 2 level is subject to crossed electric and magnetic fields. Choose your coordinate axes to make life 'simple': Choose the x and z axes in the direction of the two fields (tell me which).

a. Write down the Hamiltonian matrix.

b. Set $-3e|\mathbf{E}|a_0 = \cos\theta$ and $\mu|\mathbf{B}| = \sin\theta$. Plot the energy eigenvalues for $0 \le \theta \le 2\pi$.

1. Solution: For convenience the reference energy is taken as $E_{2S} = E_{2P}$, the energy of the degenerate 2S-2P levels in the NR hydrogen atom. $H_{pert} = -e\mathcal{E}\cdot\mathbf{r} - \mu\mathbf{L}\cdot\mathbf{B}$ and the diamagnetic term is neglected. With respect to the basis $|2S\rangle, |2P, +1\rangle, |2P, 0\rangle, |2P, -1\rangle$ the perturbation matrix is

$$-e\mathcal{E}\cdot\mathbf{r} \to -3e\mathcal{E}_z a_B \begin{bmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad -\mu B_x \begin{bmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & \sqrt{2}/2 & 0\\ 0 & \sqrt{2}/2 & 0 & \sqrt{2}/2\\ 0 & 0 & \sqrt{2}/2 & 0 \end{bmatrix}$$

For simplicity we have chosen to take the z axis along the direction of the **E** field and the x axis along the direction of the **B** field. With the substitutions $-3e\mathcal{E}_z a_B \to \cos\theta$ and $-\mu B_x \to \sin\theta$ we get

$$H_{pert} = \begin{bmatrix} 0 & 0 & \cos\theta & 0 \\ 0 & 0 & \sqrt{2}/2\sin\theta & 0 \\ \cos\theta & \sqrt{2}/2\sin\theta & 0 & \sqrt{2}/2\sin\theta \\ 0 & 0 & \sqrt{2}/2\sin\theta & 0 \end{bmatrix}$$

The eigenvalues of this matrix are 1, 0, 0, -1 for all values of θ .

2. 2-Level Oscillations: The hamiltonian describing a two-level system

is $H = \frac{\epsilon}{2}\sigma_z + \gamma\sigma_x$. At t = 0 the initial state is $\psi(t = 0) = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Plot $P(\uparrow, t)$ and $P(\downarrow, t)$ for $t \ge 0$.

Solution: In class, at the blackboard, we studied the two level problem with hamiltonian

$$H = \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix} \quad \mathbf{v}_{+} = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} \quad \mathbf{v}_{-} = \begin{bmatrix} -\sin \theta \\ \cos \theta \end{bmatrix}$$

The eigenvectors are \mathbf{v}_{\pm} and their eigenvalues are $E = \pm 1$. When the initial state is the lower energy state $\begin{bmatrix} 0\\1 \end{bmatrix}$, its resolution in terms of the eigenstates is

$$\begin{bmatrix} 0\\1 \end{bmatrix} = \sin\theta \begin{bmatrix} \cos\theta\\ \sin\theta \end{bmatrix} + \cos\theta \begin{bmatrix} -\sin\theta\\ \cos\theta \end{bmatrix}$$

The time evolution of the eigenstates is through a phase factor:

$$\begin{bmatrix} 0\\1 \end{bmatrix} \xrightarrow{t>0} \sin \theta \begin{bmatrix} \cos \theta\\\sin \theta \end{bmatrix} e^{-i(+\omega)t} + \cos \theta \begin{bmatrix} -\sin \theta\\\cos \theta \end{bmatrix} e^{-i(-\omega)t}$$

Carrying out the indicated algebra we find

$$\begin{bmatrix} 0\\1 \end{bmatrix} \xrightarrow{t>0} \begin{bmatrix} -2i\sin\theta\cos\theta\sin\omega t\\\cos\omega t+i\sin\omega t(\cos^2\theta-\sin^2\theta) \end{bmatrix} = \begin{bmatrix} -i\sin2\theta\sin\omega t\\\cos\omega t+i\cos2\theta\sin\omega t \end{bmatrix}$$

The probability of state $\begin{bmatrix} 1\\0 \end{bmatrix}$ oscillates periodically as $(\sin 2\theta)^2 \sin^2 \omega t$ and that of the state $\begin{bmatrix} 0\\1 \end{bmatrix}$ oscillates as $1 - (\sin 2\theta)^2 \sin^2 \omega t$.

3. Neutrinos with 2 Flavors: Assume neutrinos come with two flavors. The flavor eigenstates are not energy eigenstates. The two types of states are related by a 2×2 unitary transformation:

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} \cos \theta_{12} & \sin \theta_{12} \\ -\sin \theta_{12} & \cos \theta_{12} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$

Use $\sin \theta_{12} = 0.1$.

a. Assume that a decay produces a flavor-1 neutrino. Resolve this flavor state into energy states.

b. Propagate the energy states forward in time from t = 0 to arbitrary time T.

c. Assume a neutrino detector has been set up a distance L = cT away from the neutrino source to detect neutrinos with flavor 1 (or 2). Compute the probability *amplitude* for detecting neutrinos of either type. Use $E_2 =$ $10E_1 > 0$ and T large enough so your plots show interesting things.

d. Compute the probability for detecting neutrinos with flavor 1. Flavor 2.

e. Do the probabilities sum to +1? (Hint: they better!)

Solution: We solve in five steps.

Step 1. Resolve the flavor-1 neutrino in terms of the mass states:

$$|f_1\rangle = \cos\theta_{12}|m_1\rangle + \sin\theta_{12}|m_2\rangle$$

Step 2: Propagate the energy states forward in time $(\hbar = 1, c = 1)$:

$$|f_1\rangle(t) = \cos\theta_{12}|m_1\rangle e^{-im_1t} + \sin\theta_{12}|m_2\rangle e^{-im_2t}$$

Step 3: Express the mass eigenstates in terms of the flavor states:

$$|f_1\rangle(t) = \cos\theta_{12}\left(\cos\theta_{12}|f_1\rangle - \sin\theta_{12}|f_2\rangle\right)e^{-im_1t} + \sin\theta_{12}\left(\sin\theta_{12}|f_1\rangle + \cos\theta_{12}|f_2\rangle\right)e^{-im_2t}$$

Step 4: Collect terms:

$$|f_1\rangle(t) = |f_1\rangle \left(\cos^2\theta_{12}e^{-im_1t} + \sin^2\theta_{12}e^{-im_2t}\right) + |f_2\rangle \sin\theta_{12}\cos\theta_{12} \left(-e^{-im_1t} + e^{-im_2t}\right)$$

Step 5: Then flavor 1 neutrinos oscillate into flavor 2 neutrinos with an amplitude $A_{2\leftarrow 1} = \langle f_2 | f_1(t) \rangle = -i \sin 2\theta_{12} \sin \left(\frac{m_2 - m_1}{2}\right) t e^{i(m_1 + m_2)t/2}$ and with a probability $P_{2\leftarrow 1} = \sin^2 2\theta_{12} \sin^2 \frac{\Delta m}{2} t$. Further $P_{1\leftarrow 1} = 1 - \sin^2 2\theta_{12} \sin^2 \frac{\Delta m}{2} t$.

4. Rabi Oscillations: The hamiltonian describing a two-level system is

$$H = \begin{pmatrix} \frac{\epsilon}{2} & \gamma \cos \omega t \\ \gamma \cos \omega t & -\frac{\epsilon}{2} \end{pmatrix}$$

At t = 0 the initial state is $\psi(t = 0) = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Plot $P(\uparrow, t)$ and $P(\downarrow, t)$ for $t \ge 0$ and "interesting choices" of ϵ, γ, ω .

Solution: If you try to diagonalize the hamiltonian and proceed as in either of the previous two problems (time-independent hamiltonians), then you have to take into account that the unitary diagonalization matrix also varies in time, and this rapidly becomes an unpleasant problem outside the bounds of *Elementary* Quantum Mechanics. In the Old Days the great men handled this problem by making useful and intuitive approximations (*e.g.*, the rotating wave approximation (RWA)) because they didn't have computers at their fingertips. Now we do, so such approaches are no longer necessary.

The first step is to reduce the number of parameters to search over. To start, we rewrite the hamiltonian as

$$H' = H/\sqrt{(\epsilon/2)^2 + \gamma^2} = \begin{bmatrix} \cos 2\theta & \sin 2\theta \cos \omega t \\ \sin 2\theta \cos \omega t & -\cos 2\theta \end{bmatrix}$$
(1)

Here we can imagine a right triangle with perpendicular sides $\epsilon/2$ and γ and hypotenuse $\sqrt{(\epsilon/2)^2 + \gamma^2}$ with included angle 2θ .

The complex amplitudes c_i for the two states obey the first order equation

$$i\hbar\frac{dc_i}{dt} = H_{ij}(t)'c_j$$

Set $\hbar = 1$ for convenience (it can always be returned via a scaling argument). Then

$$\dot{c}_i = -iH'_{ij}c_j \quad \& \quad \dot{c}_i^* = +iH'_{ij}c_j^* \qquad \Rightarrow \frac{d}{dt}c_j^*c_j = 0$$

so that probability is conserved. Define $c_1 = x_1 + ix_2$ and $c_2 = x_3 + ix_4$ and the first order equations are

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & h_{11} & 0 & h_{12} \\ -h_{11} & 0 & -h_{12} & 0 \\ 0 & h_{21} & 0 & h_{22} \\ -h_{21} & 0 & -h_{22} & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

Here h_{ij} are the matrix elements in the hamiltonian matrix that appears in Eq. (1). The 4 × 4 matrix above is antisymmetric since $h_{12} = h_{21}$, so that

$$\frac{d}{dt}\sum_{i}x_{i}^{2}=2\sum_{i}x_{i}\dot{x}_{i}=0$$

Again, probability is conserved: $\frac{d}{dt}\sum_i c_i^* c_i = \frac{d}{dt}\sum_j x_j^2 = 0$. This means that the trajectory $x_i(t)$ lies on the surface of a sphere in $R^4 : S^3 \subset R^4$.

These equations have been integrated using a standard RK4 integrator. I used the real RK4 integrator described in *Numerical Recipes*. The results depend on the strength of the driving term $(\tan 2\theta)$ and the ratio of the driving frequency to the undriven frequency: $\omega/2$.

Remark on Problems 2 and 3: A simple way to carry out time evolution computations for time-independent hamiltonians is to insert resolutions of the identity on both sides of the time evolution operator $e^{-\frac{i}{\hbar}Ht}$:

$$e^{-\frac{i}{\hbar}Ht} \rightarrow |m_i\rangle\langle |e^{-\frac{i}{\hbar}Ht}|m_j\rangle\langle m_j|$$

Then the transition probability amplitudes for the various flavor states are

$$A_{s\leftarrow r} = \langle f_r | m_i \rangle \langle | e^{-\frac{i}{\hbar}Ht} | m_j \rangle \langle m_j | f_s \rangle$$

The matrix elements are the eigenvectors of H and can often be read from the statement of the problem. For example

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} \cos \theta_{12} & \sin \theta_{12} \\ -\sin \theta_{12} & \cos \theta_{12} \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \Rightarrow \begin{bmatrix} |f_1\rangle & |f_2\rangle \end{bmatrix} = \begin{bmatrix} |m_1\rangle & |m_2\rangle \end{bmatrix} \begin{bmatrix} \cos \theta_{12} & -\sin \theta_{12} \\ \sin \theta_{12} & \cos \theta_{12} \end{bmatrix}$$

So

$$\begin{bmatrix} \langle m_1 | f_1 \rangle & \langle m_1 | f_2 \rangle \\ \langle m_2 | f_1 \rangle & \langle m_2 | f_2 \rangle \end{bmatrix} = \begin{bmatrix} \cos \theta_{12} & -\sin \theta_{12} \\ \sin \theta_{12} & \cos \theta_{12} \end{bmatrix}$$

As a result in the flavor basis

$$U(t) = \begin{bmatrix} \cos \theta_{12} & \sin \theta_{12} \\ -\sin \theta_{12} & \cos \theta_{12} \end{bmatrix} \begin{bmatrix} e^{-im_1 t} & 0 \\ 0 & e^{-im_2 t} \end{bmatrix} \begin{bmatrix} \cos \theta_{12} & -\sin \theta_{12} \\ \sin \theta_{12} & \cos \theta_{12} \end{bmatrix}$$



Figure 1: Real and imaginary parts of the amplitudes c_1, c_2 for Rabi oscillations. $Black = Re(c_1)$, $Red = Im(c_1)$, $Blue = Re(c_2)$, $Cyan = Im(c_2)$. Parameters: $\theta = 0.3, \omega = 1.5$. The sum of the squares of the four curves is indicated by the horizontal line at 1. This acts as a self-consistency test (sanity check).



Figure 2: Probabilities $|c_1|^2$ in black and $|c_2|^2$ in red for Rabi oscillations. Parameters: $\theta = 0.3, \omega = 1.5$. Their sum is +1.