PH 500 Problem Set # 8

At this point, we've developed the formalism of quantum systems, described the possible results of measurements, and described how fixed systems evolve in time. There is one last piece of formalism to cover before we turn to calculational techniques appropriate to various situations, which is to see what happens when the system changes with time. Up to now, the states have evolved in a fixed system, for example spins in a fixed magnetic field. Now we let the magnetic field vary with time as well. In other words, we wan to consider a Hamiltonian $\hat{\mathcal{H}}(t)$ that depends explicitly on time.

Again, the things I want you to do are in **bold**.

1. Let's consider a system where the Hamiltonian $\hat{\mathcal{H}}(t)$ varies with time. The Schrödinger equation still reads

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{\mathcal{H}}(t)|\psi(t)\rangle \tag{1}$$

but it is now more complicated since both $|\psi(t)\rangle$ and $\hat{\mathcal{H}}(t)$ depend on time. In particular, the Hamiltonian at one time does not necessarily even commute with the Hamiltonian at another time! And if $[\hat{\mathcal{H}}(t_1), \hat{\mathcal{H}}(t_2)] \neq 0$, it means that *we can't find states that are eigenstates of the Hamiltonian at both times*. This makes time-dependent problems considerably more difficult, and the result is that usually the best we can do is to use some properties of the time dependence of $\hat{\mathcal{H}}$ (for example, it might be periodic or slowly varying) to construct an approximate solution.

Formally, however, the solution is a snap: If we start in the state $|\psi(t=0)\rangle$, the solution at time t is

$$|\psi(t)\rangle = \mathcal{T}e^{-\frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt'}|\psi(t=0)\rangle \tag{2}$$

For $\hat{\mathcal{H}}$ constant, this just reduces to the equation we had before (ignoring the mysterious $\mathcal{T}$ on the right–hand side for a moment). For the general case, we have to be more careful: Remember that if $[\hat{A}, \hat{B}] \neq 0$, $e^{\hat{A}}e^{\hat{B}} \neq e^{\hat{A}+\hat{B}}$. When we write out the series for the exponential, we get

$$\begin{aligned} e^{-\frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt'} &= 1 - \frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt' - \frac{1}{2\hbar^2}\int_0^t \hat{\mathcal{H}}(t')dt' \int_0^t \hat{\mathcal{H}}(t'')dt'' \\ &\quad + \frac{i}{6\hbar^3}\int_0^t \hat{\mathcal{H}}(t')dt' \int_0^t \hat{\mathcal{H}}(t'')dt'' \int_0^t \hat{\mathcal{H}}(t''')dt''' + \ldots \\ &= 1 - \frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt' - \frac{1}{2\hbar^2}\int_0^t dt' \int_0^t dt''\hat{\mathcal{H}}(t')\hat{\mathcal{H}}(t'') \\ &\quad + \frac{i}{6\hbar^3}\int_0^t dt' \int_0^t dt'' \int_0^t dt'''\hat{\mathcal{H}}(t')\hat{\mathcal{H}}(t'')\hat{\mathcal{H}}(t''') + \ldots \end{aligned} \tag{3}$$

which is already a mess. The $\mathcal{T}$ introduces another twist: it instructs us to *re-order* the $\hat{\mathcal{H}}(t')$ operators in the integrand so that the one with the latest time is on the left, the next–latest second from the left, and so on. The result is known as a *time-ordered exponential*. Note that this prescription is easy to describe in words, but quite difficult to implement in practice, since

we have to re-order every one of the infinitely many terms in the expansion of the exponential, and then re-sum the result. Our expression is now

$$\begin{aligned}\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt'} &= 1-\frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt' - \frac{1}{\hbar^2}\int_0^t dt'\int_0^{t'} dt''\hat{\mathcal{H}}(t')\hat{\mathcal{H}}(t'') \\ &\quad +\frac{i}{\hbar^3}\int_0^t dt'\int_0^{t'} dt''\int_0^{t''} dt'''\hat{\mathcal{H}}(t')\hat{\mathcal{H}}(t'')\hat{\mathcal{H}}(t''') + \ldots \end{aligned} \tag{4}$$

where in each term we have written just one of the $n!$ equal contributions to the result, and then cancelled the $n!$ in the denominator to compensate. **Show that as a formal expression, $|\psi(t)\rangle = \mathcal{T}e^{-\frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}(t')dt'}|\psi(t=0)\rangle$ provides a solution to the Schrödinger equation.** Note that such expressions are almost always impossible to compute exactly; the most general approach involves assuming that the time–dependent part is small, in which case we can separate out the time–independent piece and then do this sort of expansion for the time–independent piece, and then only keep a finite number of terms in the expansion of the exponential. This calculation is best done using *Feynman diagrams*, which we won't get into here.

2. There are a number of approximation schemes available for this purpose, whose applicability depends on the nature of the time dependence of $\hat{\mathcal{H}}$. One example is the *sudden approximation*. Suppose that at $t = 0$ we have the state

$$|\psi\rangle = |+\rangle \tag{5}$$

and the Hamiltonian is $\hat{\mathcal{H}} = \gamma B\hat{S}_y$. Then, suddenly, at $t = a$, the Hamiltonian changes to $\hat{\mathcal{H}} = \gamma B\hat{S}_z$. In the sudden approximation, we assume that the change happens so fast that *the state does not change* at that moment. Its time evolution changes from being described by the first Hamiltonian to the second (so we will likely have to change basis). **Find $|\psi(t)\rangle$ for $t > 0$ in this example.** To do so, you should time evolve with the first Hamiltonian up to $t = a$, and then take the state at $t = a$ and evolve it forward with the second Hamiltonian.

3. The *adiabatic approximation* is the opposite of the sudden approximation. In this approximation, we assume that although the Hamiltonian varies with time, it only varies very slowly. What we do is imagine a plot of the eigenvalues of the Hamiltonian as a function of time. That is, at each time, we find the eigenstates of the Hamiltonian (as if it was constant in time) and plot their eigenvalues versus t. If the potential varies gradually, these plots should be smooth lines — the eigenvalues won't jump suddenly but will just vary slowly. In the adiabatic approximation, we assume that if you start the system in a particular state, it will just move along this line, always remaining in the eigenstate corresponding to this eigenvalue. Roughly, this approximation is valid if the *difference in energy between adjacent states* times the *time scale over which the potential changes* is large compared to $\hbar$. (If the states ever *cross*, so that the difference in energy goes to zero, we are out of luck, since we don't know which state the particle will come out in. Fortunately, this bascially never happens.) We will just take this result on faith, though the approximate techniques of the previous problem set can be extended to demonstrate it more rigorously.

As an example, suppose

$$\boldsymbol{B(t)} = B_0(\hat{\boldsymbol{x}} \sin\alpha \cos\omega t + \hat{\boldsymbol{y}} \sin\alpha \sin\omega t + \hat{\boldsymbol{z}} \cos\alpha) \tag{6}$$

where α and ω are constants and our Hamiltonian is

$$\hat{\mathcal{H}} = -\gamma \boldsymbol{B} \cdot \hat{\boldsymbol{S}} \tag{7}$$

This field can be obtained by starting from $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$ and rotating by an angle α around the y-axis to obtain the $t = 0$ state, and then by rotating by an angle ωt around the z-axis. For $\mathbf{B} = B_0\hat{\boldsymbol{z}}$ the eigenstates are $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ with eigenvalue $-\frac{\gamma B_0 \hbar}{2}$ and $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ with eigenvalue $\frac{\gamma B_0 \hbar}{2}$. **Find the eigenstates of the general $\hat{\mathcal{H}}(t)$ at time t by acting with rotations on the states where $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$.**

4. (From Griffiths) Suppose the system starts with definite spin up along the direction of $\boldsymbol{B(t = 0)}$ as found in the last problem. The exact solution to the time–dependent Schrödinger equation with this initial condition is

$$|\psi(t)\rangle = \begin{pmatrix} \left[\cos\frac{\lambda t}{2} + i\frac{\omega_1+\omega}{\lambda}\sin\frac{\lambda t}{2}\right]\cos\frac{\alpha}{2}e^{-\frac{i\omega t}{2}} \\ \left[\cos\frac{\lambda t}{2} + i\frac{\omega_1-\omega}{\lambda}\sin\frac{\lambda t}{2}\right]\sin\frac{\alpha}{2}e^{\frac{i\omega t}{2}} \end{pmatrix} \tag{8}$$

where

$$\omega_1 = \gamma B_0 \qquad \text{and} \qquad \lambda = \sqrt{\omega^2 + \omega_1^2 + 2\omega\omega_1\cos\alpha} \tag{9}$$

   (a) **Show that (up to an overall phase) this exact result reduces to the state you found in the previous problem in the adiabatic limit. Find the expectation values of $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ as functions of time in the adiabatic limit.**

   Hint: First show that adiabatic limit is the same as the limit where $\omega \ll \omega_1$.

   (b) **Compare the vectors $\langle\hat{\mathbf{S}}\rangle_\psi$ (which you found in the previous subpart) and $\boldsymbol{B}$. Explain what is happening in physical terms using the adiabatic theorem.**

5. An interesting illustration of the subtleties of the adiabatic approximation is the calculation of *Berry's phase*. Surprisingly, this result was recognized only relatively recently (1984), even though all the tools necessary to derive it had been around for sixty years. (Though after Berry's paper it was realized that the central ideas were already present in the work of Pancharatnam in 1956.)

   We said that in the adiabatic approximation, if we start the system in an energy eigenstate it will stay in that eigenstate. However, while staying in that eigenstate it can pick up a time–dependent phase. In general, this phase is not very interesting, since we can always absorb it in the definition of the eigenfunctions at different times. But if we follow an adiabatic process that ends up at the same place it started, we can compare the phase at the end to the phase we started with — since we are talking about the same state, this comparison is meaningful.

The phase factor we would expect to see is just $e^{i\theta_D}$ where

$$\theta_D = -\frac{1}{\hbar}\int_0^t E(t')dt' \tag{10}$$

where $E(t')$ is the energy eigenvalue at time t'. This term just generalizes (in the adiabatic approximation) the phase $e^{-\frac{iEt}{\hbar}}$ we would get for a constant Hamiltonian. We will call this the *dynamic* phase. Clearly it depends on how fast we carry out the evolution (two different values of the total time t will give different dynamic phases, even if they are both chosen such that the adiabatic approximation is valid).

In Berry's calculation, we would like to think of the dynamical phase as the boring part. Suppose that over time t we adiabatically vary the Hamiltonian over a closed loop, so that it comes back to where it started. The system will come back to the same state, up to a phase. Subtract from that phase the dynamic phase, which we expected (for example, it shows up even if we don't change the Hamiltonian at all). What is left, called Berry's phase, can be nonzero in a wide class of problems, when it has some remarkable properties.

Consider the rotating magnetic field of the previous problem over one full cycle in the adiabatic limit. Show that the Berry's phase is equal to $-\Omega/2$, where Ω is the solid angle subtended by the loop the magnetic field took around the sphere. Note that, amazingly, this result (which generalizes to any path) is purely geometrical, independent of all the other properties of the system (as long as we are in the adiabatic limit).

Hint: You only need to show the result in the adiabatic limit, which you can show corresponds to dropping terms that vanish as $\omega/\omega_1 \to 0$. Start from the full expression for the state and then take advantage of expansions like

$$(1+x)^\beta = 1 + \beta x + \mathcal{O}(x^2)\,. \tag{11}$$

Hint: If you find your answer is off by π or 2π, check that it goes to zero as $\alpha \to 0$, which will define for you the correct definition of the zero of the phase.