PHY662, Spring 2004, Mar. 16, 2004

16th March 2004

1 Miscellaneous

1. Continue Shankar Ch. 18 for time-dependent perturbation theory.
2. I will be 5 minutes late to class on Thursday. I am out of town next week (exam on Tuesday, we will schedule a makeup class). Interest in an exam review session on Sunday afternoon?
3. Today:
   (a) Review sheet for mid-term #2. Exam is on **TUESDAY, MARCH 23** (1 week from today).
   (b) Hand out key for HWK #7, problem #3 and review HWK #8 while mentioning degenerate perturbation theory.
   (c) Start on time-dependent perturbation theory.

Last time, we used the sum $\sum_{k=1}^{\infty} \frac{1}{(2k)^2-1}$. I think someone pointed out in class that this sum collapses. Here is how:

$$\sum_{k=1}^{\infty} \frac{1}{(2k)^2-1} = \frac{1}{2}\sum_{k=1}^{\infty}\left[\frac{1}{2k-1} - \frac{1}{2k+1}\right] = \frac{1}{2}\left(1 - \frac{1}{3} + \frac{1}{3} - \frac{1}{5} + \dots\right) = \frac{1}{2}\,.$$

2 EXAM #2 NOTES

Again, review the handouts, your own notes, and understand how to solve each homework problem. You can also practice with the problems in Shankar. The format of the exam will be quite similar to the first exam. Again, a table of formulas will be provided.

2.1 Reminder of topics

The topics for this exam are the variational method we studied, the WKB approximation, and time-independent perturbation theory. Time-dependent perturbation theory will not be on the exam. Note that we relied on Griffiths for the WKB approximation, especially. So be prepared to answer questions about

- Variational method for computing approximate wavefunctions - the principles and applications.
- WKB method: how to derive and the conditions for its application.
- Use of the Airy function in deriving connection formulas.
- Quantization conditions derived from WKB.
- Applications of the WKB method, including computing bound state energies and tunneling rates.
- Time-independent perturbation theory: how to arrange the expansion.
- Perturbation theory in general: uses and dangers.
- First-order nondegenerate perturbation theory: when can it be used and how to use it. Computing corrections to the energy and to the wavefunctions.
- Second-order nondegenerate perturbation theory: conditions for use, sign of correction for the ground state, and uses.
- Degenerate perturbation theory: why is it that perturbation theory must be carried out more carefully if there are degeneracies? How to choose states for computing first-order corrections to degenerate states.
- Extra stuff that came from solving homework problems: Airy function, wave equation in presence of magnetic fields, transmission coefficients.

3 Degenerate perturbation theory

The main problem when there is degeneracy in the unperturbed problem is that the perturbed states are not necessarily continously connected to the unperturbed states, if the unperturbed states are poorly chosen. The perturbation *selects a preferred basis among the degenerate states* of the original Hamiltonian. This is called “breaking the degeneracy”.

Perturbation theory relies on the states and energies changing smoothly with varying small parameter. To get this to happen, the trick is to choose combinations of unperturbed degenerate energy eigenstates that are *eigenstates of the perturbation*. This can be done by diagonalizing the perturbation over the degenerate states or by finding an operator that commutes with the perturbation and choosing degenerate states that are eigenstates of this other operator. In any case, choosing the proper basis gives states that change continuously as the perturbation is turned on.

Last time we looked at an example of this with a 2×2 Hamiltonian. When the perturbation had only off-diagonal terms, the naive application of first-order perturbation theory gave no change to the energy eigenvalues. By rotating the basis, however, the perturbation became diagonal and the first-order corrections were easily read. You should review and understand this example and of course HWK #8.

4 Time-dependent perturbation theory

Time-dependent perturbation theory is the basis of calculating rates for many, many physical examples. There is a whole set of approaches for this problem.

If one can solve $H\psi = i\hbar\dot{\psi}$ exactly, there is of course no need for perturbation theory. Such examples are the exception, though. (One example of a non-trivial exactly solvable problem: the magnetic resonance examples we solved in lecture).

Lacking an exact solution, one might hope to be able to expand in some small parameter. The "smallness" will be assumed by splitting the Hamiltonian H into a solvable piece $H^0$and a perturbation $H'(t)$, $H(t) = H^0 + H'(t)$.

Perturbation theory, especially time-dependent perturbation theory, leads to series that are conveniently represented by diagrams, such as the Feynman diagrams for $e - e$ interactions (sketched on board). In this case, the small paramter is $\alpha = \frac{e^2}{\hbar c}$. These diagrams have mathematical meaning and a physical interpretation.

Here, we will stick mainly to first-order expansions and won't need all of this machinery. Nonetheless, it is good to keep the physical picture in mind while doing the mathematics.

The Hamiltonian H^0 provides a natural set of basis states for describing $\psi(t)$. The perspective taken is to study how $H'(t)$ can cause the state $\psi(t)$ to make transitions between the eigenstates of H^0. Note that H^0 is not the total Hamiltonian: if the initial state is ψ_n^0, the state at a later time is generally not the eigenstate ψ_n^0. But we need some way to describe $\psi(t)$, and the ψ_n^0 are useful for that.

It is also often the case that we consider a system in an eigenstate of H^0 and we then "turn on" the perturbation $H'(t)$ and then turn off the perturbation. In this case, we are certainly interested in the amplitude that the temporary perturbation took a system in a eigenstate of H^0 $|i\rangle$ to another H^0 eigenstate $|f\rangle$.

4.1 Exact transformation

We start by following the derivations in Shankar.

The total Hamiltonian H is the sum of the unperturbed Hamiltonian H^0 and the perturbation $H'(t)$. The Schrodinger equation is just

$$i\hbar\frac{\partial}{\partial t}\psi(t) = H(t)\psi(t)\,.$$

If we expand $\psi(t)$ using the complete basis ψ_n^0 for the time-independent Schrodinger equation with

$$H^0\psi_n^0 = E_n^0\psi_n\,,$$

we can by definition write

$$\psi(t) = \sum_n c_n(t)\psi_n^0\,,$$

where the coefficients of $c_n(t)$ describe the time evolution of ψ. If $H' = 0$, then $c_n(t) = e^{-iE_n^0 t/\hbar}$, so let's factor out this "trivial" dependence to get

$$\psi(t) = \sum_n d_n(t) e^{-iE_n^0 t/\hbar} |n\rangle \, ,$$

where $|n\rangle$ is used for ψ_n^0. Applying the operator $i\hbar\frac{\partial}{\partial t} - H^0 - H'$ to both sides of the equation gives

$$\begin{aligned}
0 &= \sum_n \left[i\hbar \frac{\partial}{\partial t} - H^0 - H' \right] d_n(t) e^{-iE_n^0 t/\hbar} |n\rangle \\
&= \sum_n \left[i\hbar \left(\frac{d}{dt} d_n \right) e^{-iE_n^0 t/\hbar} |n\rangle + d_n(t) E_n^0 e^{-iE_n^0 t/\hbar} |n\rangle - d_n(t) e^{-iE_n^0 t/\hbar} H^0 |n\rangle - d_n(t) e^{-iE_n^0 t/\hbar} H' |n\rangle \right] \\
&= \sum_n \left[i\hbar \dot{d}_n e^{-iE_n^0 t/\hbar} |n\rangle - d_n(t) e^{-iE_n^0 t/\hbar} H' |n\rangle \right] \, .
\end{aligned}$$

Taking the overlap (inner product) with $\langle f| e^{iE_f^0 t/\hbar}$, for some "final state" $|f\rangle$, also an eigenstate of H^0, gives

$$0 = \sum_n \left[i\hbar \dot{d}_n \langle f|n\rangle - d_n \langle f|H'|n\rangle \right] e^{i(E_f^0 - E_n^0)t/\hbar}$$

or, defining $\omega_{fn} = (E_f^0 - E_n^0)/\hbar$,

$$i\hbar \dot{d}_f = \sum_n d_n(t) \langle f|H'|n\rangle e^{i\omega_{fm} t} \, .$$

This last equation is *an exact result*. Up to the phase factor $e^{i\omega_{fn}t}$ and the $i\hbar$, this equation gives the rate of change of the amplitude to be in a final state $|f\rangle$ that is the sum over transition amplitudes from n to f that are equal to the matrix elements of H'. We say that the non-zero matrix elements of H' cause transitions between those states.

Griffiths carries out this derivation for the more specific case of a 2×2 Hamiltonian matrix.

4.2 Zeroth order

To lowest order, $\dot{d}_n = 0$. Let's take the initial condition that $\psi(0)$ is equal to some eigenstate $|i\rangle$. Then $d_f = \delta_{fi}$ to zeroth order.

4.3 First order

The first order result is found by putting in the zeroth order solution for d_n on the right hand side of the equation at the end of Sec. 4.1. This gives

$$i\hbar \dot{d}_f = \langle f|H'|i\rangle e^{i\omega_{fi} t} \, ,$$

which has solutions

$$d_f = \delta_{fi} - \frac{i}{\hbar}\int_0^t dt'\,\langle f|H'|i\rangle e^{i\omega_{fi}t}\,.$$

This is the basic first order result that will get us going on several topics.

4.4 Types of perturbations

4.4.1 Direct computation

The first-order formula for d_f can be directly applied, as Shankar does in Eqns. (18.2.10) through (18.2.13).

4.4.2 Sudden Perturbations

Shankar has a section on sudden perturbations that actually has several types of changes in the Hamiltonian:

- A brief, *finite* H': in the limit that the duration of the perturbation is short, there will be no change in $\psi(t)$. This results from the fact that for finite total H, the change in ψ over an interval of duration ϵ is zero as $\epsilon \to 0$.
- A brief "*infinite*" H'. Consider a δ-function over time change in H, with $H'(t) = \delta(t-t_0)\Delta H$. Then consider the interval $[t-\epsilon, t+\epsilon]$:

  $$\begin{aligned}\psi(t_0+\epsilon) &= \psi(t_0-\epsilon) + \int_{t-\epsilon}^{t+\epsilon} dt'\,\frac{\partial\psi(t')}{\partial t'}\\ &= \psi(t_0-\epsilon) + \frac{1}{i\hbar}\int_{t-\epsilon}^{t+\epsilon} dt'\,H(t')\psi(t')\\ &= \psi(t_0-\epsilon) + \frac{1}{i\hbar}(\Delta H)\psi(t_0)\,.\end{aligned}$$

  This is not clearly solvable in general, as $\psi(t_0)$ is not well defined ($\psi(t)$ is changing very rapidly). Taking the perturbation to be $small$ however, allows us to assume to first order that $\psi(t)$ is not changed by much. The amplitude to be in a state $|f\rangle$ at $t > t_0$ is then

  $$d_f = \frac{1}{i\hbar}\langle f|\Delta H|i\rangle\,.$$

- A *sudden* "permanent" change in H at a time t_0. Again, over a short time interval, $\psi(t)$ will not change for finite H, so $\psi(t_0+\epsilon) = \psi(t_0-\epsilon)$. For example, if a system is in its ground state for $t < t_0$ and the Hamiltonian is *rapidly* changed (much faster than the frequencies in the original H), the probability that the system will be in the ground state of the new Hamiltoinan is simply

  $$|\langle\psi_0^+|\psi_0^-\rangle|^2\,,$$

  where ψ_0^- is the ground state wave function for $t < t_0$ and $\psi_0^+$is the ground state for the Hamiltonian when $t > t_0$.

4.4.3 Adiabatic perturbations

This is a very important case that applies when the changes in $H(t)$ are *very very slow*. If $\psi_n(t)$ are the eigenstates for $H(t)$, then, when the conditions of the adiabatic theorem apply, $d_n(t)$ is *constant:* if the system is in an eigenstate at a given time, it remains in the continuously connected eigenstate at later times! For example, suppose a particle is in a box and is initially in the ground state. If the walls (boundary conditions) are moved very slowly compared to the characteristic velocity of the particle, then the particle will *remain in the ground state for all times*.

We will go over the adiabatic theorem in more detail, soon.

4.4.4 Corrections to adiabatic perturbations

See Shankar (Eqns. 18.2.28 through 18.2.31) for how first-order time-dependent perturbation theory can be used to rederive first-order time-independent perturbation theory. [Use $H(t) = H^0 + e^{t/\tau}H'$ for large τ and first-order time-dependent theory to find $d_m(0)$.]

4.4.5 Periodic perturbations

An extremely important case, which leads to Fermi's golden rule. This is especially important in understanding the interactions between matter and radiation. This will be covered in more detail after adiabatic perturbations are covered. I list it here for completeness.