PHY662, Spring 2004, Feb. 26, 2004

4th March 2004

1 Miscellaneous

1. HWK #8 due Tuesday, Mar. 16.
2. Continue to read Ch. 17 Shankar (or Griffiths Ch. 6), especially for 2nd-order perturbation theory. Start Ch. 18 for time-dependent perturbation theory for Tuesday.
3. Today: Transmission coefficients in 1D, 2nd-order perturbation theory, degenerate perturbation theory.

2 Transmission coefficients

Last time, we reviewed the problem of a plane wave Ae^{ikx} incident upon a step in the potential, $\Delta V < \frac{\hbar^2 k^2}{2m}$. Remember that we found the amplitude for the transmitted wave: $Ce^{ik'x}$, $k' = \sqrt{k^2 - \frac{2m}{\hbar^2}\Delta V}$, with $C = \left(\frac{2k}{k+k'}\right) A$.
What is the probability of transmission through the step?

3 2nd order

The second order corrections to the energy require the first order corrections to the wavefunction. (Note that the *wavefunctions* calculated using perturbation theory are generally less reliable than the energy estimates.)
In any case, the first order corrections to the wavefunction are found by computing the inner product of the first order terms in the Schrodinger equation for eigenstate n with the unperturbed eigenstate m:

$$\begin{aligned}
\langle\psi_m^0|H^0|\psi_n^1\rangle + \langle\psi_m^0|H'|\psi_n^0\rangle &= \langle\psi_m^0|E_n^0|\psi_n^1\rangle + \langle\psi_m^0|E_n^1|\psi_n^0\rangle \\
E_m^0\langle\psi_m^0|\psi_n^1\rangle + \langle\psi_m^0|H'|\psi_n^0\rangle &= E_n^0\langle\psi_m^0|\psi_n^1\rangle + E_n^1\langle\psi_m^0|\psi_n^0\rangle \\
\langle\psi_m^0|H'|\psi_n^0\rangle &= \left(E_n^0 - E_m^0\right)\langle\psi_m^0|\psi_n^1\rangle \\
\langle\psi_m^0|\psi_n^1\rangle &= \frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\,.
\end{aligned}$$

Since the set of all $|\psi_n^0\rangle$ form a complete basis, $|\psi_n^1\rangle$ can be written as a sum over $c_{m,n}^1|\psi_n^0\rangle$. Clearly, $c_{m,n}^1 = \langle\psi_m^0|H'|\psi_n^0\rangle/(E_n^0 - E_m^0)$, so

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle\,.$$

Why did we leave $|\psi_n^0\rangle$ out of the sum? Well, the first order approximation to $|\psi_n\rangle$ is $|\psi_n^0\rangle + |\psi_n^1\rangle$, so that any part of $|\psi_n^1\rangle$ that is proportional to $|\psi_n^0\rangle$ is redundant. In fact, this choice also keeps this first order wave function normalized, at least to first order:

$$\begin{aligned}\langle\psi_n|\psi_n\rangle &= (\langle\psi_n^0| + \langle\psi_n^1|)(|\psi_n^0\rangle + |\psi_n^1\rangle) \\ &= 1 + 0 + 0 + (\text{terms second order in H'})\,.\end{aligned}$$

Given this, we can now look at the second order correction to the energy, by taking the inner product of the second order part of the Schrodinger equation with $\langle\psi_n^0|$, immediately canceling the first terms on each side, due to the same trick as for first order ($\langle\psi_n^0|H^0 = \langle\psi_n^0|E^0$):

$$\begin{aligned}\langle\psi_n^0|H'|\psi_n^1\rangle &= E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2 \\ E_n^2 &= \sum_{m\neq n}\frac{\langle\psi_n^0|H'|\psi_m^0\rangle\langle\psi_m^0|H'|\psi_n^0\rangle}{(E_n^0 - E_m^0)} - 0 \\ E_n^2 &= \sum_{m\neq n}\frac{\left|\langle\psi_n^0|H'|\psi_m^0\rangle\right|}{E_n^0 - E_m^0}\,,\end{aligned}$$

an expression that again uses only matrix elements of H'.

3.1 Application

Here is a sample application (taken from problems 6.1 and 6.3 in Griffiths). Let H^0 be the square well potential for a particle confined to $0 < x < a$, so that the *normalized* unperturbed wave-functions are $\psi_n^0(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$ with $E_n^0 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}\frac{2}{a}\int_0^a \sin^2(\frac{n\pi x}{a})\,dx = \frac{n^2\pi^2\hbar^2}{2ma^2}$. If the perturbing potential is a delta-function at $x = a/2$, $H' = \alpha\delta(x - \frac{a}{2})$, then

$$\begin{aligned}E_n^1 &= \int_0^a (\psi_n^0(x))^*\alpha\delta(x - \frac{a}{2})\psi_n^0(x)\,dx \\ &= \frac{2\alpha}{a}\int_0^a \sin^2(\frac{n\pi x}{a})\delta(x - \frac{a}{2}) \\ &= \left\{\begin{array}{ll}\frac{2\alpha}{a}, & n\,\text{odd} \\ 0, & n\,\text{even}\end{array}\right.\,.\end{aligned}$$

The second order correction is

$$E_n^2 = \sum_{m\neq n}\frac{\frac{4\alpha^2}{a^2}\left[\int_0^a dx\,\sin(\frac{n\pi x}{a})\sin(\frac{m\pi x}{a})\delta(x - \frac{a}{2})\right]^2}{\frac{\pi^2\hbar^2}{4m^2a^4}(n^2 - m^2)}$$

$$
\begin{aligned}
&= \alpha^2 \frac{16m^2a^2}{\pi^2\hbar^2} \sum_{m\neq n;m,n\,\mathrm{bothodd}} \frac{(-1)^{(m+n)/2}}{n^2-m^2} \,. \\
&= \alpha^2 \frac{16m^2a^2}{\pi^2\hbar^2} \sum_{(j=1)\neq k;\; n=2k+1}^{j=\infty} \frac{1}{((2j+1)^2-(2k+1)^2)} \\
&= \ldots .
\end{aligned}
$$

4 Degenerate perturbation theory

The expressions for ψ_n^1 and E_n^2 are problematic when there is an energy degeneracy, i.e., two unperturbed states with the same energy. The energy denominators $E_n^0 - E_m^0$ can then be zero and we don't like to divide by zero. Even E_n^1 will be affected by degeneracies: this is not obvious from the expression $E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle$, but degeneracies do affect the derivation of this result.

The main problem is that the perturbation *selects a preferred basis among the degenerate states*. Consider, e.g., a two-level system with $H^0 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ and $H^0 = \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix}$. What are the unperturbed and perturbed eigenvalues? What would you get if you naively applied first-order perturbation theory?

So what do we do in the face of degeneracy? The trick is to choose combinations of unperturbed degenerate energy eigenstates that are *eigenstates of the perturbation*. As any linear combination of unperturbed energy eigenstates has the same energy, this maintains the unperturbed energies, but keeps the perturbation from "mixing" the energy eigenstates. Roughly, the relevant matrix elements in the numerator are zero, so a zero energy denominator is OK. More precisely, we are trying to diagonalize the total Hamiltonian

$$H = H^0 + H'$$

over the degenerate subspace. Let $S = \{\psi_n\}$ be a set of states degenerate under H^0, with identical values of $E_n^0 = E^0$. If we transform those states to a new basis where H' is diagonal, then it is possible to treat at least the first order part of the expansion

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$$

by rearranging to get

$$(H^0 - E^0)\psi_n^1 + H'\psi_n^0 = E_n^1\psi_n^0 \,.$$

Contracting with ψ_n^0 gives

$$\langle\psi_n^0|(H^0 - E^0)|\psi_n^1\rangle + H_n' = E_n^1 \,,$$

which is trouble-free, as $\langle\psi_n^0|(H^0 - E^0) = 0$ *and* H_n' is just the eigenvalue of H' for ψ_n^0: if ψ_n^0 were not an eigenvector of H', we could contract with $\psi_{n'}^0$, with $n' \neq n$ and $H'|\psi_n^0\rangle$ not orthogonal to $|\psi_{n'}^0\rangle$ to get

$$0 + \langle\psi_{n'}^0|H'|\psi_n^0\rangle = 0$$

a contradiction (what happens is that $|\psi_n^1\rangle$ becomes ill-defined).