PHY662, Spring 2004, Feb. 26, 2004

2nd March 2004

1 Miscellaneous

1. HWK #8 due Tuesday, Mar. 9.
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 (maybe Thursday this week).
3. Today: Review HWK #7, using maple to plot some results. Then go over 2nd-order perturbation theory.

2 Perturbation theory

Perturbation theory is an expansion about a solvable problem using a “small parameter”. Physicists often ask one another “what is the small parameter?” Typical expansion parameters include the ratios of energies, length scales or time scales. Dimensionality is often used as an expansion parameter (e.g., $\epsilon = 4-d$) as are dimensionless constants such as $\alpha = \frac{1}{137.04...}$.

Not all perturbation expansions converge nicely. Most don't. Here is a basic example of an aysmptotic expansion: let's compute an expansion in λ for

$$C(\lambda) = \int_{-\infty}^{\infty} dx\, e^{-x^2-\lambda x^4}\ .$$

The perturbative approach is to expand $e^{-\lambda x^4}$ in powers of λ. You then get

$$\begin{aligned} C(\lambda) &= \int_{-\infty}^{\infty} dx\, e^{-x^2}(1-\lambda x^4 + \frac{\lambda^2}{2}x^8 - \ldots) \\ &= \sum_{k=0}^{k=\infty} \frac{(-\lambda)^k}{k!} \int_{-\infty}^{\infty} dx\, e^{-x^2} x^{4k} \\ &= \sum_{k=0}^{k=\infty} \frac{(-\lambda)^k}{k!} \Gamma\left(2k+\frac{1}{2}\right) \end{aligned}$$

$$= \sum_{k=0}^{k=\infty} \left[\frac{(-1)^k \Gamma(2k+\frac{1}{2})}{\Gamma(k+1)} \right] \lambda^k .$$

The answer can also be written as

$$\begin{aligned} C(\lambda) &= \sum_{k=0}^{k=\infty} \frac{(-\lambda)^k}{k!} \left(\frac{\partial}{\partial a}\right)^{2k} \sqrt{\frac{\pi}{a}} \\ &= \sqrt{\pi} \sum_{k=0}^{\infty} \frac{(4k-1)!!}{k!} \left(\frac{-\lambda}{4}\right)^k . \end{aligned}$$

How do the coefficients of this series behave? They diverge exponentially in k, faster than $(\lambda)^{-k}$ for any λ. So the terms in the series *diverge*.

The series is well behaved only in the limit $\lambda \to 0$. See the plot from `maple` for examples. (There is a clue to a problem here: when $\lambda < 0$, $C(\lambda)$ diverges, so the behavior cannot be smoothly expanded about $\lambda = 0$ in powers of λ.)

3 Review of non-deg. pert. theory through 1st order

Assume we have exact eigenstates for a Hamiltonian H^0,

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

Very important note: the assumption is that ψ_n^0 is properly normalized: $\int \psi^* \psi = 1$. We wish to find the eigenstates for the Hamiltonian $H = H^0 + \lambda H'$. We can at least formally expand the new eigenstates and eigenvalues:

$$\begin{aligned} \psi_n &= \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots \end{aligned}$$

Writing $H\psi_n = E_n \psi_n$ gives, collecting equations to each order in λ,

$$\begin{aligned} H^0 \psi_n^0 &= E_n^0 \psi_n^0 & (0^{\text{th}} \text{ order in } \lambda) \\ H^0 \psi_n^1 + H' \psi_n^0 &= E_n^0 \psi_n^1 + E_n^1 \psi_n^0 & (1^{\text{st}} \text{ order in } \lambda) \\ H^0 \psi_n^2 + H' \psi_n^1 &= E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0 & (2^{\text{nd}} \text{ order in } \lambda) . \end{aligned}$$

The 0th order equation is not new. Today we will just look at the 1st order correction - this is what will be needed for homework. Take the first order equation, multiply by ψ_m^0 and integrate over the space of the wavefunction to get:

$$\langle \psi_m^0 | H^0 | \psi_n^1 \rangle + \langle \psi_m^0 | H' | \psi_n^0 \rangle = E_n^0 \langle \psi_m^0 | \psi_n^1 \rangle + E_n^1 \langle \psi_m^0 | \psi_n^0 \rangle .$$

Choosing $m = n$ gives

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle .$$

4 Second-order perturbation theory

- First order corrections to the energy are often straightforward to calculate.
- Higher order corrections usually involve infinite sums and are more difficult in general.
- Second order calculations are often the practical limit.

Here is a result that shows both the power and limits of perturbation expansion. Remember the gyromagnetic ratio of the electron? It can be computed using quantum electrodynamics (QED) in powers of $\frac{\alpha}{\pi}$, $\alpha = \frac{e^2}{hc} \approx \frac{1}{137.04}$. The answer for the QED part is

$$
\begin{aligned}
g/2 &= 1 + \\
&\frac{1}{2}(\frac{\alpha}{\pi}) + \\
&(\frac{197}{144} + \frac{\pi^2}{12} + \frac{3}{4}\zeta(3) - \frac{\pi^2 \ln 2}{2})(\frac{\alpha}{\pi})^2 + \\
&\left\{ \left[\frac{83}{72}\pi^2 + \frac{139}{18}\right]\zeta(3) - \frac{215}{24}\zeta(5) + \frac{100}{3}\left[\mathrm{Li}_4\left(\frac{1}{2}\right) + \frac{(1-\pi^2)(\ln 2)^2}{24}\right] - \frac{239}{2160}\pi^4 \right. \\
&\quad \left. \frac{298}{9}\pi^2 \ln 2 + \frac{17101}{810}\pi^2 + \frac{28259}{5184} \right\} \left(\frac{\alpha}{\pi}\right)^3 + \\
&(\text{numerical estimate}) \left(\frac{\alpha}{\pi}\right)^4 \\
&\approx 1 + 0.5\left(\frac{\alpha}{\pi}\right) - (0.328478965\ldots)\left(\frac{\alpha}{\pi}\right)^2 \\
&\quad +(1.181241456\ldots)\left(\frac{\alpha}{\pi}\right)^3 - (1.51 \pm 0.04)\left(\frac{\alpha}{\pi}\right)^4 + \ldots \\
&= 1.001\,159\,652\,\ldots
\end{aligned}
$$

Note that the third order term was solved analytically only in 1996 (ζ is the Riemann zeta function and Li_4 is a "logarithmic integral" function). The fourth order term is a numerical estimate that has required many years of work. (For a review see *Reviews of Modern Physics*, Vol. 71, pp. S133-139.)

Our goal will be a little more modest at first: computing 2nd order corrections in non-relativistic quantum mechanics.

5 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'.

5.1 Application

Here is a sample, taking problems 6.1 and 6.3 from 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 $E_n^0 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}\frac{2}{a}\int_0^a \sin^2(\frac{n\pi x}{a})\,dx = \frac{n^2\pi^2\hbar^2}{ma^2}$. If the perturbing potential is a delta-function at $x = a/2$, $H' = \alpha\delta(x - \frac{a}{2})$, then

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

The second order correction is

$$
\begin{aligned}
E_n^2 &= \sum_{m\neq n} \frac{\frac{4\alpha^2}{a^2}\left[\int_0^a dx\,\sin(\frac{n\pi x}{a})\sin(\frac{m\pi x}{a})\delta(x-\frac{a}{2})\right]^2}{\frac{\pi^2\hbar^2}{m^2a^4}(n^2-m^2)} \\
&= \alpha^2\frac{4m^2a^2}{\pi^2\hbar^2}\sum_{m\neq n;m,n\,\text{bothodd}} \frac{(-1)^{(m+n)/2}}{n^2-m^2} . \\
&= \alpha^2\frac{4m^2a^2}{\pi^2\hbar^2}\sum_{(j=1)\neq k;\,n=2k+1}^{j=\infty} \frac{1}{((2j+1)^2-(2k+1)^2)} \\
&= \alpha^2\frac{m^2a^2}{\pi^2\hbar^2n^2}\times(\text{constant}).
\end{aligned}
$$