Phys 487 Discussion 6 – Perturbation Theory: Non-Degenerate, Time-Independent

To calculate some of the multi-particle effects in atomic energy states, we turn to the study of **approximation methods**. As you might imagine, this is a substantial segment of quantum mechanics as there are rather few systems that can be solved exactly for their energy eigenvalues and eigenstates! Today, we will practice **Perturbation Theory**. Below is a summary of what we derived in class.

Suppose you have a Hamiltonian $\boldsymbol{H_0}$ that can be **solved exactly** for its eigenvalues and eigenstates.

Now **add a small perturbation** $\boldsymbol{H'}$ to H_0. The resulting Hamiltonian, $H = H_0 + H'$, is *not* exactly solvable for its eigenstates and eigenvalues … but we can approach the solution in the manner of a Taylor series: calculate smaller and smaller **corrections** to the exact eigenvalues and eigenstates, and approach the true values/states via a (probably infinite) series. Here is the notation we will use :

- "zeroth-order" Hamiltonian H_0 has <u>exact</u> eigenvalues $\left\{E_n^{(0)}\right\}$ and eigenstates $\left\{\left|n^{(0)}\right\rangle\right\}$
- *actual* Hamiltonian $H = H_0 + H'$ where H' is a <u>small correction</u> to H_0 (a "<u>perturbation</u>", $H' \ll H_0$)
- series expansion of H eigenvalues: $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$ for each n, where $E_n^{(0)} \gg E_n^{(1)} \gg E_n^{(2)} \gg \ldots$
- series expansion of H eigenstates: $|n\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle + \ldots$ for each n, where $\left|n^{(0)}\right\rangle \gg \left|n^{(1)}\right\rangle \gg \ldots$

As long as the exact eigenstates $\left\{\left|n^{(0)}\right\rangle\right\}$ are **non-degenerate** and the Hamiltonian $H = H_0 + H'$ has **no explicit time-dependence**, we get nice compact formulae for the 1st-order and 2nd-order corrections to each energy E_n. First, let H'_{mn} denote the matrix elements of H' in the unperturbed basis (the only basis we have) :

$$\boxed{H'_{mn} = \left\langle m^{(0)}\middle|H'\middle|n^{(0)}\right\rangle}.$$

Then the energy corrections are

$$\boxed{E_n^{(1)} = H'_{nn}} = \left\langle n^{(0)}\middle|H'\middle|n^{(0)}\right\rangle$$ = the expectation value of the perturbation H' in the n^{th} *exact* state, and

$$E_n^{(2)} = \sum_{m\neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$ (we will derive this one in our next lecture).

The 1st-order correction to each unperturbed eigenstate $\left|n^{(0)}\right\rangle$ is $\left|n^{(1)}\right\rangle = \sum_{m\neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}\left|m^{(0)}\right\rangle$.

I only put the $E_n^{(1)}$ formula in a box since that is the only one we will use today.

Problem 1 : Warmup Qual Problem *Qual Problem (Colorado)*

A particle of mass m is bound in a square well where $-a/2 < x < a/2$.

(a) What are the energy and eigenfunction of the ground state?

(b) A small perturbation is added, $V(x) = 2\varepsilon|x|/a$ where $\varepsilon \ll 1$. Use perturbation theory to calculate the change in the ground state energy to order $O(\varepsilon)$.

FAQ: Goodness, how can this simple problem be a qual problem? No Formula Sheet, of course. ☺ You must know how to derive the formulae above in your sleep, like Taylor's series! But more practice first.

Problem 2 : Two Identical Bosons in ∞ Well, now with a weak interaction *Griffiths 6.3*

Two identical bosons are placed in an infinite square well with $V = 0$ from $x = 0$ to $x = a$, and $V = \infty$ everywhere else. The bosons interact weakly with one another, via the potential

$$V(x_1,x_2) = -aV_0\,\delta(x_1 - x_2)$$

where V_0 is a constant with dimensions of energy.

(a) First, ignoring the interaction between the particles, find the ground state and the first excited state — both the wave functions and the associated energies. (This is our standard Sandbox system, so by all means just write down what the single-particle wavefunctions without any/much derivation.)

(b) Use first-order perturbation theory to estimate the effect of the particle-particle interaction above on the energies of the ground state and the first excited state.

Problem 3 : Qual Problem with Spin *Qual Problem (MIT)*

Consider two electrons bound to a proton by Coulomb interaction. Neglect the Coulomb repulsion between the two electrons.

(a) What are the ground state energy and wave function for this system?

(b) Consider that a weak potential exists between the two electrons of the form

$$V(\vec{r}_1 - \vec{r}_2) = V_0\ \delta^3(\vec{r}_1 - \vec{r}_2)\ \vec{s}_1 \cdot \vec{s}_2$$

where V_0 is a constant and $\vec{s}_j$ is the spin operator for electron j (neglect the spin-orbit interaction) . Use first-order perturbation theory to estimate how this potential alters the ground state energy.