Physics 487 – Homework #5   **due Friday 1 pm**

Here are the perturbation theory (non-degenerate, time-independent) results we introduced in discussion 5 and will prove in lecture. If you have

- a "zeroth-order" Hamiltonian H_0 that has <u>exact</u> eigenvalues $\{E_n^{(0)}\}$ and eigenstates $\{|n^{(0)}\rangle\}$,

- an *actual* Hamiltonian $H = H_0 + H'$ where H' is a <u>small correction</u> to H_0 (a "<u>perturbation</u>", $H' \ll H_0$),

- a series expansion of H eigenvalues: $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + ...$ for each n where $E_n^{(0)} \gg E_n^{(1)} \gg E_n^{(2)} \gg ...$

- & a series expansion of H eigenstates: $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + ...$ for each n, where $|n^{(0)}\rangle \gg |n^{(1)}\rangle \gg ...$

then as long as
- the exact eigenstates $\{|n^{(0)}\rangle\}$ are **non-degenerate** and
- the Hamiltonian $H = H_0 + H'$ has **no explicit time-dependence**,

then 1st-order and 2nd-order corrections to each unperturbed energy E_n / unperturbed eigenstate $|n^{(0)}\rangle$ are:

$$\boxed{E_n^{(1)} = \langle n^{(0)}|H'|n^{(0)}\rangle}\ = \text{the expectation value of the perturbation } H' \text{ in the } n^{\text{th}} \textit{ exact} \text{ state.}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m^{(0)}|H'|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \qquad\qquad |n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle m^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}|m^{(0)}\rangle$$

Problem 1 : Two Identical Bosons in ∞ Well, now with a weak interaction between them   *Griffiths 6.3*

Two <u>identical bosons</u> 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

$$V_{\text{INT}}(x_1, x_2) = -a V_0\, \delta(x_1 - x_2)$$

where V_0 is a constant with dimensions of energy.

(a) First, ignoring the interaction V_{INT} 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 2 : Spherical Harmonic Oscillator + Spin-Orbit Interaction

Consider a particle in a spherically-symmetric harmonic oscillator potential : the Hamiltonian is

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2 r^2}{2} \quad \text{where } m \text{ and } \omega \text{ are known constants.}$$

(a) Using separation of variables in <u>spherical coordinates</u>, in the form $\psi(r,\theta,\phi) = Y_l^m(\theta,\phi)R(r)$ that always works for a central potential $V(r)$, find the radial equation for $R(r)$ and solve it for

- the ground state of the *s*-shell ($l = 0$) and

- the ground state of the *p*-shell ($l = 1$).

You do NOT have to normalize your $R(r)$ functions.

(b1) Obtain the <u>energies</u> and <u>degeneracies</u> of the lowest-lying s-shell and p-shell states you have just found.

(b2) There is another way of thinking / calculating the 3D SHO : using separation of variables in Cartesian coordinates. Since the kinetic energy is proportional to $p^2 = p_x^2 + p_y^2 + p_z^2$ and the potential energy is proportional to $r^2 = x^2 + y^2 + z^2$, the Hamiltonian is the sum of three identical 1D SHO Hamiltonians: $H_{3D} = H_{1D,x} + H_{1D,y} + H_{1D,z}$. The energy spectrum of a 1D SHO is $E_n = (n + 1/2)\hbar\omega$, so the energy of a 3D SHO is $E_{n_x n_y n_z} = (n_x + n_y + n_z + 3/2)\hbar\omega$. From this way of thinking, find the <u>energies</u> and <u>degeneracies</u> of the ground state and 1st-excited state(s) of the 3D SHO. Comparing your results to (b1) should provide happiness!

(c) Suppose the particle in the SHO is an electron. Let's add to the Hamiltonian a <u>spin-orbit interaction</u> term,

$$V_{SO} = \frac{\hbar^2}{2m^2c^2}\frac{1}{r}\frac{dV_{SHO}(r)}{dr}\vec{L}\cdot\vec{S} \qquad \text{where} \qquad V_{SHO} = \frac{m\omega^2 r^2}{2}$$

Use perturbation theory to estimate how the SHO's lowest two energy eigenvalues are altered by the addition of the (small) spin-orbit interaction.

TECHNIQUE : This is your first problem involving a **spin-orbit interaction** so it's time to learn a new technique! The issue is how to evaluate the term $\vec{L}\cdot\vec{S}$. If you are working with a particle in an state $|LS\,M_L\,M_S\rangle$, you have have the eigenvalues of L^2, S^2, L_z, and S_z at your disposal. However, $\vec{L}\cdot\vec{S} = L_x S_x + L_y S_y + L_z S_z$, and your particle $|LS\,M_L\,M_S\rangle$ is not in an eigenstate of those x or y components. Oh dear! The way to go is to *switch bases* and work with your particle in a state $|LS\,J\,M_J\rangle$ instead, where $\vec{J} \equiv \vec{L} + \vec{S}$. Now you have the eigenvalues L^2, S^2, J^2, and J_z at your disposal. You can obtain $\vec{L}\cdot\vec{S}$ in terms of these eigenvalues by expanding the right-hand-side of $J^2 = |\vec{L} + \vec{S}|^2$. (The formula you require can be found in §6.3.2 of Griffiths or Ch.XII §23 of Messiah.)

Problem 3 : δ-Function Bump in the ∞ Square Well ™   *adapted from Griffiths 6.1 & 6.4(a)*

Suppose we put a δ-function bump in the center of an infinite square well that runs from $x = 0$ to $x = a$. The bump adds the following term to the Hamiltonian :

$$H' = \alpha\,\delta\left(x - \frac{a}{2}\right) \quad \text{where } \alpha \text{ is a constant.}$$

You can use without proof any results for the unperturbed InfiniteWell™ as you have worked with it so much.

(a) Find the first-order energy corrections $E_n^{(1)}$ caused by the bump. Hint: you should find that the bump has a very different effect on the energy for even and odd values of n.

(b) Now let's calculate the first-order modifications that the bump produces in the energy eigen<u>states</u> rather than the energy eigen<u>values</u>. The energy eigenstates of the unperturbed ∞ well are $|n^{(0)}\rangle$. First-order perturbation theory provides a correction $|n^{(1)}\rangle$ for each unperturbed state $|n^{(0)}\rangle$, given as a sum over contributions from the *other* unperturbed states $|m^{(0)}\rangle$:

$$\left|n^{(1)}\right\rangle = \sum_{m \neq n} \frac{\left\langle m^{(0)}\left|H'\right|n^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}} \left|m^{(0)}\right\rangle.$$

Calculate the first three non-zero terms in this sum for the ground state ($n = 1$).

(c) Calculate the second-order energy corrections $E_n^{(2)}$ caused by the bump. You will obtain an infinite sum that you can actually *do*, which is rather wondrous. The main trick is to use

$$\frac{1}{a^2 - b^2} = \frac{1}{2a}\left(\frac{1}{a+b} + \frac{1}{a-b}\right)$$

to rewrite the sum you have to do. If you write out explicitly (in actual numbers) the first few terms in the resulting series, you will see what happens. It will be very pleasing. ☺

Problem 4 : Helium Ground State Energy

(a) The helium atom consists of two electrons bound by a doubly-charged nucleus. The most crude approximation you can make to its Hamiltonian is the sum of two hydrogen-like Hamiltonians, i.e. one for each of the two electrons, treating them as if they are interacting with just the Z (nuclear charge) = 2 nucleus and not at all with each other. Making use of the hydrogen-like solutions on the formula sheet and/or the hydrogen-like energy formula that will shortly be added to the formula sheet,

$$E_n = -\frac{(Z\alpha)^2}{2n^2}(m_e c^2),$$

calculate the energy of the helium ground state in the approximation that Helium $\approx$ two non-interacting electrons sitting in the field of a $Z{=}2$ nucleus. Express your result in eV.

(b) The measured energy of the helium ground state is –79 eV, so our two-non-interacting-particle approximation is not very accurate (almost 40% off the true value). Happily, almost all of the discrepancy with experiment can be accounted for by adding an **electron-electron repulsion term, V_{ee},** to the Hamiltonian and calculating the energy shift it produces in first-order perturbation theory. Off you go! After you apply your correction you should be about 5% away from the experimental ground state energy instead of 40% ... an excellent correction indeed!