All solutions must clearly show the steps and/or reasoning you used to arrive at your result. You will lose points for poorly written solutions or incorrect reasoning. Answers given without explanation will not be graded: our master rule for homework and exams is <u>NO WORK = NO POINTS</u>. However, unless otherwise specified, you may use any relation from the **formula sheets** on our website, from the introductions to **this or previous homework / discussions**, or from **non-QM courses** without proof. Here's a rule of thumb: Write enough so that it will MAKE SENSE <u>TO YOU</u> IN 5 YEARS, i.e. so that it provides you with useful future notes.

For this homework, you may also use <u>wolframalpha.com</u>, <u>wolframcloud.com</u>, or any similar tool to evaluate your integrals **after you set them up** in a form that can be **directly entered** into such tools.

Here are the perturbation theory (time-independent, non-degenerate) results we have proved or 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:  $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots$  for each *n* where  $E_n^{(0)} \gg E_n^{(1)} \gg E_n^{(2)} \gg \dots$
- & a series expansion of *H* eigenstates:  $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + \dots$  for each *n*, where  $|n^{(0)}\rangle \gg |n^{(1)}\rangle \gg \dots$

then as long as

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

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

 $E_n^{(1)} = \langle n^{(0)} | H' | n^{(0)} \rangle$  = the expectation value of the perturbation H' in the n<sup>th</sup> exact state.

$$\frac{E_{n}^{(k)} = \langle n^{(0)} | H' | n^{(k-1)} \rangle}{E_{n}^{(0)} = \sum_{m \neq n} \frac{\langle m^{(0)} | H' | n^{(0)} \rangle}{E_{n}^{(0)} - E_{m}^{(0)}} | m^{(0)} \rangle} \text{ so } E_{n}^{(2)} = \sum_{m \neq n} \frac{\left| \langle m^{(0)} | H' | n^{(0)} \rangle \right|^{2}}{E_{n}^{(0)} - E_{m}^{(0)}}$$

**Reading for week 6 :** Griffiths §6.2 (Degenerate PT)

## Problem 1 : Two Identical Bosons in $\infty$ Well, 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

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

where  $V_0$  is a constant with dimensions of energy. As you can see, this potential describes an attractive "contact interaction", i.e. one that is so short-range that it only acts when the particles are at the same place.

(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 — the easiest QM system to play with — 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 : δ-Function Bump in the** ∞ Square Well <sup>™</sup>

Suppose we put a  $\delta$ -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 :

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

You can use without proof any results for the unperturbed InfiniteWell<sup>™</sup> 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 eigenstates rather than the energy eigenvalues. The energy eigenstates of the unperturbed  $\infty$  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  $|m^{(0)}\rangle$ . 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.  $\odot$ 

Also, hints from the Sunday crew: (1) Don't confuse your summation index "m" with mass, and (2) remember that you are summing over *m*, while *n* is a fixed value that will appear in the final result for  $E_n^{(2)}$ .

## **Problem 3: A Spin-Spin Interaction in Matrix Form**

An interaction between two spin-1/2 particles is given by

 $V = a + b \vec{\sigma}_1 \cdot \vec{\sigma}_2$ 

where a and b are constants. To clarify how the matrix-representation of states and operators works when two different spins are involved, please read through the solution for Discussion 5 Question 2 and/or watch the little video **Hwk05-assistance-Spin1Matrices.mp4** in the homework folder before starting on this problem. The little video goes through a relevant example problem.

(a) Derive the matrix representation for V in the basis  $|SM\rangle$  where the ordered basis states are

$$\left[ |e_1\rangle, |e_2\rangle, |e_3\rangle, |e_4\rangle \right] \equiv \left\{ |00\rangle_{SM}, |1+1\rangle_{SM}, |10\rangle_{SM}, |1-1\rangle_{SM} \right\}$$

(b) Derive the <u>matrix representation</u> for V in the basis  $|m_1 m_2\rangle$  where the ordered basis states are

$$\left\{ |e_1\rangle, |e_2\rangle, |e_3\rangle, |e_4\rangle \right\} \equiv \left\{ |\uparrow\uparrow\rangle_{m_1m_2}, |\uparrow\downarrow\rangle_{m_1m_2}, |\downarrow\uparrow\rangle_{m_1m_2}, |\downarrow\downarrow\rangle_{m_1m_2}, |\downarrow\downarrow\rangle_{m_1m_2} \right\}$$

Here, the up and down arrows are convenient shorthand for  $+\frac{1}{2}$  and  $-\frac{1}{2}$ .

▶ HINT: There are two ways to solve this problem, one involving all the Pauli matrices, and the other involving Clebsch-Gordan coefficients & some of your work from part (a).

## **OPTIONAL** Problem 4: Spherical Harmonic Oscillator + Spin-Orbit Interaction

Qual Problem

This is not for points, but please do read it through as it contains an important derivation.

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

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

Last semester you used separation of variables in spherical coordinates, in the form

$$\psi(r,\theta,\phi) = Y_l^m(\theta,\phi)R(r)$$

that *always* works for a central potential V(r), to find the radial equation for R(r). You used the asymptoticbehaviour × Frobenius–series method to obtain a recursion relation and quantization condition for the eigenstates  $R_{nl}(r)$ . It was SUPER FUN! *IF* you need any of that, you'll have to derive it again! (\*^ - ^\*)

(a) Find the <u>energies</u> and <u>degeneracies</u> of the lowest-lying s-shell state(s) and the lowest-lying p-shell state(s) of the 3D SHO.

▶ Hint: One possible way to proceed is to convert the problem to *Cartesian* coordinates and use some things from the file Formulae-SHO-reference.pdf ... BUT: If you switch from  $(r, \theta, \phi)$  to (x, y, z), you lose the explicit connection to angular momentum and the quantum numbers of your states won't be  $(n, l, m_l)$  but (something else). When you find the lowest-lying states, you must make some argument to convince yourself that they should be identified with the "s-shell" and "p-shell" states mentioned in the question. An argument involving the degeneracies of the Cartesian states that you found would do the trick, for example.

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

$$H'_{\text{S-O}} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV_{\text{SHO}}(r)}{dr} \vec{L} \cdot \vec{S}$$
 where  $V_{\text{SHO}} = \frac{m\omega^2 r^2}{2}$ 

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

(c) Hmm, the above form for the spin-orbit potential energy isn't the same as the one in Griffiths §6.3.2 [6.61] :

$$H'_{\rm S-O} = \frac{1}{2} \left( \frac{e^2}{4\pi\varepsilon_0} \right) \frac{1}{m^2 c^2 r^3} \vec{L} \cdot \vec{S} .$$

This Griffiths formula is the special-case result for an electron in a hydrogen atom; the more general formula

$$H'_{\text{S-O}} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \vec{L} \cdot \vec{S}$$

from part (b) works for an **electron** moving in **any** central potential V(r) of electrostatic origin. We didn't derive  $V_{S-O}$  in class, so here's a chance to do it. Griffiths starts with the classical magnetic field seen at the center of a current loop. That works great for an electron in an atom, which sees the nucleus orbiting around it. To derive the more general formula in the box, instead with the conceptual origin of the spin-orbit interaction,

$$H_{\text{S-O}} = -\vec{\mu}_{\text{due to SPIN of electron}} \cdot B_{\text{due to ORBIT of electron within an }\vec{E}}$$
 field

and this relation from special relativity,

$$\vec{B} = -\frac{\vec{v}}{c^2} \times \vec{E} ,$$

which gives the magnetic field seen by a particle of speed  $\vec{v}$  moving through an electric field  $\vec{E}$ . After the first couple of steps, the derivation matches the atom-specific one in Griffiths §6.3.2, by all means follow along! WARNING: Near the start of your derivation, you must obtain  $\vec{E}$  from the central potential V(r) that describes it, but watch out  $\rightarrow$  in E&M, V means "voltage" while in QM and Lagrangian CM, V means "potential energy"!