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 without proof any relation from the **formula sheets** on our website, from the introductions to **this or previous homework / discussions**, or from **non-QM courses**. 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 is a summary of our perturbation theory results so far. If you have

- an "**unperturbed**" Hamiltonian H_0 that has known eigen-things $\{E_n^{(0)}\}$ and $\{|n^{(0)}\rangle\}$,
- an *actual* Hamiltonian $H = H_0 + H'$ where H' is a <u>small correction</u> to H_0 (a "**perturbation**", $H' \ll H_0$),
- a series expansion of *H*'s 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*'s eigenstates: $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + |n^{(2)}\rangle + \dots$ for each *n*, where $|n^{(0)}\rangle \gg |n^{(1)}\rangle \gg \dots$,

and you define the matrix elements Q_{mn} of an operator \hat{Q} to be written in the <u>unperturbed basis</u>,

$$Q_{mn} \equiv \left\langle m^{(0)} \right| \hat{Q} \left| n^{(0)} \right\rangle$$

then as long as

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

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

$$\begin{bmatrix} E_n^{(1)} = H'_{nn} \end{bmatrix} \equiv \left\langle n^{(0)} \left| H' \right| n^{(0)} \right\rangle = \text{the expectation value of the perturbation } H' \text{ in the } n^{\text{th}} unperturbed \text{ state.}$$

$$\begin{bmatrix} E_n^{(k)} = \left\langle n^{(0)} \left| H' \right| n^{(k-1)} \right\rangle \end{bmatrix} \text{ and } \left| n^{(1)} \right\rangle = \sum_{m \neq n} \frac{H'_{nn}}{E_n^{(0)} - E_m^{(0)}} \left| m^{(0)} \right\rangle \end{bmatrix} \text{ so } E_n^{(2)} = \sum_{m \neq n} \frac{\left| H'_{nn} \right|^2}{E_n^{(0)} - E_m^{(0)}}$$

If an unperturbed energy you are trying to correct is part of a **degenerate subspace** of states, you must do a partial change of basis before applying these formulae. This procedure is summarized on the first page of Discussion 7.

Problem 1 : δ-Function Bump in the ∞ Square Well ™

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 :

$$H' = \alpha \delta \left(x - \frac{a}{2} \right)$$
 where α 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 $|m^{(0)}\rangle$. 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. ③

Also, hints from past students: (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 2: 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 <u>two different spins</u> are involved, please read through the solution for Discussion 6 Question 3 before doing this problem.

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

$$\left\{ \left| e_{1} \right\rangle, \left| e_{2} \right\rangle, \left| e_{3} \right\rangle, \left| e_{4} \right\rangle \right\} \equiv \left\{ \left| 00 \right\rangle_{SM}, \left| 1+1 \right\rangle_{SM}, \left| 10 \right\rangle_{SM}, \left| 1-1 \right\rangle_{SM} \right\}$$

(b) Derive the matrix representation for V in the basis $|m_1m_2\rangle$ where the ordered basis states are

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

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 { your result from part (a), Clebsch-Gordan coefficients , and the change-of-basis procedure discussed / reviewed at the end of Lecture 7B $\}$.

► ALTERNATE HINT: You can also solve part (b) first, then use { that result + Clebsch-Gordan coefficients + change-of-basis procedure discussed / reviewed at the end of Lecture 7B } to solve part (a).

Problem 3 : The Stark Effect

When an atom is placed in a uniform external electric field E_{ext} , the energy levels are shifted — a phenomenon known as the **Stark effect**. In this problem we analyze the Stark effect for the n = 1 and n = 2 states of hydrogen. Let the field point in the *z* direction, so the potential energy of the electron is

$$H'_{S} = e E_{\text{ext}} z = e E_{\text{ext}} r \cos \theta$$

Treat this as a perturbation on the simple "Bohr" Hamiltonian for the hydrogen atom,

$$H_0 = -\frac{\hbar^2 \nabla^2}{2m} - \frac{e^2}{4\pi \varepsilon_0 r} \,.$$

Spin is irrelevant to this problem so ignore it.

(a) Show that the ground state energy is not affected by this perturbation, to first order.

(b) The first excited state is 4-fold degenerate: ψ_{200} , ψ_{211} , ψ_{210} , ψ_{21-1} . Using degenerate perturbation theory, determine the first-order corrections to the energy. Into how many levels does E₂ split?

(c) What are the " β " wave functions for part (b), i.e. the ones that diagonalize the perturbation H'_s ? (Griffiths calls these "good" wavefunctions.) Find the expectation value of the electric dipole moment ($\vec{p}_e = -e\vec{r}$) in each of these "good" states. Notice that the results are independent of the applied field — evidently hydrogen in its first excited state can carry a *permanent* electric dipole moment.

► **HINT**: There are a lot of integrals in this problem, but almost all of them are ZERO. So study each one carefully before you do any calculations! For example, if the ϕ integral vanishes, there's not much point in doing the *r* and θ integrals \odot . Partial answer: $H'_{13} = H'_{31} = -3ea_0 E_{ext}$ where a_0 is the Bohr radius as usual; all other elements of $\mathbf{H}'_{ij} \equiv \langle \beta_i^{(0)} | H' | \beta_j^{(0)} \rangle$ are zero \odot .