Homework 9

Due: April 13 at 11:59 PM. Submit on Canvas.

Problem 1: Consider two interacting particles in a rotationally invariant three-dimensional harmonic oscillator. Think of the particles as distinguishable quantum particles. The unperturbed Hamiltonian is

$$H_0 = \frac{p_{x1}^2 + p_{x2}^2 + p_{y1}^2 + p_{y2}^2 + p_{z1}^2 + p_{z2}^2}{2m} + \frac{1}{2}m\omega^2 \left(x_1^2 + x_2^2 + y_1^2 + y_2^2 + z_1^2 + z_2^2\right).$$
 (1)

The eigenstates of H_0 can be labeled as $|n_{x1}n_{x2}n_{y1}n_{y2}n_{z1}n_{z2}^{(0)}\rangle$ where each *n* labels the energy level of the corresponding (decoupled) oscillator.

Now consider a perturbation that causes the particles to couple together: $H = H_0 + \lambda V$ where δ is a small parameter, and

$$V = -\delta \left(x_1 x_2 + y_1 y_2 + z_1 z_2 \right).$$
⁽²⁾

- 15 A: This problem is about the effect of the perturbation V on the first excited states of the oscillator.
 - A1. Show that the energy of the first excited state is $E_1 = 4\hbar\omega$.
 - A2. Show that this energy level has a degeneracy of 6, and write down the degenerate eigenvectors of H_0 .
 - A3. Find the matrix elements of V between these six eigenstates.
- 10 **B**: While in principle you can diagonalize the 6×6 matrix V found in A3 to deduce the first order perturbation to the energy levels of H, we can also use the fact that H_0 and V are both symmetric under particle exchange:

$$P_{12}|n_{x1}n_{x2}n_{y1}n_{y2}n_{z1}n_{z2}^{(0)}\rangle = |n_{x2}n_{x1}n_{y2}n_{y1}n_{z2}n_{z1}^{(0)}\rangle.$$
(3)

You do not need to show $[H_0, P] = [V, P] = 0$ explicitly, but can use the result as appropriate.

- B1. Explain why the eigenvectors of H must be either even or odd under particle exchange.
- B2. Combine the results of A3 and B1 to find the first order corrections to the energy level $4\hbar\omega$, along with the eigenstates of H up to first order in perturbation theory. You should find that the energy level $4\hbar\omega$ splits into two energy levels, each of which has degeneracy 3.
- 10 C: Now, think of the perturbation as $V = -\delta \mathbf{r}_1 \cdot \mathbf{r}_2$.
 - C1. Argue that the perturbation preserves three-dimensional rotational symmetry.
 - C2. Conclude that the resulting three-fold degeneracies that you found in part **B** are protected by symmetry, and will thus persist to all orders in perturbation theory.

We can thus use a combination of particle exchange and rotation symmetry to completely fix the eigenvectors of H (at first order)!

Problem 2: Find the eigenvalues of the Hamiltonian H to second order in ϵ , using perturbation theory:

$$H = \begin{pmatrix} 0 & \epsilon & \epsilon & \epsilon \\ \epsilon & 0 & 0 & 0 \\ \epsilon & 0 & 1 & -3\epsilon \\ \epsilon & 0 & -3\epsilon & 4 \end{pmatrix}.$$
 (4)

Problem 3 (Stark effect): In this problem, we will describe the response of a hydrogen atom to a uniform background electric field $\mathcal{E}\hat{\mathbf{z}}$. This corresponds to taking the hydrogen atom H_0 , and deforming it by potential

$$V = e\mathcal{E}z.$$
(5)

In this problem, you may find the hydrogen wave functions in Table 8.2 in McIntyre helpful. For simplicity in this problem, assume that the spectrum of hydrogen contains only the n = 1 and n = 2 states.

- **20** A: Let us begin by studying the response of the ground state: n = 1, l = m = 0.
 - A1. Show that the first order correction to the energy $E_{100}^{(1)} = 0$.
 - A2. Since the ground state is not degenerate, we can use non-degenerate second order perturbation theory for this state only. Deduce that, within our approximations,

$$E_{100}^{(2)} \approx \frac{2^{20}}{3^{11}} \pi \epsilon_0 a_0^3 \mathcal{E}^2.$$
 (6)

where $a_0 \approx 5 \times 10^{-11}$ m is the Bohr radius.

A3. The polarizability of the hydrogen atom can be defined as

$$\alpha = -\left.\frac{1}{\mathcal{E}} \frac{\partial E_{100}}{\partial \mathcal{E}}\right|_{\mathcal{E} \to 0}.$$
(7)

Evaluate α for hydrogen (within our approximations).

A4. For a *dilute* gas with ρ atoms per unit volume, the index of refraction is

$$n \approx 1 + \frac{\rho \alpha}{2\epsilon_0}.\tag{8}$$

For a gas with the density of air (in ambient conditions), $\rho \sim 10^{26} \text{ m}^{-3}$. Estimate ρ for hydrogen gas, assuming all atoms are in the ground state. Is the answer surprising?

- 20 **B**: Now let us discuss what happens in the n = 2 levels, which are four-fold degenerate.
 - B1. For degenerate perturbation theory, we will need to evaluate the matrix elements $\langle 2lm|V|2l'm'\rangle$. By considering these integrals over the angular coordinates θ and ϕ , conclude that all matrix elements vanish except for $\langle 200|V|210\rangle$ and $\langle 210|V|200\rangle$.
 - B2. Evaluate out the integrals explicitly to show that

$$\langle 200|V|210\rangle = -3e\mathcal{E}a_0. \tag{9}$$

B3. Deduce the energy splitting in the n = 2 levels at first order in \mathcal{E} .

Problem 4 (Crystal field splitting): A toy model for the energy levels of atomic orbitals associated to the individual atoms that make up a crystal is as follows. Take the hydrogen atom, and subject it to a perturbing potential of the form

$$V = c \left(x^2 + y^2 + z^2\right) + bxy + \cdots .$$
(10)

In general, the perturbing potential would need to incorporate the symmetries of the whole crystal, but in this problem we will just consider the three terms above.

For convenience, restrict your attention in this problem to just the n = 3 energy levels of hydrogen, which are degenerate in the absence of perturbation V. Also, you do not have to evaluate any integrals in this problem, if you can deduce the answer without calculating them explicitly. In this problem the only questions will concern what states (if any) remain degenerate within first order perturbation theory.

- 10 A: Let us begin by assuming that $c \neq 0$ but b = 0. In this case, explain why you expect that the n = 3 level will split into three distinct energy levels of degeneracies 1, 3 and 5.
- 10 **B**: Now, consider turning on $b \neq 0$ as small perturbations to the already perturbed spectrum.¹ Describe how the energy levels will split.

¹This will make your life a little simpler, since now degenerate perturbation theory requires studying fewer matrix elements.