Quantum Physics III (8.06) — Spring 2016

Assignment 1

Readings

This week, and in general, you should consider the Griffiths reading as required and the others as optional.

- Griffiths, Chapter 6
- Cohen-Tannoudji, Chapter XI
- Shankar, Chapter 17
- Sakurai, Sections 5.1-5.3

Problem Set 1

1. **The Joy of 2×2 Hermitian Matrices (10 points)**

   (a) Compute $(\vec{a}\cdot\vec{\sigma})^2$ (using the formula $\sigma_i\sigma_j = \delta_{ij}I + \sum_{k=1}^{3} i\epsilon_{ijk}\sigma_k$) and write down its eigenvalues. Using also the fact that $\mathrm{tr}\vec{a}\cdot\vec{\sigma} = 0$, what can you conclude about the eigenvalues of $\vec{a}\cdot\vec{\sigma}$? What about the eigenvalues of $a_0 I + \vec{a}\cdot\vec{\sigma}$?

   (b) Let $\vec{a} = (\alpha, 0, \beta)$. Write down the exact eigenvalues of $\vec{a}\cdot\vec{\sigma}$. Write down the dominant terms and the first *two* correction terms in the cases when $|\alpha| \ll |\beta|$ and when $|\alpha| \gg |\beta|$. Compare with the results you obtain from second-order perturbation theory.

   (c) Define the inner product $\langle A, B\rangle \equiv \mathrm{tr}[A^\dagger B]$. Suppose that $A = \frac{a_0 I + \vec{a}\cdot\vec{\sigma}}{2}$. Write down Hermitian matrices Q_0, Q_1, Q_2, Q_3 such that $a_i = \langle A, Q_i\rangle$.

2. **Anharmonic Oscillator (25 points)**

   Consider the anharmonic oscillator with Hamiltonian

   $$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} + \lambda x^3 \ ,$$

   treating the λx^3 term as a perturbation. [Hint: you should not find yourself doing any integrals as you do this problem; you should find yourself manipulating harmonic oscillator creation and annihilation operators and harmonic oscillator energy eigenstates.]

   (a) Show that the first order shift in the ground state energy is zero. Calculate the shift to order λ^2.

   (b) Calculate the ground state wave function to order λ. (You may just write your answer as a sum of harmonic oscillator states.)

(c) Sketch the potential $V(x)$ as a function of x for small λ. Is the state you found in (b) anything like the true ground state? What effect has perturbation theory failed to find?

3. **Perturbation of the Three-Dimensional Harmonic Oscillator (30 points)**

The spectrum of the three-dimensional harmonic oscillator has a high degree of degeneracy. In this problem, we see how the addition of a perturbation to the Hamiltonian reduces the degeneracy. This problem is posed in such a way that you can work through it before we even begin to discuss degenerate perturbation theory in lecture.

Consider a quantum system described by the Hamiltonian

$$H = H_0 + \delta H \tag{1}$$

where

$$H_0 = \frac{1}{2m}\vec{p}^{\,2} + \frac{1}{2}m\omega^2\vec{x}^{\,2} \tag{2}$$

where $\vec{x} = (x_1, x_2, x_3)$ and $\vec{p} = (p_1, p_2, p_3)$. The perturbing Hamiltonian δH is given by

$$\delta H = \kappa L_2 \tag{3}$$

where κ is a constant and where $L_2 = x_3 p_1 - x_1 p_3$.

In parts (a)-(e) of this problem, we study the effects of this perturbation within the degenerate subspace of states which have energy $E = (5/2)\hbar\omega$ when $\kappa = 0$.

(a) Set $\kappa = 0$. Thus, in this part of the problem $H = H_0$. Define creation and annihilation operators for "oscillator quanta" in the 1, 2 and 3 directions. Define number operators N_1, N_2, N_3. Denote eigenstates of these number operators by their eigenvalues, as $|n_1, n_2, n_3\rangle$. What is the energy of the state $|n_1, n_2, n_3\rangle$? How many linearly independent states are there with energy $E = (5/2)\hbar\omega$? [That is, what is the degeneracy of the degenerate subspace of states we are studying?]

(b) Express the perturbing Hamiltonian δH in terms of creation and annihilation operators.

(c) What is the matrix representation of δH in the degenerate subspace you described in part (a)?

(d) What are the eigenvalues and eigenstates of δH in the degenerate subspace? What are the eigenvalues and eigenstates of $H = H_0 + \delta H$ in the degenerate subspace?

(e) What is the matrix representation of $H_0 + \delta H$ in the degenerate subspace if you use the eigenvectors of δH as a new basis? (i.e. instead of the original $|n_1, n_2, n_3\rangle$ basis.)

[Note: As we shall see in part (f), this problem is "too simple" in important ways. The aspect of this problem which *will* generalize when we consider more generic perturbations is that if a perturbation breaks a degeneracy, then even an arbitrarily small but nonzero perturbation has qualitative consequences: it selects one particular choice of energy eigenvectors, within the previously degenerate subspace. In the present problem, this can be described as follows: if κ were initially zero and you were happily using the $|n_1, n_2, n_3\rangle$ states as your basis of energy eigenstates, and then somebody "turns on" a very small but nonzero value of κ, this forces you to make a qualitative change in your basis states. The "rotation" you must make from your previous energy eigenstates to the new states which are now the only possible choice of energy eigenstates is not a small one, even though κ is arbitrarily small.]

(f) Suppose that $|\psi\rangle$ and $|\phi\rangle$ are eigenstates of H_0 with *different* energy eigenvalues. That is, $|\psi\rangle$ and $|\phi\rangle$ belong to different degenerate subspaces. Show that $\langle\phi|\delta H|\psi\rangle = 0$ for any two such states. Relate this fact to a statement you can make about the operators H_0 and δH, without reference to states.

[The fact that $\langle\phi|\delta H|\psi\rangle = 0$ if $|\psi\rangle$ and $|\phi\rangle$ and belong to different degenerate subspaces means that δH is a "non-generic" perturbation of H_0; a more general perturbation would not have this property. It is only for perturbations with this property that the analysis you have done above — which focusses on one degenerate subspace at a time — is complete. Notice also that in order to analyze $H = H_0 + \delta H$, we did not have to assume that κ was in any sense small. If δH were "generic", we would have had to assume that κ was small in order to make progress.]

4. **Polarizability of a Particle on a Ring; the Ethane Molecule (15 points)**

Consider a particle of mass m constrained to move in the xy-plane on a circular ring of radius a. The only variable of the system is the azimuthal angle, which we will call ϕ. The state of the system is described by a wave function $\psi(\phi)$ that must be periodic

$$\psi(\phi + 2\pi) = \psi(\phi)$$

and normalized:

$$\int_0^{2\pi} |\psi(\phi)|^2 d\phi = 1 \ .$$

(a) The kinetic energy of the particle can be written:

$$H_0 = \frac{L_z^2}{2ma^2} \tag{4}$$

where $L_z = -i\hbar d/d\phi$. Calculate the eigenvalues and eigenfunctions of H_0. Which of the energy levels are degenerate?

(b) Now assume that the particle has a charge q and that it is placed in a uniform electric field ε in the x-direction. We must therefore add to the Hamiltonian the perturbation

$$\delta H = -q\varepsilon a \cos\phi.$$

Calculate the new wave function of the ground state to first order in ε. Use this wave function to evaluate the induced electric dipole moment in the x-direction: $\langle\psi|qx|\psi\rangle$. Determine the proportionality constant between the dipole moment and the applied field ε. This proportionality constant is called the "polarizability" of the system.

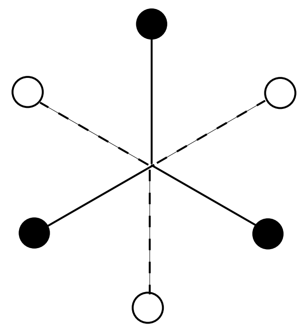

Figure 1: A cartoon of an ethane molecule in its most favorable orientation, seen end on.

(c) Now turn off the electric field of part (b) and consider the ethane molecule CH_3—CH_3. We will consider the rotation of one CH_3 group relative to the other, about the straight line joining the two carbon atoms, as sketched in figure 1. Here, the solid circles represent the H atoms in one CH_3 group, which rotate relative to the open circles representing the H atoms in the other CH_3 group.

To a zeroth approximation, this rotation is free, and the Hamiltonian H_0 of (4) describes the rotational kinetic energy. (The constant $2ma^2$ must be replaced by some new constant times the moment of inertia of a CH_3 group with respect to the rotational axis. However, for simplicity, we will just keep calling the constant $2ma^2$.)

We now take the electrostatic interaction energy between the two CH_3 groups into account as a perturbation. To take into account the threefold symmetry, we add to H_0 a term of the form

$$\delta H = b \cos 3\phi \ ,$$

where b is a real constant. Calculate the energy and wave function of the new ground state (to first order in b for the wave function and to second order for the energy). Give a physical interpretation of the result.

5. **Energy Shift Due to Finite Nuclear Size (20 points)**

When you studied the hydrogen atom in 8.04/8.05, you assumed that the Coulomb potential extended all the way to the origin. In reality, the proton's charge is smeared out over a sphere of roughly 10^{-13} cm in radius. This has a small effect on the energy levels of the hydrogen atom. Let's find out how small.

You will model the electric charge distribution of the proton as a uniformly charged sphere of radius R. You may ignore the fine structure, Lamb shift, and hyperfine splittings of hydrogen for this problem.

(a) Find the electrostatic potential energy of the electron for all r.

[Hint: Use Gauss's law $\vec{\nabla} \cdot \vec{E} = 4\pi\rho$ to find the electric field everywhere and then integrate $\vec{F} = -e\vec{E}$ to obtain the potential energy.]

Your answer should have the features that for $r > R$ you should have $V(r) = -e^2/r$ and for all values of r, $V(r)$ is continuous.

(b) Use lowest order perturbation theory to calculate the shift in the energy of the ground state of hydrogen due to this modification of the potential. Evaluate your answer numerically, taking $R = 10^{-13}$ cm, and express your answer as a fraction of the binding energy of the ground state (13.6 eV). [Hint: You can simplify the integrals by noticing that the unperturbed wave function varies only slowly over the range $0 < r < R$ and can thus be replaced by the value at $r = 0$.]

(c) Why is this effect most important for states with orbital angular momentum zero? Without doing any calculation, make an estimate of the factor by which this effect is smaller for an $\ell = 1$ state as compared to an $\ell = 0$ state.

(d) Experimentally, the most precise measurement of the proton radius comes from the PSI experiment:

$$R = 0.84184(67) \times 10^{-13}\ \text{cm}. \tag{5}$$

[R. Pohl *et al.*, "The size of the proton," Nature **466**, 213 (2010).] This measurement is controversial, since it differs by 4% from the CODATA world average ($R = 0.8768(69) \times 10^{-13}$ cm). Putting the controversy aside, explain why the PSI experiment could get such impressive accuracy using muonic hydrogen (a muon-proton bound state) instead of ordinary hydrogen (an electron-proton bound state). [Hint: Recall that the muon has basically the same properties as an electron, except it is 206.8 times heavier.]