Quantum Physics III (8.06) — Spring 2016

Assignment 2

Readings

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

- Griffiths, Chapter 8
- Cohen-Tannoudji, Chapter XII
- Shankar, Section 16.2

Problem Set 2

1. **Stark Effect (Adapted from Griffiths Problem 6.36, 35 points)**

   When an atom is placed in a uniform external electric field $\vec{E}_{\text{ext}}$, the energy levels are shifted, a phenomenon known as the **Stark effect**. This is the electrical analog to the magnetic Zeeman effect. In this problem, you will analyze the Stark effect for the $n = 1$ and $n = 2$ states of hydrogen. Let the electric field point in the $\hat{z}$ direction, so the electrostatic potential of the electron is

   $$\delta H_{\text{Stark}} = eE_{\text{ext}}z \tag{1}$$

   Treat this as a perturbation on the Bohr Hamiltonian

   $$H_0 = \frac{\vec{p}^{\,2}}{2m} - \frac{e^2}{r}, \tag{2}$$

   for now ignoring spin and fine structure effects.

   (a) *[This part is just math, but will make the later calculations much easier.]* Suppose that a, b, c are nonnegative integers and $f(r)$ is a function. Prove that

   $$\int dx\,dy\,dz\,x^a y^b z^c f(r) = 0 \tag{3}$$

   unless a, b, c are *each* even. Here $r \equiv \sqrt{x^2 + y^2 + z^2}$ and you may assume that $f(r)$ is a function such that the integral in (3) is always defined.

   (b) Show that the ground state energy $E_{1,0,0}$ is not affected by the perturbation in (1), to first order in perturbation theory.

   (c) The second-order shift to $E_{1,0,0}$ is nonzero and is not so easy to calculate. In this part you will compute a bound on the shift.

i. Calculate $\sum_\alpha |\langle\alpha|z|1,0,0\rangle|^2$, where α runs over all states of the Hydrogen atom, bound or unbound. [*Hint:* Dimensional analysis can be a good sanity check of this result.]

ii. The quantity

$$\frac{1}{E^0_{1,0,0} - E^0_\alpha} \tag{4}$$

is always negative for all $\alpha \neq (1,0,0)$. What is the lowest (i.e. closest to $-\infty$) possible value for (4)?

iii. Conclude by arguing that the second order shift

$$E^2_{1,0,0} \geq -Ca_0^3 E^2_{\text{ext}}, \tag{5}$$

for some C. What is C?

Discussion: This calculation shows an upper bound on the ground-state polarizability of the Hydrogen atom. Why? A system has polarizability α if applying field $\vec{E}$ induces dipole moment $\vec{p} = \alpha\vec{E}$. A dipole $\vec{p}$ in an electric field $\vec{E}$ has energy $-\vec{p}\cdot\vec{E}$; thus polarizability α corresponds to energy $-\alpha E^2$ in an electric field with $E = |\vec{E}|$. Conversely, if the term $-\alpha E^2$ appears in a Hamiltonian, it corresponds to a system with polarizability α. Carrying out the calculation of $E^2_{1,0,0}$ exactly requires integrating over the unbound states, which is doable using 8.06 methods but a lot of work. This leads to the value $C_{\text{exact}} = \frac{9}{4}$. The value of C that you calculate should be consistent with this! Calculating the polarizability is a step towards calculating the van der Waals force.

(d) The first excited state of H_0 is 4-fold degenerate, with $|n,\ell,m\rangle$ states $|2,0,0\rangle$, $|2,1,1\rangle$, $|2,1,0\rangle$, $|2,1,-1\rangle$. Using degenerate perturbation theory, determine the first-order corrections to the energy. Into how many levels do these $n=2$ states split? (Ignore spin.)

(e) What are the "good" wave functions for part (d)? Find the expectation value of the electric dipole moment ($\vec{p}_e \equiv -e\vec{r}$) in each of these "good" states.

(f) Now we consider electron spin, and the fine-structure splitting between the $2S$ and $2P$ levels. Calculate the electric field strength (in V/cm) at which the energy of the Stark shift calculated above becomes equal to the fine-structure splitting between the $2S$ and $2P$ energy levels.

A common household electric field strength is roughly 100V/cm. For example, the live and neutral wires in an electrical socket have a voltage difference of 110V and if they are 1.1cm apart then there will be a field of 100V/cm between them. In this case, a hydrogen atom that happened to be between the two wires would experience a field of strength 100V/cm. At this field strength would this atom become polarized according to your result in part (d), or would the fine-structure splitting be dominant? [Regardless of what you calculate, please do not try any version of this at home.]

2. **Quantum Mechanics of a Bouncing Ball (15 points)**

The semiclassical approximation can also be used to estimate the energy eigenvalues and eigenstates for potentials that cannot be treated exactly so easily. This problem is loosely based on Griffiths 8.6. (See Griffiths 8.5 if you'd like to learn how to treat this quantum mechanical problem exactly, using Airy functions.)

Consider the quantum mechanical analogue to the classical problem of a ball of mass m bouncing elastically on the floor, under the influence of a gravitational potential which gives it a constant acceleration g.

(a) Find the semiclassical approximation to the allowed energies E_n, in terms of m, g, and $\hbar$.

(b) Estimate the zero point energy of a neutron "at rest" (i.e. in the quantum mechanical ground state) on a horizontal surface in the earth's gravitational field. Express your answer in eV. [This may sound artificial to you, but the experiment has been done. See V. V. Nesvizhevsky *et al.*, Nature **415**, 297 (2002) and arXiv:hep-ph/0306198 for an experimental measurement of the quantum mechanical ground state energy for neutrons bouncing on a horizontal surface in the earth's gravitational field. This experiment got a lot of press at the time, because it involves both gravity and quantum mechanics, which made for an eye catching press release. It of course has *nothing* to do with quantum gravity.]

(c) Now imagine dropping a ball of mass 1 gram from rest from a height of 1 meter, and letting it bounce. Do the 8.01 "calculation" of the classical energy of the ball. The quantum mechanical state corresponding to a ball following this classical trajectory must be a coherent superposition of energy eigenstates, with mean energy equal to the classical energy. How large is the mean value of the quantum number n in this state?

3. Application of the Semiclassical Method to the Double Well Potential (25 points)

Do Griffiths Problem 8.15.

This is not as difficult a problem as its length would indicate. Griffiths leads you through all the steps. This is an instructive problem in quantum dynamics. You should recall that this is the potential that we used to describe the physics of the ammonia molecule, early in 8.05. Back then, we had to wave our hands a little when we talked about tunneling splitting the degeneracy between the even and odd states. Now, you can do this calculation for real.

Hint for (a) and (b): The steps suggested by Griffiths are: work out the wave function ψ_1 in region (i); from ψ_1 use the connection formulae at x_2 to obtain the wave function ψ_2 in regions (ii); use ψ_2 and the connection formulae at x_1 to obtain the wave function ψ_3 in region (iii). Equation (8.59) can be found by requiring that ψ_3 should satisfy $\psi_3(0) = 0$ or $\psi_3'(0) = 0$ at $x = 0$.

It is a bit easier (and more transparent) to use a slightly different approach from what Griffiths suggests. Given that the wave function should be an even or odd function of

x, the wave function in region (iii) can be written down immediately. For example in the even case,

$$\psi(x) = \frac{C}{\sqrt{\kappa(x)}} \cosh\left[\frac{1}{\hbar}\int_0^x dy\, \kappa(y)\right], \qquad -x_1 < x < x_1 \tag{6}$$

using our standard notations. (6) is an example where by symmetry, the exponentially small piece in a classically forbidden region is known exactly. The wave function ψ_2 in region (ii) then can be obtained using two ways: from ψ_1 in region (i) via connection formulae at x_2, or from ψ_3 in region (iii) via connection formulae at x_1. The consistency of two wave functions leads to equation (8.59) of Griffiths.

4. **Hydrogen medley (25 points)** Let m_e denote the mass of an electron and e its charge. The 8.04 version of the Hydrogen Hamiltonian is

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{r}.$$

In this problem we will consider the spin of the electron (whose corresponding operator we call $\vec{S}$) but we will ignore the spin of the proton.

(a) **Complete sets of commuting observables (CSCO).** A CSCO is a set of commuting operators whose simultaneous eigenspaces are each one dimensional. Equivalently, specifying all the eigenvalues of all the operators in a CSCO uniquely specifies a state (up to multiplication by a scalar). You may use without proof the fact that $H_0, \vec{L}^2, L_z, S_z$ form a CSCO with eigenbasis $\{|n, l, m_l, m_s\rangle\}$. For each of the following sets of operators, either (a) explain why they are CSCOs and justify this by expressing its eigenstates in terms of the $\{|n, l, m_l, m_s\rangle\}$ eigenstates, or (b) explain why they are *not* CSCOs. For simplicity, consider only bound states.

i. $H_0, \vec{L}^2, \vec{L}\cdot\vec{S}, J_z$.
ii. $H_0, \vec{L}^2, L_z, S_x$.
iii. $H_0, \vec{L}^2, J_z, S_z$.
iv. $H_0, \vec{J}^2, J_z, S_z$.
v. $H_0, \vec{J}^2, \vec{L}\cdot\vec{S}, J_z$.

(b) **Strong-field Zeeman effect.** In the strong-field Zeeman effect, the unperturbed eigenstates are $|n, l, m_l, m_s\rangle$. The fine structure can be thought of as contributing a term

$$H_{\text{fs}} = -\frac{m_e c^2 \alpha^4}{2n^3}\left(\frac{1}{\hat{j}+1/2} - \frac{3}{4n}\right),$$

where $\hat{j}$ is an operator satisfying $J^2 = \hbar^2 \hat{j}(\hat{j}+1)$. To compute the first-order energy shifts here we need to evaluate

$$\langle n, l, m_l, m_s|\frac{1}{\hat{j}+1/2}|n, l, m_l, m_s\rangle. \tag{7}$$

i. Use the following strategy to evaluate (7). First compute the expectation value of J^2 on the $|n, l, m_l, m_s\rangle$ state. Now imagine that we measure $\hat{j}$. Use your calculation to find the probabilities of the two outcomes $j = l + 1/2$ and $j = l - 1/2$. Finally use the fact that(7) equals

$$\frac{\Pr[j = l + 1/2]}{l + 1} + \frac{\Pr[j = l - 1/2]}{l} \tag{8}$$

to reproduce the known result for the strong-field Zeeman effect (see lecture notes or Griffiths).

ii. The shifts in (7) used non-degenerate perturbation theory. But since the unperturbed energies are a function of $m_l + 2m_s$ there will be degeneracies. Explain why, despite this, the above argument is still correct.

5. **Tunneling and the Stark Effect (preview)**
Do not turn in this problem with pset 2. It will appear on pset 3.

The Stark effect concerns the physics of an atom in an electric field. In this problem, you will explore the possibility that in an electric field, the electron in an atom can tunnel out of the atom, making the atomic bound states unstable. We consider this effect in a simpler one-dimensional analog problem.

Suppose an electron is trapped in a one-dimensional square well of depth V_0 and width d:

$$\begin{aligned} V(x) &= -V_0 \text{ for } |x| < d/2 \\ &= 0 \quad \text{for } |x| \geq d/2 \; . \end{aligned}$$

Suppose a weak constant electric field in the x-direction with strength $\mathcal{E}$ is turned on. That is $V \to (V - e\mathcal{E}x)$. Assume throughout this problem that $e\mathcal{E}d \ll \hbar^2/2md^2 \ll V_0$.

(a) Set $\mathcal{E} = 0$ in this part of the problem. Estimate the ground state energy (i.e. the amount by which the ground state energy is above the bottom of the potential well) by pretending that the well is infinitely deep. (Because $\hbar^2/2md^2 \ll V_0$, this is a good approximation.) Use this estimate of the ground state energy in subsequent parts of the problem. Note that the true ground state energy is lower than what you've estimated, why?

(b) Sketch the potential with $\mathcal{E} \neq 0$ and explain why the ground state of the $\mathcal{E} = 0$ potential is no longer stable when $\mathcal{E} \neq 0$.

(c) Use the semiclassical approximation to calculate the barrier penetration factor for the ground state. [You should use the fact that $e\mathcal{E}d \ll \hbar^2/2md^2$ to simplify this part of the problem.]

(d) Use classical arguments to convert the barrier penetration factor into an estimate of the lifetime of the bound state.

(e) Now, lets put in numbers that are characteristic of an atomic system. Calculate the lifetime for $V_0 = 20$ eV, $d = 2 \times 10^{-8}$ cm and an electric field of 7×10^4 V/cm. Compare the lifetime you estimate to the age of the universe.

(f) Show that the lifetime goes like $\exp(1/\mathcal{E})$, and explain why this result means that this "instability" could not be obtained in any finite order of perturbation theory, treating $\mathcal{E}$ as a perturbation to the Hamiltonian.

8.06 Quantum Physics III
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