Quantum Physics III (8.06) — Spring 2018 Assignment 2

Posted: Wednesday, February 14, 2018

Announcements

• Please put your name and section at the top of what you hand in.

Readings

- Griffiths, Chapter 6 (Time-independent perturbation theory)
- Cohen-Tannoudji, Chapter XI and Chapter XII
- Shankar, Chapter 17 (very nice chapter!)

Problem Set 2

- 1. Higher order and normalization in non-degenerate perturbation theory (10 points)
 - (a) Calculate the second order state correction $|n^{(2)}\rangle$ and the third order energy correction $E_n^{(3)}$.
 - (b) The state $|n\rangle_{\lambda}$ is not normalized. Use the expression for this state including the first correction proportional to λ to calculate to order λ^2 the quantity $Z_n(\lambda)$ defined by

$$\frac{1}{Z_n(\lambda)} \equiv \lambda \langle n | n \rangle_{\lambda} \quad . \tag{1}$$

What is the probability that the state $|n\rangle_{\lambda}$ will be observed to be along its unperturbed version $|n^{(0)}\rangle$?

2. Polarizability of a particle on a ring revisited (15 points)

Consider again 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 ϕ . The state of the system is described by a wave function $\psi(\phi)$ that must be periodic with period 2π . The energy eigenstates were found in the previous homework

$$\psi_n(\phi) = \langle \phi | n \rangle = \frac{1}{\sqrt{2\pi}} e^{in\phi} , \ n \in \mathbb{Z}$$
 (2)

$$E_n = \frac{\hbar^2 n^2}{2ma^2} = E_1 n^2$$
, with $E_1 = \frac{\hbar^2}{2ma^2}$. (3)

The ground state n = 0 has zero energy and is non-degenerate. All other states are doubly-degenerate because the states with $\pm n$ have the same energy level.

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

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

Consider the degenerate $|\pm 1\rangle$ states. Calculate the second order corrections to the energy of the states and the corrected states to zeroth order in the perturbation.

3. **3-by-3 matrix and degenerate perturbation (Adapted from Schiff, 15 points)** Sakurai calls this problem "a challenge for the experts."

Consider the matrix

$$\begin{pmatrix} E_1 & 0 & \epsilon_1 \\ 0 & E_1 & \epsilon_2 \\ \epsilon_1^* & \epsilon_2^* & E_2 \end{pmatrix}$$
(4)

Where $E_1 \neq E_2$ and the ϵ_i 's are perturbations. The degeneracy of the E_1 eigenvectors is not lifted to first order in the perturbation.

- (a) Calculate the exact eigenvalues and find their expansion to second order in the perturbations. Calculate the corresponding eigenstates to first order in the perturbation.
- (b) Use perturbation theory (both non-degenerate and degenerate) to reproduce the above results for the eigenvalues, and the zeroth-order result for the eigenvectors.

4. Feynman-Hellman (FH) for hydrogen atom expectation values (Adapted from Griffiths Problem 6.33, p.288, 10 points)

The effective Hamiltonian for radial wavefunctions is given by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - \frac{e^2}{r}.$$
 (5)

The hydrogen atom energies are

$$E_n = -\frac{e^2}{2a_0}\frac{1}{n^2}, \quad a_0 = \frac{\hbar^2}{me^2}.$$
 (6)

In solving the radial equation one sets $n = N + \ell + 1$, where N is the degree of the radial polynomial. (The Feynman-Hellmann lemma is explained in Problem 6.32, and in the posted lecture notes from 8.05 (Chapter 14))

- (a) Use the FH lemma for parameter $\lambda = e^2$ to derive $\langle 1/r \rangle$.
- (b) Use the FH lemma for parameter λ = ℓ to derive (1/r²) (Imagine, not so rigorously, that ℓ can be treated as a continuous variable. Otherwise consult Shankar, p. 470, exercise 17.3.4).

5. Stark Effect (Adapted from Griffiths Problem 6.36, 30 points)

When an atom is placed in a uniform external electric field \vec{E}_{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

$$\delta H_{\rm Stark} = e E_{\rm ext} z \tag{7}$$

Treat this as a perturbation on the Bohr Hamiltonian

$$H_0 = \frac{\vec{p}^2}{2m} - \frac{e^2}{r},$$
(8)

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

$$\int dx \, dy \, dz \, x^a y^b z^c f(r) = 0 \tag{9}$$

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 (9) is always defined.

(b) Show that the ground state energy $E_{1,0,0}$ is not affected by the perturbation in (7), 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

$$\frac{1}{E_{1,0,0}^0 - E_\alpha^0} \tag{10}$$

is always negative for all $\alpha \neq (1, 0, 0)$. What is the lowest (i.e. closest to $-\infty$) possible value for (10)?

iii. Conclude by arguing that the second order shift

$$E_{1,0,0}^2 \ge -Ca_0^3 E_{\text{ext}}^2,\tag{11}$$

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 $E_{1,0,0}^2$ 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.]

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