

Physics 580: Quantum Mechanics I
Department of Physics, UIUC
Fall Semester 2006
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Problem Set No. 7/ Final Exam:
Time Independent Perturbation Theory
Due Date: 12/8/2006

Note: the solutions must be sent to me as a pdf file to my e-mail address efradkin@uiuc.edu. You can either have a typed solution and send me the pdf file or have your handwritten solution scanned and saved as a pdf file which you will send to me. If you choose the “handwritten solution” you should make sure to use a pen with ink that is dark enough and your handwritting clear enough for me to be able to see it. I cannot guess what you write! You should send me the solutions on or before Friday december 8 at 5:00 pm central Standard Time. Since I have a hard deadline to submit the grades I will not be able to accept late solutions. You should **not** give the solutions to the TA **nor** put them in the Physics 580 homework box. **No late sets will be accepted.** Please note that this Problem set is a take home Final Exam. You must turn in your solutions to pass this course.

1 The Anharmonic Oscillator

Consider a linear harmonic oscillator of mass m and angular frequency ω in one dimension. The Hamiltonian is

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega\hat{X}^2$$

where \hat{X} and \hat{P} are the position and momentum operators which satisfy canonical commutation relations, $[\hat{X}, \hat{P}] = i\hbar$. Let \hat{a} and \hat{a}^\dagger be their associated annihilation and creation operators,

$$\begin{aligned}\hat{a} &= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} \hat{X} + i \frac{1}{\sqrt{m\hbar\omega}} \hat{P} \right) \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} \hat{X} - i \frac{1}{\sqrt{m\hbar\omega}} \hat{P} \right)\end{aligned}$$

which satisfy $[\hat{a}, \hat{a}^\dagger] = 1$. In this notation of eigenstates $\{|n\rangle\}$, where $n = 0, 1, 2, \dots$, of the oscillator are

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle$$

where $\hat{a}|0\rangle = 0$. The Hamiltonian now reads $\hat{H} = \hbar\omega (\hat{a}^\dagger\hat{a} + \frac{1}{2})$, and the energy of these states is $E_n = \hbar\omega(n + \frac{1}{2})$.

In this problem you will consider the effects of the perturbation $\hat{V} = \lambda\hat{X}^4$ on the states of the harmonic oscillator. Use the algebra of creation and annihilation operators to do all calculations.

1. Consider first an arbitrary unperturbed eigenstate $|n\rangle$. What states $|m\rangle$ are mixed with $|n\rangle$ by the perturbation \hat{V} ? Why?
2. Use the algebra of the creation and annihilation operators to compute the non-vanishing matrix elements of $\langle n|\hat{V}|0\rangle$.
Hint: Organize your calculation by writing \hat{V} in terms of \hat{a} and \hat{a}^\dagger , and use the commutation relations to write \hat{V} as a sum of terms such that in every factor all annihilation operators are to the right of all creation operators. (This arrangement is called normal ordering.)
3. Use the algebra of the creation and annihilation operators to compute the first order shift of the energy of an arbitrary eigenstate $|n\rangle$.
4. Compute the first correction to the eigenstate $|n\rangle$.
5. Use these methods to compute the corrections to the ground state energy to first and second order perturbation theory in λ .

2 Charged Particle in a Magnetic Field

Consider a particle of mass M and charge $q = -e$ restricted to move on a plane of linear size L parallel to the xy plane. There is a uniform magnetic field of strength B perpendicular to the plane. The magnetic flux is $\Phi = BL^2 = N_\phi\phi_0$, where N_ϕ is a positive integer and the combination of fundamental constants $\phi_0 = hc/e$ is called the flux quantum (Hence, N_ϕ is the number of flux quanta.) For simplicity we will assume that the plane is a strip of width L along the y axis, with $-L/2 \leq y < L/2$, and that the strip is infinitely long on the x axis with $-\infty < x < \infty$.

We showed before that there is close connection between this problem and the one-dimensional linear harmonic oscillator. The quantum mechanical Hamiltonian for this problem is

$$\hat{H} = \frac{1}{2M} \left(\vec{P} - \frac{e}{c} \vec{A}(\vec{R}) \right)^2 + V(\vec{R})$$

where $V(\vec{R})$ is a potential which we will regard as a perturbation. The vector potential \vec{A} for a uniform magnetic field, in the Landau gauge $A_x = 0$, is

$$A_x = 0 \quad A_y = BX$$

In this gauge the Hamiltonian reduces to

$$\hat{H} = \frac{1}{2M} \hat{P}_x^2 + \frac{1}{2M} \left(\hat{P}_y - \frac{eB}{c} \hat{X} \right)^2 + V(\hat{X})$$

Here we have assumed that the in-plane electrostatic potential $V(\vec{R})$ depends only on X . From now on we will work with a potential of the form

$$V(X) = V_0 e^{-\frac{X^2}{2a^2}}$$

where V_0 plays the role of the coupling constant and a is a range. We will assume that V_0 is small and we will use it as the small parameter to do perturbation theory.

1. In the absence of the potential the eigenstates of this system are the Landau levels. *Verify* that in the Landau gauge the eigenstates have the factorized form

$$\langle x, y | n, k \rangle = \Psi_{n,k}(x, y) = \frac{1}{\sqrt{L}} e^{iky} \phi_n(x - x_0(k))$$

where $\ell = \sqrt{\frac{\hbar c}{eB}}$ is the magnetic length, and $\phi_n(x - x_0(k))$, with $n \geq 0$, are the wave functions of a one-dimensional harmonic oscillator with angular frequency given by the cyclotron frequency $\omega_c = \frac{eB}{Mc}$, and that $x_0(k) = k\ell^2$. Show that the unperturbed energy eigenvalues are $E_{n,k} = \hbar\omega_c(n + 1/2)$. Show that these eigenstates are also eigenstates of the operator \hat{P}_y , and for a system with periodic boundary conditions along the y direction and N_ϕ flux quanta the allowed values we must have the quantization condition $k = k_m = \frac{2\pi}{L}m$, where m is an integer quantum number in the range $-\frac{N_\phi - 1}{2} \leq m \leq \frac{N_\phi - 1}{2}$, for N_ϕ even. In other terms, each Landau level has an N_ϕ -fold degeneracy.

Note: In these notation, the harmonic oscillator wave functions that we discussed in the Lectures are

$$\phi_n(x) = (\pi\hbar\ell^2 4^n (n!)^2)^{-1/4} H_n\left(\frac{x}{\ell}\right) e^{-\frac{x^2}{2\ell^2}}$$

where $H_n(x)$ are the Hermite polynomials (for details see my lecture notes or any textbook). For the purposes of this problem we will need only in the first two Hermite polynomials, $H_0(x) = 1$ and $H_1(x) = 2x$.

2. Use symmetry arguments to show that the matrix elements $\langle n', k_{m'} | \hat{V} | n, k_m \rangle$ of any potential of the form $V(x, y) \equiv V(x)$ obey a selection rule of the form $\langle n', k_{m'} | \hat{V} | n, k_m \rangle = \delta_{m,m'} \langle n', k_m | \hat{V} | n, k_m \rangle$.
3. Compute the matrix elements $V_{0,0}(k) = \langle 0, k | \hat{V} | 0, k \rangle$, $V_{1,1}(k) = \langle 1, k | \hat{V} | 1, k \rangle$, $V_{0,1}(k) = \langle 0, k | \hat{V} | 1, k \rangle$ and $V_{1,0}(k) = \langle 1, k | \hat{V} | 0, k \rangle$, for the potential given above.

Hint: You will have to do a number of gaussian integrals. The following result will be useful for you

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{\alpha}{2}x^2 + \beta x} = \frac{1}{\sqrt{\alpha}} e^{\frac{\beta^2}{2\alpha}}$$

- Use first order perturbation theory in V_0 to compute the energy shift of the states $|0, k\rangle$ and $|1, k\rangle$. Draw a qualitative plot of the k dependence of the perturbed energy levels. Has the potential lifted the degeneracy? Is there any degeneracy left? Explain and justify your answers.
- Find the form of the perturbed wave functions to first order in perturbation theory. Use this result to compute the current,

$$\vec{J} = \frac{\hbar}{2mi} \int_{-\infty}^{\infty} dx \int_{-L/2}^{L/2} dy \left(\Psi_{n,k}(x, y)^* \vec{\nabla} \Psi_{n,k}(x, y) - \Psi_{n,k}(x, y) \vec{\nabla} \Psi_{n,k}(x, y)^* \right)$$

Which component is not zero? Why? How does J_y depend on k ? Give a physical explanation for these results.

Hint: Think of the classical motion of a charged particle in crossed electric and magnetic fields.

- Show that there is a critical value of V_0 at which the first-order perturbed energy levels become degenerate. For which value of k does this first occur? Use almost degenerate perturbation theory (or Brillouin-Wigner perturbation theory if you prefer) to resolve this degeneracy. Discuss what changes does this Landau level mixing have on the k -dependence of the energy levels.

3 Model of a Hydrogen-like atom

We model a hydrogen atom as a point-like proton and a point-like electron interacting through an attractive Coulomb interaction. There are many hydrogen-like atoms of atomic number Z , namely those in the first column of the periodic table, which have a single outer electron while the remaining $Z - 1$ electrons are in closed shells which are more tightly bound to the nucleus. A crude model of these atoms (which neglects the effects of the Pauli exclusion principle) is the following. We will regard the electrons on the closed shells as a core of radius d which repels the outer electron and partially screen the charge of the nucleus. A simple model for this hydrogen-like atom is that of a single electron of charge $-e$ and mass M interacting to the nucleus and the core through a spherically-symmetric potential of the form

$$U(r) = \begin{cases} -\frac{e^2}{r} & \text{for } r > d \\ V_0 & \text{for } r \leq d \end{cases}$$

where $V_0 > 0$. In what follows it will be convenient to write this potential as

$$U(r) = -\frac{e^2}{r} + W(r)$$

end to regard $W(r)$ as a perturbation.

In this problem we will consider the effects of this perturbation on the eigenstates and energy levels of the Hydrogen atom. Recall that the eigenstates are $|n, l, m\rangle$, where $n = 1, 2, \dots$, $l = 0, 1, \dots, n-1$ and $|m| \leq l$. The energy levels are

$$E_n^{(0)} = -\frac{e^2}{2a_0 n^2}$$

where $a_0 = \hbar^2/M_e e^2$ is the Bohr radius and, in spherical coordinates (r, θ, φ) , where $0 \leq r < \infty$, $0 \leq \theta \leq \pi$ and $0 \leq \varphi < 2\pi$, the wave functions are

$$\psi_{nlm}(r, \theta, \varphi) = \langle \vec{r} | n, l, m \rangle = R_{nl}(r) Y_{lm}(\theta, \varphi)$$

where $Y_{lm}(\theta, \varphi)$ are the spherical harmonics, and, up to a normalization, the radial wave functions $R_{nl}(r)$ are

$$R_{nl}(r) \propto e^{-r/na_0} \left(\frac{r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$$

where $L_q^p(x)$ are the associated Laguerre polynomials. In this problem we will work mostly with the $|1S\rangle = |1, 0, 0\rangle$, the $|2S\rangle = |2, 0, 0\rangle$ and $|2P\rangle = |2, 1, m\rangle$ states. Their normalized wave functions are

$$\begin{aligned} \psi_{1,0,0}(r, \theta, \varphi) &= \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0} \\ \psi_{2,0,0}(r, \theta, \varphi) &= \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0} \\ \psi_{2,1,0}(r, \theta, \varphi) &= \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \frac{r}{a_0} e^{-r/2a_0} \cos \theta \\ \psi_{2,1,\pm 1}(r, \theta, \varphi) &= \mp \left(\frac{1}{64\pi a_0^3}\right)^{1/2} \frac{r}{a_0} e^{-r/2a_0} \sin \theta e^{\pm i\varphi} \end{aligned} \tag{1}$$

1. Use commutation relations to show that due to rotational invariance the matrix elements of the perturbation \hat{W} obey the selection rule

$$\langle n', l', m' | \hat{W} | n, l, m \rangle = \delta_{l', l} \delta_{m', m} \langle n', l, m | \hat{W} | n, l, m \rangle$$

2. Use the potential given above to compute the following matrix elements: $\langle 1, 0, 0 | \hat{W} | 1, 0, 0 \rangle$, $\langle 2, 0, 0 | \hat{W} | 2, 0, 0 \rangle$, $\langle 2, 1, 0 | \hat{W} | 2, 1, 0 \rangle$, $\langle 2, 1, \pm 1 | \hat{W} | 2, 1, \pm 1 \rangle$, and $\langle 1, 0, 0 | \hat{W} | 2, 0, 0 \rangle$.

3. Use the matrix elements you computed above to find the first order shift in the energy of the ground state of the hydrogen atom.
4. Show that this perturbation lifts the 4-fold degeneracy of the $n = 2$ states $|2, 0, 0\rangle$ and $|2, 1, m\rangle$ states of hydrogen and give an expression for the energy splitting. What is the residual degeneracy? Can you generalize this result to other central potentials?