Physics 113 Spring 2009
Quantum Theory Seminar #11

Readings:

Zettili - Chapter - 9 (remaining sections)
Boccio - Chapter - 10 (remaining sections)

This week we continue our study of time-independent perturbation theory and also look at the variational method.

Presentations:

Wigner-Eckart Theorem (Do Proof) _Orion____
(Section 10.7.3)

Variational Method _Andrew K_
(Section 10.8)

Zettili Problems:

1. **Z9-21 Angular Momentum Perturbations (EVERYONE)**
2. **Z9-22 Mess with Matrices (EVERYONE)**
3. **Z9-27 Variational Method (Jean)**
4. **Z9-33 Variational Method (Jono)**

Boccio Problems:

1. Perturbed Oscillators(Ari)

(a) A particle of mass m is moving in the 3-dimensional harmonic oscillator potential

$$V(x,y,z) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2)$$

A weak perturbation is applied in the form of the function

$$\Delta V(x,y,z) = kxyz + \frac{k^2}{\hbar\omega} x^2 y^2 z^2$$

where k is a small constant.

Calculate the shift in the ground state energy to **second order in k.**

(b) Now consider the system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2\alpha}(1 - e^{-\alpha x^2})$$

(1) Calculate an approximate value for the ground state energy using first-order perturbation theory, perturbing the harmonic oscillator Hamiltonian

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

(2) Calculate an approximate value for the ground state energy using the variational method with a trial function $\psi = e^{-\beta x^2/2}$. Assume that $\alpha << m\omega/\hbar$

2. Helium from Hydrogen - 2 Methods(Dan)

(a) Using a simple hydrogenic wave function for each electron, calculate by perturbation theory the energy in the ground state of the He atom associated with the electron-electron Coulomb interaction. Use this result to estimate the ionization energy of Helium.
(b) Calculate the ionization energy by using the variational method with an effective charge λ in the hydrogenic wave function as the variational parameter.
(c) Compare (a) and (b) with the experimental ionization energy

$$E_{ion} = 1.807 E_0 \quad , \quad E_0 = \frac{\alpha^2 mc^2}{2} \quad , \quad \alpha = \text{fine structure constant}$$

You will need

$$\psi_{1s}(r) = \sqrt{\frac{\lambda^3}{\pi}} \exp(-\lambda r) \quad , \quad a_0 = \frac{\hbar^2}{me^2} \quad , \quad \iint d^3 r_1 d^3 r_2 \frac{e^{-\beta(r_1 + r_2)}}{|\vec{r}_1 - \vec{r}_2|} = \frac{20\pi^2}{\beta^5}$$

That last integral is very hard to evaluate from first principles.

3. Hydrogen atom + xy perturbation(Robert) - An electron moves in a Coulomb field centered at the origin of coordinates. The first excited state (n=2) is 4-fold degenerate. Consider what happens in the presence of a non-central perturbation

$$V_{pert} = f(r)xy$$

where $f(r)$ is some function only of r, which falls off rapidly as $r \to \infty$. To first order this perturbation splits the 4-fold degenerate level into several distinct levels (some might still be degenerate).

(a) How many levels are there?
(b) What is the degeneracy of each?

(c) Given the energy shift, call it ΔE, for one of the levels, what are the values of the shifts for all the others?

4. Rigid rotators in electric and magnetic fields(Kevin)

(a) Suppose that the Hamiltonian of a rigid rotator in a magnetic field is of the form

$$\hat{H} = A\hat{\vec{L}}^2 + B\hat{L}_z + C\hat{L}_y$$

Assuming that $A,B >> C$, use perturbation theory to lowest nonvanishing order to get approximate energy eigenvalues.

(b) Consider a rigid body with moment of inertia I, which is constrained to rotate in the xy-plane, and whose Hamiltonian is

$$\hat{H} = \frac{1}{2I}\hat{L}_z^2$$

Find the eigenfunctions and eigenvalues (zeroth order solution).

Assume the rotator has a fixed dipole moment $\vec{p}$ in the plane. An electric field $\vec{\varepsilon}$ is applied in the plane. Find the change in the energy levels to first and second order in the field.

5. Perturbation with 2 Spins(Karen) - Let $\vec{S}_1$ and $\vec{S}_2$ be the spin operators of two spin-1/2 particles. Then

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

is the spin operator for this two-particle system.

(a) Consider the Hamiltonian

$$\hat{H}_0 = \alpha(\hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2)/\hbar^2$$

Determine its eigenvalues and eigenvectors.

(b) Consider the perturbation $\hat{H}_1 = \lambda(\hat{S}_{1x} - \hat{S}_{2x})$. Calculate the eigenvalues in first-order perturbation theory.

Now consider a system with the unperturbed Hamiltonian

$$\hat{H}_0 = -A(\hat{S}_{1z} + \hat{S}_{2z})$$

with a perturbing Hamiltonian of the form

$$\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y})$$

(c) Calculate the eigenvalues and eigenvectors of H_0.

(d) Calculate the exact eigenvalues of $H_0 + H_1$.

(e) By means of perturbation theory, calculate the first- and the second-order shifts of the ground state energy of H_0, as a consequence of the perturbation H_1. Compare these results with those of (d).

Electric and Magnetic Fields as Perturbations

6. Spherical cavity with electric/magnetic fields(Jonah) - Consider a spinless particle of mass m and charge e confined in spherical cavity of radius R, that is, the potential energy is zero for r < R and infinite for r > R.

(a) What is the grounds state energy of this system?
(b) Suppose that a weak uniform magnetic field of strength B is switched on. Calculate the shift in the ground state energy.
(c) Suppose that, instead a weak uniform electric field of strength ε is switched on. Will the ground state energy increase or decrease? Write down, but do not attempt to evaluate, a formula for the shift in the ground state energy due to the electric field.
(d) If, instead, a very strong magnetic field of strength B is turned on, approximately what would be the ground state energy? **8**

7. Hydrogen in electric and magnetic fields(Sarah) - Consider the n=2 levels of a hydrogen-like atom. Neglect spins. Calculate to lowest order the energy splittings in the presence of both electric and magnetic fields $\vec{B} = B\hat{e}_z$, $\vec{\varepsilon} = \varepsilon\hat{e}_x$.

8. n=3 Stark effect in Hydrogen(Andrew Z) - Work out the Stark effect to lowest nonvanishing order for the n=3 level of the hydrogen atom. Obtain the energy shifts and the zeroth order eigenkets.

9.

FINAL #1

Perturbation of the n=3 level in Hydrogen - Spin-Orbit and Magnetic Field corrections(This is a big, messy problem which will tell me whether you know all aspects of time-independent perturbation theory - I expect all details to be carried out, however messy they are!) - In this problem we want to calculate the 1st-order correction to the n=3 unperturbed energy of the hydrogen atom due to spin-orbit interaction and magnetic field interaction for arbitrary strength of the magnetic field. We have $\hat{H} = \hat{H}_0 + \hat{H}_{so} + \hat{H}_m$ where

$$\hat{H}_0 = \frac{\vec{p}_{op}^{\,2}}{2m} + V(r) \quad , \quad V(r) = -e^2\left(\frac{1}{r}\right)$$

$$\hat{H}_{so} = \left[\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\right]\vec{S}_{op}\cdot\vec{L}_{op}$$

$$\hat{H}_m = \frac{\mu_B}{\hbar}(\vec{L}_{op} + 2\vec{S}_{op})\cdot\vec{B}$$

We have two possible choices for basis functions, namely,

$$\left|n\ell s m_\ell m_s\right\rangle \quad \text{or} \quad \left|n\ell s j m_j\right\rangle$$

The former are easy to write down as direct-product states

$$\left|n\ell s m_\ell m_s\right\rangle = R_{n\ell}(r)Y_\ell^{m_\ell}(\theta,\phi)\left|s,m_s\right\rangle$$

while the latter must be constructed from these direct-product states using addition of angular momentum methods.

The perturbation matrix is not diagonal in either basis.

The number of basis states is given by

$$\sum_{\ell=0}^{n-1=2}(2\ell+1)\times 2 = 10 + 6 + 2 = 18$$

All the 18 states are degenerate in zero-order. This means that we deal with an 18 x 18 matrix (mostly zeroes) in degenerate perturbation theory.

Using the direct-product states

(a) Calculate the nonzero matrix elements of the perturbation and arrange them in block-diagonal form.
(b) Diagonalize the blocks and determine the eigenvalues as functions of B.
(c) Look at the $B \to 0$ limit. Identify the spin-orbit levels. Characterize them by ($\ell s j$).
(d) Look at the large B limit. Identify the Paschen-Bach levels.
(e) For small B show the Zeeman splittings and identify the Lande g-factors.
(f) Plot the eigenvalues versus B.