QUANTUM MECHANICS B (PHY–5646)

HOMEWORK 19

(March 8, 2017)

Due on Tuesday, March 21, 2017

PROBLEM 55

The Hamiltonian for a particle moving in the presence of a one dimensional 'quadratic-plus-quartic' potential is given by the following expression:

$$\hat{H} = \frac{\hat{P}^2}{2} + \frac{\hat{X}^2}{2} + \lambda \hat{X}^4,$$

where the Hamiltonian has been written in terms of properly scaled variables. We have shown in class that to first order in λ the energy of the system is given by

$$E_n = \left(n + \frac{1}{2}\right) + \frac{3}{4}\lambda\big(2n^2 + 2n + 1\big).$$

(a) Compute the *ground-state* energy of the system correct up to second order in λ. That is, evaluate the value of the dimensionless constant κ in the following expression:

$$E_0 = \frac{1}{2} + \frac{3}{4}\lambda + \kappa\lambda^2.$$

Before you start you should already know whether κ is positive or negative. After you compute the value κ comment on whether you think that the perturbative series will converge.

(b) Using a variational wave-function of the form

$$\phi(x) = \frac{1}{(\pi c^2)^{1/4}} \exp(-x^2/2c^2),$$

where c is the variational parameter, provide an estimate of the ground-state energy of the full Hamiltonian as a function of λ. For 'small' values of λ compare your answer against the perturbative estimate obtained in part (a).

PROBLEM 56 – (Shankar 17.2.4)

An important result in atomic, condensed-matter, and nuclear physics is the *Thomas-Reiche-Kuhn* ("TRK") sum rule that states that:

$$M_1 \equiv \sum_{n'} \big(E_{n'} - E_n\big)\Big|\langle n'|\hat{X}|n\rangle\Big|^2 = \frac{\hbar^2}{2m},$$

where $|n\rangle$ and $|n'\rangle$ are exact eigenstates of a generic Hamiltonian given by

$$\hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{X}).$$

(a) Show that by eliminating the energy factor $\left(E_{n'} - E_n\right)$ in favor of $\hat{H}$, M_1 can be written as the expectation value in state $|n\rangle$ of a suitable "double commutator".

(b) Using this result, prove the TRK sum rule for the generic Hamiltonian given above. Note that this result holds *regardless* of the form of $\hat{V}$.

(c) Test the validity of the TRK sum rule in the particular case of the one-dimensional harmonic oscillator: $\hat{V}(\hat{X}) = \frac{1}{2}m\omega^2\hat{X}^2$.

PROBLEM 57

The interaction of the electron spin with the magnetic field of the proton gives rise to the following interaction energy known as the "*spin-orbit*" interaction:

$$\hat{H}_{\text{so}} = \left(\frac{e^2}{2m^2c^2}\right)\frac{1}{r^3}\,\mathbf{S}\cdot\mathbf{L}\,,$$

where m is the mass of the electron, and $\mathbf{S}$ and $\mathbf{L}$ are the spin and orbital angular momentum operators of the electron. In this problem you will calculate the first-order shift in the energy levels of the hydrogen atom due to the spin-orbit interaction.
Given that the Coulomb potential is spherically symmetric, we can write the eigenstates of the hydrogen atom in terms of the spherical harmonics: $|nlm_l\rangle$, where l and m_l are the quantum numbers associated with $\hat{L}^2$ and $\hat{L}_z$. Now we have to incorporate the intrinsic spin-1/2 nature of the electron. We can do so in two ways: (a) the direct product basis: $|nlm_lm_s\rangle$ or (b) the total angular momentum basis: $|nljm\rangle$.

(a) Show that the spin-orbit operator is *diagonal* in the total angular momentum basis. That is, show that

$$\mathbf{S}\cdot\mathbf{L}|nljm\rangle = C_{lj}|nljm\rangle\,.$$

Provide an expression for C_{lj} and note that it is independent of both n and m.

(b) Using *Kramer's rule*, one can evaluate the following matrix element in closed analytic form:

$$\left\langle nl\,\left|\frac{1}{r^3}\right|nl\right\rangle = \frac{2}{n^3l(l+1)(2l+1)a_0^3}\,,$$

where a_0 is the Bohr radius. Verify the validity of this expression for all the eigenstates with principal quantum numbers $n=1$ and $n=2$.

(c) Using the results obtained in parts (a) and (b), conclude that the first-order shift in the energy levels of the hydrogen atom due to the spin-orbit interaction may be written as follows:

$$E^{(1)}_{nlj} = \frac{\alpha^4mc^2}{2n^3}\left[\frac{j(j+1) - l(l+1) - 3/4}{l(l+1)(2l+1)}\right]\,.$$

Evaluate explicitly the first-order shift for all the eigenstates with principal quantum numbers $n = 1$, $n = 2$, and $n = 3$ — and compare it against the corresponding unperturbed value of the energy.