Quantum Mechanics

September 9, 2005

Work 4 of the 5 problems. Please put each problem solution on a separate sheet of paper and your name on each sheet.

Problem 1

(Kyle)
Take the spin Hamiltonian for the hydrogen atom in an external magnetic field B_0 in the z direction to be

$$H = \frac{2A}{\hbar^2}\mathbf{S_1} \cdot \mathbf{S_2} + \omega_\mathbf{0}\mathbf{S_{1z}}$$

where $\omega_0 = geB_0/2mc$, with m the mass of the electron. Determine the energies of this system. Examine your results in the limiting cases $A >> \hbar\omega_0$ and $A << \hbar\omega_0$ by expanding the energy eigenvalues in a Taylor series or binomial expansion through the first non-vanishing order.

Problem 2

Kiefer

In quantum mechanics, it is often assumed that the nucleus can be treated as a point particle. Is this a justifiable approach? In this problem, you will consider the effect of a finite size nucleus on the electronic ground state. As an example, consider a hydrogen-like atom resulting when an aluminum atom ($Z = 13; A = 27$) is stripped of all but one of its electrons.

a.) [3 points] Assuming that the nuclear charge is spread uniformly over a sphere of radius R, show that the potential energy of the electron is

$$V(r) = \begin{cases} \frac{Ze^2}{2R}\left(\frac{r^2}{R^2} - 3\right) & \text{for } r \leq R \\ -\frac{Ze^2}{r} & \text{for } r \geq R \end{cases}$$

b.) [1 point] Since we are treating a two-body problem, the question arises whether we should transform the problem from the coordinate system in which the nucleus represents the origin into the center of mass reference frame. Estimate the effect of neglecting the transformation to a moving reference frame.

c.) [5 points] Use first order perturbation theory to calculate the change of the electronic ground state energy; remember that the radius of the nucleus is much smaller than the Bohr radius of the electronic $1s$-state. (Hint: Treat the potential in the region $r < R$ as a perturbation).

d.) [1 point] Evaluate this difference using a radius of the aluminum nucleus of $R = 6.8 \cdot 10^{-5} a_B$ and compare it to the $1s$ energy level.

Note:

The $1s$ state of a hydrogen-like atom is given by:

$$\psi_{1s} = \frac{2}{\sqrt{4\pi}} \cdot \gamma^{3/2} \cdot \exp(-\gamma r)$$

with $\gamma = Z/a_B$ where a_B is the Bohr radius.

Problem 3

(Burkardt)
These are multiple choice questions. Do **NOT** show your work! Each correct checkmark counts as 1 point. Each incorrect checkmark counts as –0.5 point.

1. Consider a particle in a potential with an "ellipsoidal deformation", i.e. a Hamiltonian of the form
$$H = \frac{\vec{p}^2}{2M} + f(x^2 + y^2 + a \cdot z^2)$$
with $a \neq 1$. Check which of the following statements is true

    a. $\vec{L}^2$ is conserved ○
    b. L_z is conserved ○
    c. L_x is conserved ○
    d. $L_x + iL_y$ is conserved ○
    e. states with the same $\vec{L}^2$ but different L_z are degenerate ○
    f. there is a degeneracy between states with $l_z = m$ and $l_z = -m$ ○
    g. none of the above ○

2. Consider a particle in a central potential with a small perturbation $\propto L_y$
$$H = \frac{\vec{p}^2}{2M} + V(r) + \varepsilon L_y,$$
where $r = \sqrt{x^2 + y^2 + z^2}$. Since ε is supposed to be small the term $\propto \varepsilon$ can be treated in perturbation theory. Compare the ground state energy for nonzero but small ε with the one for $\varepsilon = 0$. Is $E_0(\varepsilon \neq 0) - E_0(\varepsilon = 0)$

    a. always positive ○
    b. always negative ○
    c. zero ○
    d. sign depends on details ○

3. Consider now a Hamiltonian of the form
$$H = \frac{\vec{p}^2}{2M} + V(r) + \varepsilon \cdot y.$$
Which of the following statements are true

    a. $\vec{L}^2$ is conserved ○
    b. L_x is conserved ○

c. L_y is conserved ○

d. L_z is conserved ○

e. $L_z + iL_x$ is conserved ○

f. For small ε, the ground state energy depends at most linearly on ε ○

g. For small ε, the ground state energy depends at most quadratically on ε ○

h. Since the ground state has even parity, its energy does not depend on ε ○

4. Decide if the following statements are true (T) or false (F)

   a. Only states with $l \geq 2$ can have a non-vanishing quadrupole moment $Q = \int d^3\mathbf{r}\,(3z^2 - r^2)\,|\psi(\vec{r})|^2$ T ○ F ○

   b. An eigenstate of a parity invariant Hamiltonian must be a parity eigenstate . T ○ F ○

   c. The ground state of a rotationally invariant single particle Hamiltonian $H = \frac{\vec{p}^2}{2m} + V(r)$ has always l=0 T ○ F ○

   d. The spatial part of a two-electron wavefunction (both electrons have spin $\uparrow$) can always be written in the form $\psi(\vec{r}_1, \vec{r}_2) = \phi_A(\vec{r}_1)\phi_B(\vec{r}_2) - \phi_B(\vec{r}_1)\phi_A(\vec{r}_2)$. T ○ F ○

   e. Every Hamiltonian $H = \frac{1}{2m}\vec{p}^2 + V(\vec{r})$ that satisfies $V(\vec{r}) < 0$ for all $\vec{r}$ has at least one negative energy eigenvalue. T ○ F ○

Problem 4

(Papavassiliou)
A particle of mass m moves in a one-dimensional potential of the form

$$V(x) = -\frac{\hbar^2 C}{m}\delta(x^2 - a^2),$$

where $C > 0$.

(a) Calculate the bound states of this system, for different values of C; sketch the potential and the solutions that you found (5 points)

(b) What is the parity of the various solutions? (2 points)

(c) Explain each solution as a superposition of two functions (3 points)

Problem 5

(Urquidi)
Let a particle of mass m in one dimension be governed by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + a|x|$$

a.) Use the normalized trial wave function

$$\phi_b(x) = \left(\frac{2b}{\pi}\right)^{1/4} \exp(-bx^2)$$

to estimate the energy of the ground state of this system using the variational principle, by evaluating the expectation value of the energy as a function of b.

b.) Optimize b to obtain the best approximation to the ground state energy of this system in the space of trial wave functions of the form ϕ_b given above. The numerically calculated exact ground state energy is

$$0.808616\hbar^{2/3}m^{-1/3}a^{2/3}$$

What is the percent error in your variational value?