Candidacy Exam Fall 2005

Quantum Mechanics

1. (30 pts.) In a quantum-electronics laboratory, a molecular-sized device was developed with the properties:

a) it had only one degree of freedom characterized by two states: $|\text{ON}\rangle$ and $|\text{OFF}\rangle$

b) it had the Hamiltonian matrix elements $\langle\text{OFF}|\text{H}|\text{ON}\rangle = \langle\text{ON}|\text{H}|\text{OFF}\rangle = \lambda/d$, where λ is a constant and d is a distance representing the proximity of an external probe, and the diagonal elements of H could be taken as zero,

c) any change between $|\text{ON}\rangle$ and $|\text{OFF}\rangle$ could be electronically and visually monitored.

An engineer suggested the tentative name "quantum pixel" and observed that the frequency f of ON/OFF oscillation varied with d.

You, as the laboratory physicist, are requested to derive the formula for $f(d)$.

2. (35 pts.) The Hamiltonian for the Helium atom is $\text{H} = \text{h}_1 + \text{h}_2 + \text{e}^2/\text{r}_{12}$, where $r_{12} = |\vec{r}_1 - \vec{r}_2|$, the nucleus is considered to be infinitely heavy, $\text{h}_1 = \text{p}_1^2/2\text{m} - \text{Ze}^2/\text{r}_1$, and similarly for h_2 and the nuclear charge is $\text{Z} = 2$. The ground state solution of $\text{h}\,|\phi_0\rangle = \varepsilon_0|\phi_0\rangle$ is $\varepsilon_0 = -\text{Z}^2$, where

$$\phi_0(\vec{r}) = \left[\frac{Z^3}{\pi a_0^3}\right]^{\frac{1}{2}} e^{-Zr/a_0},$$

energy is measured in units of $e^2/2a_0 = 13.6\text{eV}$, a_0 is the Bohr radius, and ϕ_0 is normalized. By experiment, the Helium ground state energy is $E_0 = -5.808$.

a) (10 pts.) Find an approximate E_0 and the corresponding expression for the normalized wave function $\Psi(Z, \vec{r}_1, \vec{r}_2)$ when the repulsion between electrons is ignored. You must include the spin degree of freedom in the wave function, and comment on your choice of total spin quantum number.

b) (10 pts.) Find an improved approximation to E_0 by including the interaction between electrons to first order.

$$\left[\text{ you may use } \iint d^3r\, d^3r' \frac{e^{-2b(r+r')}}{|\vec{r} - \vec{r}'|} = \frac{5}{8}\frac{\pi^2}{b^5} \right]$$

c) (15 pts.) Use the variational principle to obtain another estimate of E_0.
In particular, minimize $\langle H \rangle$ with respect to Z' where
$\langle H \rangle = \langle \Psi(Z')|H(Z=2)|\Psi(Z')\rangle = 2Z'(Z' - 27/8)\ e^2/2a_0$, and $\Psi(Z')$ is the wave function in a) except that Z has been converted to the variational parameter Z'. What is the variational estimate of E_0? What new physics is thereby included compared to b)?

3. (35 pts) A particle moves in three dimensions governed by $H = p^2/2m + V(r)$, and V is real.

a) (10 pts) If L_i is a rectangular component of orbital angular momentum, derive the result for $[L_1, L_2]$ by using only the result for $[p_i, r_j]$, showing clearly all the steps.

b) (15 pts) Prove that $[L_i, H] = 0$, showing clearly all steps.

c) (10 pts) If a time-independent Hermitian operator commutes with H, the corresponding observable is called a constant of the motion. Derive this result mathematically.