PHY306 Advanced Quantum Mechanics Jan-Apr 2024: Assignment 7

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1. Prove the corollary to the variational principle that if $\langle\psi|\psi_g\rangle = 0$, then $\langle H\rangle \geq E_f$ where E_f is the energy of the first excited state. What kinds of trial functions should one use in order to get an upper bound on the first excited state?

2. Find the best bound on the first excited state of the one-dimensional harmonic oscillator using the trial function $\psi(x) = Axe^{-bx^2}$

3. Use the variational principle to prove that first-order nondegenerate perturbation theory always overestimates (or never underestimates) the ground state energy. Use this to confirm that second-order correction to the ground state is always negative.

4. Apply the variational principle to hydrogen molecule ion which has a single electron in the Coulomb field of two protons. Use a trial wave function $\psi(x) = A[\psi_g(r_1) - \psi_g(r_2)]$. Express the total energy of the system in units of $-E_1$ and as a function of $x \equiv R/a_0$ where $E_1 = -13.6\text{eV}$ is the ground-state energy of atomic hydrogen, a_0 is the Bohr radius and R is the distance between the two protons. Find the total energy of the system $F(x)$, and construct the graph $F(x)$ versus x and show that there is no evidence of bonding.

5. Consider a two-level system with unperturbed Hamiltonian H_0 and eigenstates ψ_a, ψ_b and $E_a < E_b$. Turn on a perturbation H' with diagonal elements 0 and off-diagonal elements h. Estimate the ground-state energy of the perturbed system using the variational principle with a trial wavefunction $\psi = \cos\phi\psi_a + \sin\phi\psi_b$, where ϕ is an adjustable parameter. Now consider an electron at rest in a uniform magnetic field $B = B_z\hat{k}$ with the Hamiltonian $H_0 = \frac{eB_z}{m}S_z$ with eigen spin wave functions χ_a, χ_b (which are eigenstates of S_z) and energies E_a, E_b. Turn on a perturbation which is a uniform field in the x direction with the Hamiltonian $H' = \frac{eB_x}{m}S_x$. Find the matrix elements of H' and what is h in this case? Use the above more general results to find the variational bound on the ground-state energy.

6. Consider a helium-like system in which Coulomb forces are replaced by Hooke's law forces

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}m\omega^2(r_1^2 + r_2^2) - \frac{\lambda}{4}m\omega^2|r_1 - r_2|^2$$

Make a change of variable from r_1, r_2 to $u = \frac{1}{\sqrt{2}}(r_1+r_2), v = \frac{1}{\sqrt{2}}(r_1-r_2)$ and show that the Hamiltonian turns into two independent 3D harmonic oscillators. Find the exact ground state energy for this system. Apply the variational method to the Hamiltonian in its original form (without change of variables) but ignore shielding. Compare this result with the exact ground state energy.

7. Consider the H^- ion (has two electrons but nuclear charge $Z = 1$). Use a trial wave function of the form $\psi(r_1, r_2) = A[\psi_1(r_1)\psi_2(r_2) + \psi_2(r_1)\psi_1(r_2)]$ where $\psi_1(r) = \sqrt{\frac{Z_1^3}{\pi a_0^3}}e^{-Z_1 r/a_0}$ and $\psi_2(r) = \sqrt{\frac{Z_2^3}{\pi a_0^3}}e^{-Z_2 r/a_0}$. Find $\langle H \rangle$ in terms of parameters x, y by choosing the adjustable parameters Z_1, Z_2 such that $x = Z_1 + Z_2$ and $y = 2\sqrt{Z_1 Z_2}$ and show that you can get $\langle H \rangle$ less than -13.6eV.