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FY2045 Problem set 11 fall 2023

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Problem 1

The Hamiltonian of the hydrogen atom moving in a Coulomb potential is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{k}{r}, \tag{1}$$

where $k = \frac{e^2}{4\pi\epsilon 0}$. The normalized ground-state wavefunction of the hydrogen atom is

$$\psi_0(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}, \tag{2}$$

where $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ is the Bohr radius. In this problem, we shall apply the variational principle to the hydrogen atom in the ground state. A trail wavefunction is

$$\psi(r) = A\sqrt{r}e^{-\alpha r}, \tag{3}$$

where α is a real positive variational parameter and A is a normalization constant.

a) Determine the normalization constant A.

b) Calculate the expectation value of the kinetic energy T, $\langle T\rangle = \langle\psi|T|\psi\rangle$, using the trial wavefunction.

c) Calculate the expectation value of the potential energy V, $\langle V \rangle = \langle \psi | V | \psi \rangle$, using the trial wavefunction.

d) Find the value of α that minimizes the expectation value of the total energy, $\langle E \rangle = \langle T \rangle + \langle V \rangle$, and the energy for this value. Compare the result with the exact value $E_0 = -\frac{\hbar^2}{2ma_0^2}$.

Problem 2

A particle moves within the potential

$$V(x) = \begin{cases} \frac{1}{2} m\omega x^2, & x > 0, \\ \infty, & x \leq 0. \end{cases} \tag{4}$$

a) Verify (without calculations!) what the exact ground state energy is $E_0 = \frac{3}{2}\hbar\omega$.

b) Use the variational method and the trial function

$$\psi(x) = \begin{cases} cxe^{-\alpha x}, & x > 0, \\ 0, & x \leq 0, \end{cases} \tag{5}$$

to estimate the ground state energy. How good is the estimate?