Physics 5403

Problem Set 7 – Due October 30, 2009

Problem 1

The Hamiltonian of the Helium atom is

$$\begin{aligned} H &= H_0 + H_1 \\ H_0 &= -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 - \frac{\hbar^2}{2m}\vec{\nabla}_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} \\ H_1 &= \frac{e^2}{r_{12}} \end{aligned}$$

where $Z = 2$, m is the mass of the electron; $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the two electrons, $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$, and $r_i = |\vec{r}_i|, i = 1, 2$.

Let us adopt a trial function of the form

$$\psi_0(r_1, r_2) = \frac{Z^3}{\pi a_0^3} e^{-Z(r_1+r_2)/a_0}$$

where we choose Z to be the variational parameter which would determine the effective charge of the nucleus.

(a). Show that

$$\int d^3r_1 d^3r_2 \; \psi_0^*(r_1, r_2) \left(-\frac{\hbar^2}{2m}\vec{\nabla}_1^2 \right) \psi_0(r_1, r_2) = Z^2 \left(\frac{me^4}{2\hbar^2} \right) .$$

(b). Show that

$$\int d^3r_1 d^3r_2 \; \psi_0^*(r_1, r_2) \left(-\frac{2e^2}{r_1} \right) \psi_0(r_1, r_2) = \frac{-2Ze^2}{a_0} = -4Z \left(\frac{me^4}{2\hbar^2} \right) .$$

(c). Show that

$$\int d^3r_1 d^3r_2 \; \psi_0^*(r_1, r_2) \left(\frac{e^2}{r_{12}} \right) \psi_0(r_1, r_2) = \frac{5Z}{4} \left(\frac{me^4}{2\hbar^2} \right) .$$

This integral becomes simpler if we scale both coordinates

$$\begin{aligned} \vec{r}_1 &= \frac{a_0}{2Z}\vec{s}_1 \\ \vec{r}_2 &= \frac{a_0}{2Z}\vec{s}_2 \, . \end{aligned}$$

(d). Apply the variational method to find Z_{min}, and calculate the ground state energy ($E_0 = \langle H \rangle_{\text{min}}$) of the Helium atom with $H = H_0 + H_1$,

Problem 2

A particle is subject to the linear potential $V(x) = mgx$ but with an infinite potential barrier at $x = 0$, namely

$$V(x) = \begin{cases} mgx & \text{for } x > 0, \text{ and} \\ \infty & \text{for } x \leq 0 \,. \end{cases}$$

Let us choose

$$\psi_\alpha(x) = xe^{-\alpha x}, \qquad \alpha > 0$$

as a trial wave function for the ground state.

(a) Find $\langle \psi_\alpha | \psi_\alpha \rangle$.

(b) Find the expectation value of the Hamiltonian $\langle H \rangle$.

(c) Determine the best bound on the ground state energy of this system using the variational method and the trial wave function given above.

Problem 3

Let us consider a Hydrogen atom in its ground state ($|\alpha\rangle = |0\rangle$) and it is subject to an oscillating electric field. Thus

$$\begin{aligned} H_1(t) &= -2e\vec{r} \cdot \vec{\mathcal{E}} \sin(\omega t) \\ &= 2\hat{V} \sin(\omega t) \\ \hat{V} &= -e\vec{r} \cdot \vec{\mathcal{E}} \,. \end{aligned}$$

This is not a realistic system. However, the idea is that a travelling electromagnetic wave can have such high frequencies associated with it and hence can cause the Hydrogen atom to be ionized. Apply the perturbation theory for transition from a discrete level to continuum and find the differential ionizability ($dW/d\Omega$) into the solid angle Ω for the electron in the final state ($|\beta\rangle = |k\rangle$) with momentum $\vec{k}$.