## NANO 705 Homework 3 Due: F-2/28, 10:00 AM

Show all work. Use additional sheets.

The spherical wave function

$$\phi(r) = \frac{1}{\sqrt{2\pi R}} \cdot \frac{\mathrm{e}^{-r/R}}{r}$$

describes an electron in a bound state outside a very narrow, deep potential well, where  $\hat{H} = \hat{K} = \hat{p}^2/2m$ .

1) Find an expression for its kinetic energy K. [Hint: use  $\hat{K}_r = -(\hbar^2/2m)\nabla_r^2$ , where  $\nabla_r^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r$ .]

2) Find an expression for the radial electron density  $\sigma(r) = 4\pi r^2 |\phi(r)|^2$ .

3) Assume other electrons are in the well and the electron-electron energy is

$$U_{ee}(r) = \frac{q^2}{6\pi\varepsilon_0 R} \cdot \left(\frac{a_0}{R}\right)^2 \cdot e^{-2r/R}$$

where

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{mq^2} = 0.053 \text{ nm}$$

Find an expression for the expectation value of the  $U_{ee}$  using

$$U_{ee} = \int_{r=0}^{\infty} dr \cdot \sigma(r) \cdot U_{ee}(r)$$

4) Find the value  $R = R_{best}$  that mimizes the total energy  $E = K + U_{ee}$ . Express  $R_{best}$  as a constant times  $a_0$ . 5) Find the minimum energy  $E_{best} = E|_{R=R_{best}}$ . Express  $E_{best}$  in rydbergs, where

$$1 \text{ Ryd} = \frac{\hbar^2}{2m{a_0}^2} = 13.6 \text{ eV}$$