PHY140Y

Spring Term – Week 9 Discussion Solutions

15 March, 1999

1. (a) The boundary conditions on the wave function are that the wave function and its derivative with respect to x are both continuous. By direct substitution, one can see that to within rounding errors this is true for the given wave function.

   (b) We calculate the probability of the particle being outside the well by squaring the wave function in that region and integrating the resulting probability density. Since the problem has symmetry in x, we just have to do one integral: Let $k = 7.60/L$. Then

$$\begin{aligned} P_{out} &= 2\int_{L/2}^{\infty} |\psi(x)|^2\,dx && (1)\\ &= 2\int_{L/2}^{\infty} \frac{1}{L}e^{-2kx}\,dx && (2)\\ &= -\frac{2}{2kL}\left[e^{-2kx}\right]_{L/2}^{\infty} && (3)\\ &= \frac{1}{kL}\,e^{-kL} && (4)\\ &= \frac{1}{7.60}e^{-7.60} = 6.6\times 10^{-5}. && (5) \end{aligned}$$

   (c) The average distance the particle is outside the square well is given by what we call the "expectation value" of x when the particle is in the ground state. It is calculated by taking the weighted mean of x when the particle is out of the well, ie. by weighting each value of x with the probability of finding the particle outside the box, now normalized assuming that the probability of finding the particle outside the box is unity. This is mathematically

$$\begin{aligned} <x> &= \int_{L/2}^{\infty} x\,|\psi(x)|^2\,dx/(P_{out}/2) && (6)\\ &= \int_{L/2}^{\infty} \frac{x}{L}e^{-2kx}\,dx/(P_{out}/2) && (7)\\ &= -\frac{1}{2Lk^2}\left[e^{-2kx}\right]_{L/2}^{\infty}/(P_{out}/2) && (8)\\ &= \frac{L}{2(7.60)^2}\,e^{-kL}/(P_{out}/2) && (9)\\ &= (4.33\times 10^{-6})\,L/(P_{out}/2) = 1.32\ \text{Å}. && (10) \end{aligned}$$

   So it doesn't stray too far. Why?

   (d) We can use the Heisenberg uncertainly relationship, assuming that $\Delta x \simeq L$, to get

$$\begin{aligned} \Delta p_x &\geq \frac{\hbar}{\Delta x} && (11)\\ &= \frac{\hbar}{L} = \frac{(1.055\times 10^{-34})}{(10^{-9})} = 1.1\times 10^{-25}\ \text{kg m/s}. && (12) \end{aligned}$$

2. This calculation is identical to the one performed in the text on Pg 1092, except that we substitute $10a_\circ$ for the limit of integration. The probability is

$$P(r > 10a_\circ) \quad = \quad 5e^{-20} = 1.0 \times 10^{-8}. \tag{13}$$

3. Even this is optimistic since once the electrons starts to range out to those radii, it can eventually feel the effect of neighbouring nuclei and be possible stripped off.