Answers to HW #1

1. $\psi = \varphi_1 + \varphi_2 = e^{-ax^2} + xe^{-ax^2}$

a) Normalize ψ.

$$\langle \varphi_1 + \varphi_2 | \varphi_1 + \varphi_2 \rangle = \langle \varphi_1 | \varphi_1 \rangle + \langle \varphi_2 | \varphi_2 \rangle + \underbrace{2\langle \varphi_1 | \varphi_2 \rangle}_{\phi}$$

$$\langle \varphi_1 | \varphi_1 \rangle = \sqrt{\frac{\pi}{2a}}$$

$$\langle \varphi_2 | \varphi_2 \rangle = \sqrt{\frac{\pi}{2}} \frac{1}{4a^{3/2}}$$

$$\psi = \frac{e^{-ax^2}(1+x)}{\sqrt{\sqrt{\frac{\pi}{2a}}\left(1+\frac{1}{4a}\right)}}$$

b) what is the probability of the particle being between -1 and 1?

$$\int_{-1}^{1} (\varphi_1+\varphi_2)^2 dx \Big/ \int_{-\infty}^{\infty} (\varphi_1+\varphi_2)^2 dx$$

$$= \left[\operatorname{erf}(\sqrt{2a}) - \frac{e^{-2a}}{2a\left(\sqrt{\frac{\pi}{2a}}\right)\left(1+\frac{1}{4a}\right)}\right]$$

c) $\langle \varphi_1 | \varphi_2 \rangle = 0$ since it is an integral over an odd function

2. $V=\infty \;|\; V=0$, $x=a$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

$$\psi(a) = Ae^{ika} + Be^{-ika} = 0$$

$$\Rightarrow B = -Ae^{2ika}$$

$$\psi(x) = A\left(e^{ikx} - e^{2ika}e^{-ikx}\right)$$

$$= Ae^{ika}\left(e^{ik(x-a)} - e^{-ik(x-a)}\right)$$

$$= 2iAe^{ika}\sin k(x-a)$$

$E = \frac{\hbar^2 k^2}{2m}$ where k is any positive real number.

3. What is the ZPE of an election in a box with L= 10 Bohr.

$$E = \frac{\pi^2}{2(1)(100)} = 0.0493 \text{ a.u.}$$

$\rightarrow 1.34$ eV