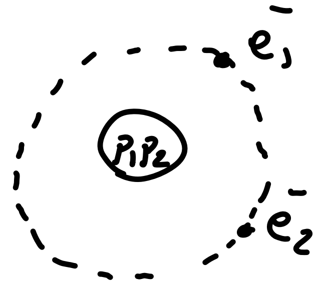
HW2

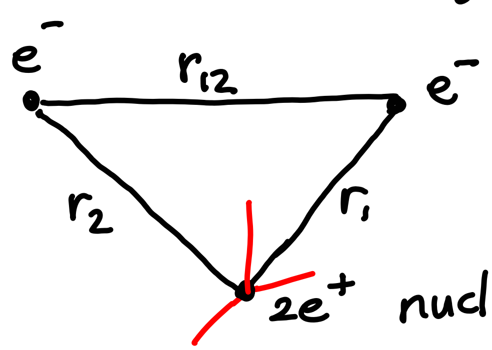
Note Title 2/4/2008

Problem 1: Hamiltonian for Helium atom?



Solution:

For the complete Hamiltonian, one has to consider the nuclear force between the protons too - we will this and take the nucleus as a single charge of +2e



nucleus at origin

$$\hat{H} = T_{e_1} + T_{e_2} + T_p + V_{e_1 e_2} + V_{e_1 p} + V_{e_2 p}$$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2_{r_1} - \frac{\hbar^2}{2m_e}\nabla^2_{r_2} + \frac{(-e)(2e)}{4\pi\epsilon_0 r_1} + \frac{(-e)(2e)}{4\pi\epsilon_0 r_2}$$

$$+ \frac{(-e)(-e)}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$$

$$= -\frac{\hbar^2}{2m_e}\left(\nabla^2_{r_1} + \nabla^2_{r_2}\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)$$

Problem 2   Levi, prolem 2.4

ⓐ $$\langle x\rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2 dx$$

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} x\,|\psi(x,t)|^2 dx = \int_{-\infty}^{\infty} x \underbrace{\frac{\partial}{\partial t}|\psi(x,t)|^2}\, dx$$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{\partial}{\partial t}(\psi^*\psi) = \psi \underbrace{\frac{\partial \psi^*}{\partial t}}_{\frac{1}{-i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}+V\psi^*\right)} + \psi^* \underbrace{\frac{\partial \psi}{\partial t}}_{\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi\right)}$$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = -\frac{i\hbar}{2m}\psi\frac{\partial^2\psi^*}{\partial x^2} + \cancel{\frac{i}{\hbar}V\psi\psi^*} + \frac{i\hbar}{2m}\psi^*\frac{\partial^2\psi}{\partial x^2} - \cancel{\frac{i}{\hbar}V\psi^*\psi}$$

$$= \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2} + \frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x} - \frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}\right)$$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

So we have:

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)dx$$

Since $\langle p\rangle = m\langle v\rangle = m\dfrac{d\langle x\rangle}{dt} \Rightarrow$

$$\langle P\rangle = \frac{i\hbar}{2}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx$$

(b) Integrate by part:

$$\int_{-\infty}^{\infty} UV'\,dx = [UV]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} U'V\,dx$$

Assume $U = x$ and $V' = \frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right) \Rightarrow$

$$\langle p\rangle = \frac{i\hbar}{2}\left(\underbrace{\left[x\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)\right]_{-\infty}^{\infty}}_{=0 \text{ as } \psi(\infty)=0} - \int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx\right)$$

$$= \frac{i\hbar}{2}\left(0 - \int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx\right)$$

$$= \frac{-i\hbar}{2}\int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx$$

Integrate by part again assuming $U = \psi$, $V' = \frac{\partial\psi^*}{\partial x} \Rightarrow$

$$\langle p\rangle = \frac{-i\hbar}{2}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x} + \underbrace{\frac{i\hbar}{2}\int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial x}\psi\,dx}_{\text{integrate by part}}$$

$$= \frac{-i\hbar}{2}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x} + \frac{i\hbar}{2}\left(\underbrace{[\psi^*\psi]_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}\,dx\right)$$

$$= -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}$$

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi^*\underbrace{\left(-i\hbar\frac{\partial}{\partial x}\right)}_{\hat{p}\ \text{momentum operator}}\psi$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

Problem 3 Levi 2-11

Start with $\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\psi(x,t)|^2 dx$

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{\partial}{\partial t}(\psi^*\psi) = \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}$$

Substitute $\frac{\partial\psi}{\partial t}$ & $\frac{\partial\psi^*}{\partial t}$ from Schrod. equation as in Prob-2 $\Rightarrow$

$$= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

Evaluating the integral:

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi|^2 dx = \frac{i\hbar}{2m}\left[\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right]_{-\infty}^{\infty} = 0$$

bcause $\Psi\Big|_{x \to \pm\infty} = 0$

Hence, if Ψ is normalized at a time, it is normalized for all time, because it doesn't change with time.