436(5): Expectation Values of the Schroedinger Equation

Consider the Schroedinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial r^2} + U(r)\psi = i\hbar\frac{\partial \psi}{\partial t}. \quad -(1)$$

using the separation of variables:

$$\psi = \psi_1(r)\psi_2(t) \quad -(2)$$

eq. (1) divides into:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_1}{\partial r^2} + U(r)\psi_1 = E\psi_1 \quad -(3)$$

and

$$i\hbar\frac{\partial \psi_2}{\partial t} = E\psi_2 \quad -(4)$$

Eq. (4) has the solution:

$$\psi_2(t) = \exp\left(-\frac{iEt}{\hbar}\right) \quad -(5)$$

The expectation value of energy is:

$$\langle E \rangle = \int \psi^* E \psi \, d\tau \quad -(6)$$

$$= \int \psi_1^*(r)\psi_2^*(t) E \psi_1(r)\psi_2(t) \, d\tau$$

From eq. (5):

$$\psi_2^*(t)\psi_2(t) = 1 \quad -(7)$$

so $\psi_2^*(t)$ is the complex conjugate of $\psi_2(t)$.

From eq. (3):

2)

$$\langle E \rangle = -\frac{\hbar^2}{2m}\int \psi_1^* \frac{\partial^2 \psi_1}{\partial r^2}\, d\tau + \int \psi_1^* U(r) \psi_1 \, d\tau$$

$$= \int \psi_1^* E \psi_1 \, d\tau \qquad -(8)$$

From eq. (4):

$$\langle E \rangle = i\hbar \int \psi_2^* \frac{\partial \psi_2}{\partial t}\, d\tau = \int \psi_2^* E \psi_2 \, d\tau \qquad -(9)$$

In m space:

$$\psi_2(t) = \exp\left(-\frac{iE}{\hbar} m^{1/2}(r)\, t \right) \qquad -(10)$$

so

$$\frac{\partial \psi_2}{\partial t} = -i\frac{E}{\hbar} m^{1/2}(r) \psi_2 \qquad -(11)$$

and

$$\langle E \rangle = E \int \psi_2^* m^{1/2}(r) \psi_2 \, d\tau \qquad -(12)$$

$$= E \int m^{1/2}(r)\, d\tau$$

In m space, eq. (8) becomes:

$$\langle E \rangle = -\frac{\hbar^2}{2m}\int \psi_1^*\left(\frac{r}{m(r)^{1/2}}\right) \frac{\partial^2}{\partial r^2}\left(\psi_1\left(\frac{r}{m(r)^{1/2}}\right)\right) d\tau$$

$$+ \int \psi_1^*\left(\frac{r}{m(r)^{1/2}}\right) U\left(\frac{r}{m(r)^{1/2}}\right) \psi_1\left(\frac{r}{m(r)^{1/2}}\right) d\tau$$

$$-(13)$$

) The expectation values from eqs. (12) and (13) must be the same, so the right hand side of eq. (13) is equal to:

$$\langle E \rangle = E \int m^{1/2}(r)\, d\tau \quad -(14)$$

So:

$$E = \frac{1}{\int m^{1/2}(r)\, d\tau} \left[-\frac{\hbar^2}{2m} \int \phi_1^*\left(\frac{r}{m(r)^{1/2}}\right) \frac{\partial^2}{\partial r^2}\left(\phi_1\left(\frac{r}{m(r)^{1/2}}\right)\right) d\tau + \int \phi_1^*\left(\frac{r}{m(r)^{1/2}}\right) U\left(\frac{r}{m(r)^{1/2}}\right) \phi_1\left(\frac{r}{m(r)^{1/2}}\right) d\tau \right] \quad -(15)$$
