427(2): Comparison of Hamilton Jacobi and Schroedinger Equations

Consider the classical hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \quad -(1)$$

for the interaction of an electron and proton. Here p is the classical momentum of the electron, m its mass, e the charge on the proton, $-e$ the charge on the electron, ϵ_0 the vacuum permittivity and r the distance between the electron and proton.

The Hamilton Jacobi equation corresponding to eq. (1) can be obtained using:

$$p^2 = p_r^2 + \frac{p_\phi^2}{r^2} \quad -(2)$$

in the notation of immediately preceding notes and papers. It is

$$\frac{1}{2m}\left(\frac{\partial S_r}{\partial r}\right)^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{L^2}{2mr^2} = E \quad -(3)$$

where

$$L = \frac{\partial S_\phi}{\partial \phi} \quad -(4)$$

is a constant of motion:

$$\frac{dL}{dt} = 0 \quad -(5)$$

and is the total angular momentum. The total action is

$$S = S_r + S_\phi \quad -(6)$$

The functions S_r and S_ϕ can be found by integrating Eqs. (3) and (4).

Schroedinger quantization of eq. (1) is defined by:

2)

$$\underline{\hat{p}} = -i\hbar\underline{\nabla} \quad -(7)$$

i.e.:

$$\underline{\hat{p}}\,\psi = -i\hbar\underline{\nabla}\psi \quad -(8)$$

and

$$\hat{p}^2\psi = -\hbar^2\nabla^2\psi \quad -(9)$$

where ψ is the wave function. The latter is factorized into:

$$\psi = R(r)\,Y(\theta,\phi) \quad -(10)$$

where Y are the spherical harmonics and $R(r)$ the radial wave functions.

Define

$$\underline{\hat{P}}(r) = r\hat{R}(r) \quad -(11)$$

and it follows that:

$$-\frac{\hbar^2}{2m}\frac{d^2 P}{dr^2} - \left(\frac{e^2}{4\pi\epsilon_0 r} - \frac{l(l+1)\hbar^2}{2mr^2}\right)\underline{P} = E\underline{P} \quad -(12)$$

in which the angular momentum is quantized as:

$$\hat{L}^2\psi = l(l+1)\hbar^2\psi \quad -(13)$$

and

$$\hat{L}\psi = m\hbar\psi \quad -(14)$$

where

$$m = l, l-1, \ldots, -l \quad -(15)$$

It follows that:

$$L = \langle\hat{L}\rangle = m\hbar\int\psi^*\psi\,d\tau = m\hbar \quad -(16)$$

so

$$\boxed{\frac{\partial S_\phi}{\partial\phi} = m\hbar} \quad -(17)$$

3) Similarly:
$$\boxed{\left(\frac{\partial S_\phi}{\partial \phi}\right)^2 = l(l+1)\hbar^2} \quad -(18)$$

From eqs. (3) and (12),
$$p_r = \langle \hat{p}_r \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial r} d\tau \quad -(19)$$

so
$$\frac{\partial S_r}{\partial r} = -i\hbar \int \psi^* \frac{\partial \psi}{\partial r} d\tau \quad -(20)$$

Similarly:
$$p_r^2 = \left(\frac{\partial S_r}{\partial r}\right)^2 = -\hbar^2 \int \psi^* \frac{\partial^2 \psi}{\partial r^2} d\tau \quad -(21)$$

The classical expectation values can be found from eq. (3):
$$\frac{1}{2m}\left(\frac{\partial S_r}{\partial r}\right)^2 - \frac{e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2mr^2} = E \quad -(22)$$

For the hydrogen atom the total energy levels are
$$E_n = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(23)$$

where n is the principal quantum number. Therefore $\partial S_r/\partial r$ is quantized in terms of l and n.

Defining:
$$S = S_r + S_\phi \quad -(24)$$

the Schroedinger equation:
$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi \quad -(25)$$

becomes the Hamilton Jacobi equation:

4)

$$\frac{1}{2m}\left(\frac{\partial S}{\partial r}\right)^2 - \frac{e^2}{4\pi\epsilon_0 r} = E \quad -(26)$$

using

$$\left(\frac{\partial S}{\partial r}\right)^2 \psi = -\hbar^2 \nabla^2 \psi \quad -(27)$$

So

$$\boxed{\left(\frac{\partial S}{\partial r}\right)^2 = \left\langle \left(\frac{\partial S}{\partial r}\right)^2 \right\rangle = -\hbar^2 \int \psi^* \nabla^2 \psi \, d\tau} \quad -(28)$$

where

$$\psi = R(r)\, Y(\theta, \phi) \quad -(29)$$

The quantized actions S, S_r and S_ϕ may be computed from these equations.

We are now ready to consider quantization in special relativity and in theory