Hamiltonians & Quantum Mechanics

In classical mechanics, the Hamiltonian is:

$$H(x,p) = \underset{\text{kinetic energy}}{\frac{p^2}{2m}} + \underset{\text{potential energy}}{U(x)} = E \leftarrow \text{total energy, a constant.}$$

we obtain eqns of motion via:

$$\dot{x} = \frac{\partial H}{\partial p} \quad \& \quad \dot{p} = -\frac{\partial H}{\partial x}$$

$$\dot{x} = p/m \Rightarrow p = m\dot{x} \qquad \dot{p} = -\frac{dU}{dx} \Rightarrow m\ddot{x} = -\frac{dU}{dx} \ \checkmark$$

One can "generate" Schrödinger's eqn from the classical Hamiltonian by taking $p \to \frac{\hbar}{i}\frac{\partial}{\partial x}$, & acting on $\psi(x)$:

$$E = p^2/2m + U(x) \longrightarrow E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x)$$

which, together w/ b.c. is the eigenvalue problem that determines the measurable values of the particle's energy.

Unlike the classical H, for which the eqns of motion are the fundamental tool for quantitative prediction, in QM, all you get is Schrödinger's eqn.

? Classically $U(x) \to U(x) + \underset{\text{const.}}{U_0}$ does nothing to the eqns of motion.

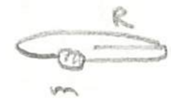
In QM: $U(x) \to U(x) + U_0$ shows up immediately

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (U(x)+U_0)\psi(x) = E\psi(x)$$

is this okay ?

=

Bead on a Wire (QM)



a mass m is constrained to move on a ring of radius R.

Schrödinger's eqn. is: $-\frac{\hbar^2}{2m}\frac{1}{R^2}\frac{d^2\psi(\phi)}{d\phi^2} = E\psi(\phi)$

w/ b.c. $\psi(\phi + 2\pi) = \psi(\phi)$.

solve $\frac{d^2\psi}{d\phi^2} = -\frac{2mR^2}{\hbar^2}E\psi \Rightarrow \psi = e^{\pm i \underbrace{\sqrt{\frac{2mR^2E}{\hbar^2}}}_{\equiv \alpha}\phi}$

& the b.c. gives: $e^{\pm i\alpha(\phi+2\pi)} = e^{\pm i\alpha\phi} \cdot \underbrace{e^{\pm i\alpha \cdot 2\pi}}_{=1} \Rightarrow \alpha = ?$

α must be an integer: $\alpha = j \Rightarrow \frac{2mR^2E}{\hbar^2} = j^2 \Rightarrow E_j = \frac{j^2\hbar^2}{2mR^2}$ $j = 0, 1, 2, \ldots$

the wave function is:

$\psi(\phi) = \underset{\text{normalization}}{A} e^{\pm ij\phi}$ w/ the same E_j for + (ccw) or − (cw) travellers.

Magnetism in QM

When a magnetic field is present, w/ $\vec{B} = \nabla \times \vec{A}$, the Hamiltonian becomes:

$$H = \frac{1}{2m}(\vec{p} - q\vec{A})\cdot(\vec{p} - q\vec{A}) + \cancel{V} = E$$

assume no other interaction

the H depends on $\vec{A}$, but the eqn.s of motion are still

$$m\ddot{\vec{r}}(t) = q\vec{v}(t) \times \vec{B}(\vec{r}(t)) \qquad (*)$$

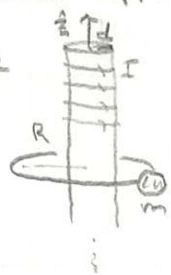
the eqn.s of motion are "gauge invariant" (sending $\vec{A} \to \vec{A} + \nabla\varphi$ leaves $\vec{B}$, & hence (*) unchanged)

Schrödinger's eqn. now becomes:

$$E\Psi = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)\cdot\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)\Psi$$

(which would appear to be sensitive to $\vec{A} \to \vec{A} + \nabla\varphi$ ...)

Example



An infinite solenoid has $\vec{B} = B_0\hat{z}$ inside of it.

Our mass constrained to the ring is outside the solenoid, where $\vec{B} = 0$, but $\vec{A} \neq 0$ (why not?)

In general, $\vec{A} = A(s)\hat{\phi}$, & at the particle location, it's a constant $\vec{A} = A(R)\hat{\phi}$. Schrödinger's eqn. reads, in this one dimensional setting:

$$\frac{1}{2m}\left(\frac{\hbar}{iR}\frac{d}{d\phi} - qA\right)^2\Psi = E\Psi$$

assume we retain the $e^{\pm ij\phi}$ solution for Ψ, then:

$$\frac{\hbar^2}{2mR^2}\left(\pm j - q\frac{AR}{\hbar}\right)^2\Psi = E\Psi$$

and
$$E_j = \frac{\hbar^2}{2mR^2}\left(\pm j - q\frac{AR}{\hbar}\right)^2 \qquad (*)$$

this time, the energy is different for $+j$ & $-j$, ccw & cw travellers have detectably different energies...

we can interpret $q\frac{AR}{\hbar}$ physically:

$$\int_S \vec{B}\cdot d\vec{a} = \int_S (\nabla\times\vec{A})\cdot d\vec{a} = \oint_{\partial S} \vec{A}\cdot d\vec{\ell}$$

take the surface to a disk of radius R, then

independent of gauge choice

$$\Phi = B_0 \pi d^2 = A(R)\cdot 2\pi R \Rightarrow AR = \frac{\Phi}{2\pi}$$

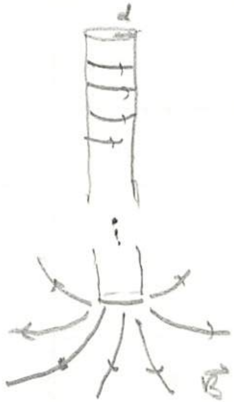
& we can write (*) as:

$$E_j = \frac{\hbar^2}{2mR^2}\left(\pm j - \frac{q\Phi}{2\pi\hbar}\right)^2$$

this detectability is related to the Aharonov-Bohm effect.

Dirac String

A ½-infinite solenoid:



magnetic field lines spray out of the open end, mimicking a magnetic monopole.

A "Dirac string"

As part of the Dirac string construction, Dirac proposed the "Dirac veto" – the string should be undetectable.

Undetectability amounts to $q\frac{\Phi}{2\pi\hbar} = n$ an integer then

$$q = \left(\frac{2\pi\hbar}{\Phi}\right)n \qquad (*)$$

the q here refers to the "detecting" charge, the mass on the ring.

Physically, (*) tells us that if charge is quantized, the 'string' is undetectable.