1 Quantizing in Curvilinear Coordinates

Classical mechanics can be written in any coordinate system, and the usual Lagrangian and Hamiltonian methods apply. In this section, we explore the question of how to quantize a system in curvilinear coordinates, using plane polar coordinates as an example. Suppose we have a Lagrangian written in plane polar coordinates.

$$L = \frac{m}{2}\left((\frac{dr}{dt})^2 + (r\frac{d\phi}{dt})^2 \right) - V(r,\phi) \tag{1}$$

Our first task is to find the classical Hamiltonian. From the Lagrangian of Eq.(1), we have

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}, \;\; p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2\dot{\phi},$$

where in general

$$\dot{O} = \frac{dO}{dt}$$

The classical Hamiltonian is given by

$$H_{cl} = p_r\dot{r} + p_\phi\dot{\phi} - L = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V,$$

and the classical equations of motion are

$$\dot{r} = \frac{\partial H_{cl}}{\partial p_r} = \frac{p_r}{m}, \;\; \dot{p}_r = -\frac{\partial H_{cl}}{\partial r} = -\frac{p_\phi^2}{mr^3} - \frac{\partial V}{\partial r}$$

$$\dot{\phi} = \frac{\partial H_{cl}}{\partial p_\phi} = \frac{p_\phi}{mr^2}, \;\; \dot{p}_\phi = -\frac{\partial V}{\partial \phi}$$

Let us try to quantize this system directly in plane polar coordinates. We label our position kets by $|r,\phi>$. Writing the norm of a state, we have

$$< \Psi|\Psi >= \int r dr d\phi < \Psi|r,\phi >< r,\phi|\Psi > .$$

We have again "sandwiched the identity" so we must have

$$I = \int r dr d\phi |r,\phi >< r,\phi|.$$

This must satisfy

$$I|r',\phi' >= |r',\phi' > .$$

Writing this out, we have

$$|r',\phi' >= \int r dr d\phi |r,\phi >< r,\phi|r',\phi' >$$

For this integral to give $|r',\phi' >$, we must have

$$< r,\phi|r',\phi' >= \frac{1}{\sqrt{rr'}}\delta(r-r')\delta(\phi-\phi')$$

Operators We expect there to be operators R, P_r, Φ, P_ϕ. If we follow the procedure used in Cartesian coordinates, we would write commutation rules,

$$[R, P_r] = i\hbar, \quad [\Phi, P_\phi] = i\hbar$$

These are satisfied if

$$< r, \phi|P_r|\Psi >= \frac{\hbar}{i}\frac{\partial}{\partial r} < r, \phi|\Psi >,$$

and

$$< r, \phi|P_\phi|\Psi >= \frac{\hbar}{i}\frac{\partial}{\partial \phi} < r, \phi|\Psi >,$$

We may now ask if P_r and P_ϕ defined this way are self-adjoint. It will turn out that P_ϕ is self-adjoint but P_r is not. Let us consider P_ϕ first. If P_ϕ is self-adjoint, we must have

$$< \Psi_2|P_\phi\Psi_1 >=< P_\phi\Psi_2|\Psi_1 >$$

Defining the right hand side as (a), and the left hand side as (b), we have

$$(a) = \int \Psi_2^*(r, \phi)(\frac{\hbar}{i}\frac{\partial}{\partial \phi}\Psi_1(r, \phi))rdrd\phi,$$

and (b) is

$$(b) = \int (\frac{\hbar}{i}\frac{\partial}{\partial \phi}\Psi_2(r, \phi))^*\Psi_1(r, \phi)rdrd\phi$$

Showing that $(a) = (b)$ is a simple exercise in integration by parts on ϕ, using the physical requirement that wave functions must be periodic, i.e. $\Psi(r, 0) = \Psi(r, 2\pi)$. So we have that

$$P_\phi = (P_\phi)^\dagger,$$

so quantizing naively was fine for P_ϕ.

Let us turn to asking the same question for P_r. If P_r is self-adjoint, we will have

$$< \Psi_2|P_r\Psi_1 >=< P_r\Psi_2|\Psi_1 >$$

Again writing left and right hand sides out, we define

$$(a) =< \Psi_2|P_r\Psi_1 >= \int \Psi_2^*(r, \phi)(\frac{\hbar}{i}\frac{\partial}{\partial r}\Psi_1(r, \phi))rdrd\phi,$$

and

$$(b) =< P_r\Psi_2|\Psi_1 >= \int (\frac{\hbar}{i}\frac{\partial}{\partial r}\Psi_2(r, \phi))^*\Psi_1(r, \phi)rdrd\phi$$

We can get the relation between (a) and (b) by integration by parts in r. Doing so on (a), we have

$$(a) = \int (\frac{\hbar}{i}\frac{\partial}{\partial r}r\Psi_2(r, \phi))^*\Psi_1(r, \phi)drd\phi$$

(The surface terms in the integration by parts vanish because $r\Psi_r(r,\phi)\Psi_1(r,\phi)$ vanishes at both $r=0$ and $r=\infty$.) Our expression after integration by parts is

$$(a) = \int (\frac{\hbar}{i}\frac{\partial}{\partial r}\Psi_2(r,\phi))^* \Psi_1(r,\phi) r dr d\phi + \int (\frac{\hbar}{i}\Psi_2(r,\phi))^* \Psi_1(r,\phi) dr d\phi$$

$$= < P_r\Psi_2|\Psi_1 > + \int (\frac{\hbar}{i}\Psi_2(r,\phi))^* \Psi_1(r,\phi) dr d\phi.$$

The presence of the extra integral term on the right hand side of the last equation means that P_r is not self-adjoint. The problem is of course that the integration weight $rdrd\phi$ depends on r.

Modified Radial Momentum It turns out to be possible to modify P_r so the result is self-adjoint. We define a new radial momentum operator by

$$< r,\phi|\tilde{P}_r|\Psi > \equiv \frac{\hbar}{i}(\frac{\partial}{\partial r} + \frac{1}{2r}) < r,\phi|\Psi >$$

This operator satisfies

$$\tilde{P}_r = (\tilde{P}_r)^\dagger.$$

We may now try to construct a quantum Hamiltonian by using $\tilde{P}_r$. This would give

$$\tilde{H} = \frac{\tilde{P}_r^2}{2m} + \frac{P_\phi^2}{2mr^2} + V$$

Using this as on a wave function we would get

$$< r,\phi|\tilde{H}|\Psi > = \left\{ -\frac{\hbar^2}{2m}\left[(\frac{\partial}{\partial r} + \frac{1}{2r})(\frac{\partial}{\partial r} + \frac{1}{2r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \right] + V \right\} < r,\phi|\Psi >$$

Working out the derivatives in terms of the Laplacian, we have

$$< r,\phi|\tilde{H}|\Psi > = \left\{ -\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2}{4mr^2} + V \right\} < r,\phi|\Psi >,$$

where the Laplacian is the usual plane polar expression,

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}$$

Our modified Hamiltonian has produced a sensible result, involving an extra term $O(\hbar^2)$ that must be added to the original potential. The fact that this extra term is $O(\hbar^2)$ means that it would disappear on going to the classical limit. However we can argue against including this term by considering a free particle with $V=0$. Here we surely believe that the wave function can be built up out of plane waves, where

$$< \vec{x}|\vec{p} > = \frac{1}{2\pi\hbar}\exp(i\frac{\vec{p}\cdot\vec{x}}{\hbar}),$$

and all vectors are two-dimensional. For these plane waves the correct quantum Hamiltonian is (still free particle)

$$< r, \phi|H|\Psi >= -\frac{\hbar^2}{2m}\Delta < r, \phi|\Psi > .$$

Here we can certainly rule out the term $\hbar^2/4mr^2$. Going back to the presence of a potential, if the extra term is ruled out for a free particle, it should also be ruled out when a potential is present.

Summary While it may be possible to construct momentum operators in curvilinear coordinates which are self-adjoint, the correct procedure is to use the Laplacian as the kinetic energy term in the Schrödinger equation, and not try to express the kinetic energy as sums of squares of the modified momentum operators.

So for plane polar coordinates, if the classical Hamiltonian is

$$H_c = \frac{1}{2m}p_r^2 + \frac{1}{2mr^2}p_\phi^2 + V,$$

The correct quantum Hamiltonian is defined by

$$< r, \phi|H|\Psi >= \left\{-\frac{\hbar^2}{2m}\Delta + V\right\} < r, \phi|\Psi >,$$

where

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}.$$

Likewise, in spherical coordinates, the classical Hamiltonian will be of the form

$$H_c = \frac{1}{2m}p_r^2 + \frac{1}{2mr^2}p_\theta^2 + \frac{1}{2mr^2\sin^2\theta}p_\phi^2 + V.$$

The quantum Hamiltonian is defined by

$$< r, \theta, \phi|H|\Psi >= \left\{-\frac{\hbar^2}{2m}\Delta + V\right\} < r, \theta, \phi|\Psi >,$$

where Δ is the usual Laplacian in spherical coordinates,

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2},$$

and in spherical coordinates, we have

$$< r, \theta, \phi|r', \theta', \phi' >= \frac{\delta(r-r')}{rr'}\frac{\delta(\theta-\theta')}{\sqrt{\sin\theta\sin\theta'}}\delta(\phi-\phi').$$