HAMILTONIAN IN NON-RECTANGULAR COORDINATES

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 7.4, Exercise 7.4.10.

The standard procedure for quantizing a classical hamiltonian is to write the classical hamiltonian in terms of position and momentum variables in rectangular coordinates and then convert the position and momentum variables to operators satisfying the usual commutation relations. However, in some cases, another coordinate system makes solving the differential equation resulting from the Schrödinger equation easier (as, for example, with the hydrogen atom, where the system has spherical symmetry).

As a 2-d example, suppose we have the classical hamiltonian

$$H=\frac{p_x^2+p_y^2}{2m}+a\sqrt{x^2+y^2} \tag{1}$$

for some constant a. Since the system has radial symmetry, polar coordinates should make things easier. That is, we'd like to transform to

$$\rho = \sqrt{x^2+y^2} \tag{2}$$

$$\phi = \arctan\frac{y}{x} \tag{3}$$

In the rectangular position basis, the quantized operators are

$$P_x = -i\hbar\frac{\partial}{\partial x} \tag{4}$$

$$P_y = -i\hbar\frac{\partial}{\partial y} \tag{5}$$

$$X = x \tag{6}$$

$$Y = y \tag{7}$$

so the quantum hamiltonian is

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+a\sqrt{x^2+y^2} \tag{8}$$

The first term contains the Laplacian derivative operator, which can be written in polar coordinates as

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}=\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} \tag{9}$$

Thus the quantum hamiltonian in polar coordinates is

$$H=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+a\rho \tag{10}$$

The question is: can we instead convert the hamiltonian 1 to polar coordinates and then quantize the result, rather than converting the rectangular coordinates after the hamiltonian is written? The answer turns out to be surprisingly complicated, and I'm not sure I follow everything Shankar says, but here's the argument anyway. Comments, as usual, are welcome.

We first convert the rectangular momentum coordinates to polar momentum coordinates by means of the substitutions

$$p_\rho = \hat{\mathbf{r}}\cdot\mathbf{p}=\frac{xp_x+yp_y}{\sqrt{x^2+y^2}} \tag{11}$$

$$p_\phi=\ell_z = xp_y-yp_x \tag{12}$$

Note that the two components of polar momentum have different units: p_ρ has the dimensions of linear momentum while p_ϕ is actually the angular momentum about the z axis ℓ_z. In terms of these new momenta, the classical hamiltonian 1 becomes

$$H=\frac{p_\rho^2}{2m}+\frac{p_\phi^2}{2m\rho^2}+a\rho \tag{13}$$

This can be verified either by inverting equations 11 and 12 to get p_x and p_y in terms of p_ρ and p_ϕ and then plugging these into 1 (very messy), or else just starting with 13 and showing it reduces to 1. We'll do the latter.

$$p_\rho^2+\frac{p_\phi^2}{\rho^2} = \left[\frac{xp_x+yp_y}{\sqrt{x^2+y^2}}\right]^2+\frac{(xp_y-yp_x)^2}{x^2+y^2} \tag{14}$$

$$= \frac{1}{\rho^2}\left(x^2p_x^2+y^2p_y^2+2xyp_xp_y+x^2p_y^2+y^2p_x^2-2xyp_xp_y\right) \tag{15}$$

$$= \frac{1}{\rho^2}\left(x^2+y^2\right)\left(p_x^2+p_y^2\right) \tag{16}$$

$$= p_x^2+p_y^2 \tag{17}$$

We can now try quantizing 13 by creating a couple of quantum momentum operators according to the standard rule:

$$P_\rho = -i\hbar\frac{\partial}{\partial\rho} \tag{18}$$

$$P_\phi = -i\hbar\frac{\partial}{\partial\phi} \tag{19}$$

These operators satisfy the usual commutation rule, in the sense that

$$\left[\rho, P_\rho\right] = \left[\phi, P_\phi\right] = i\hbar \tag{20}$$

However, substituting them into 13 gives

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + a\rho \tag{21}$$

Comparing with 10 we see that the middle term with the first order derivative is missing. The problem is due to the fact that 18 is actually not a hermitian operator, which we can see by calculating the bracket as follows:

$$\left\langle\psi_1\left|P_\rho\right|\psi_2\right\rangle = -i\hbar\int_0^{2\pi}\int_0^\infty \psi_1^*\frac{\partial\psi_2}{\partial\rho}\rho\,d\rho\,d\phi \tag{22}$$

We can do the ρ integral by parts and, assuming that $\rho\psi_1^*\psi_2 \to 0$ at both $\rho \to 0$ and $\rho \to \infty$, we have

$$\int_0^\infty \psi_1^*\frac{\partial\psi_2}{\partial\rho}\rho\,d\rho = \rho\psi_1^*\psi_2\big|_0^\infty - \int_0^\infty \psi_2\frac{\partial\left(\rho\psi_1^*\right)}{\partial\rho}\,d\rho \tag{23}$$

$$= -\int_0^\infty \psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho\,d\rho - \int_0^\infty \psi_1^*\psi_2 d\rho \tag{24}$$

Substituting back into 22 we get

$$\left\langle\psi_1\left|P_\rho\right|\psi_2\right\rangle = i\hbar\int_0^{2\pi}\int_0^\infty\left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho + \psi_1^*\psi_2\right]d\rho\,d\phi \tag{25}$$

If P_ρ is to be hermitian, we need to satisfy

$$\left\langle\psi_1\left|P_\rho\right|\psi_2\right\rangle = \left\langle P_\rho\psi_1\left|\psi_2\right.\right\rangle \tag{26}$$

$$= i\hbar\int_0^{2\pi}\int_0^\infty \psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho\,d\rho\,d\phi \tag{27}$$

We can see that the presence of the second term in the integrand of 25 messes things up. This term arises from the presence of the extra factor of ρ that is present in a polar area integral.

We can, in fact, attempt to fix this by defining the radial momentum operator to be, instead of 18:

$$P_\rho = -i\hbar\left(\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\right) \tag{28}$$

We first verify that this is hermitian:

$$\begin{aligned}
\left\langle\psi_1\left|P_\rho\right|\psi_2\right\rangle &= -i\hbar\int_0^{2\pi}\int_0^\infty \psi_1^*\left[\frac{\partial\psi_2}{\partial\rho}\rho + \frac{\psi_2}{2}\right]d\rho\,d\phi &(29)\\
&= i\hbar\int_0^{2\pi}\int_0^\infty\left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho + \psi_1^*\psi_2 - \frac{1}{2}\psi_1^*\psi_2\right]d\rho\,d\phi &(30)\\
&= i\hbar\int_0^{2\pi}\int_0^\infty\left[\psi_2\frac{\partial\psi_1^*}{\partial\rho}\rho + \frac{1}{2}\psi_1^*\psi_2\right]d\rho\,d\phi &(31)\\
&= \left\langle P_\rho\psi_1\left|\psi_2\right.\right\rangle &(32)
\end{aligned}$$

In the second line we did the same integration by parts on the first term and used the result in 24. Thus this new P_ρ is indeed hermitian. If we now insert this along with the old P_ϕ from 19 into 13 we get

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\right)^2 + a\rho \tag{33}$$

To work out the differential part of the hamiltonian we can apply it to a test function.

$$\begin{aligned}
\left(\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\right)^2\psi &= \left(\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\right)\left(\frac{\partial\psi}{\partial\rho} + \frac{\psi}{2\rho}\right) &(34)\\
&= \frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{2\rho}\frac{\partial\psi}{\partial\rho} - \frac{\psi}{2\rho^2} + \frac{1}{2\rho}\frac{\partial\psi}{\partial\rho} + \frac{\psi}{4\rho^2} &(35)\\
&= \frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} - \frac{\psi}{4\rho^2} &(36)
\end{aligned}$$

The hamiltonian then becomes

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{1}{4\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + a\rho \tag{37}$$

Comparing this with 10 we see that now we have an extra term $-\frac{1}{4\rho^2}$. Shankar doesn't really explain in detail what the problem is, except to state that when converting from a classical to a quantum hamiltonian, terms of order $\hbar$ or higher may be present in the quantum version that are absent in the classical version. Presumably he means terms of order $\hbar$ that don't involve derivatives, since the entire momentum-dependent part of the hamiltonian is multiplied by a factor of $\hbar^2$. In any case, we'll have to leave it at that.