# Momentum Operator in General Coordinates

## Abstract

It is common practice in quantum physics textbooks to define the 1-particle momentum operator as a hermitian operator given by $\boldsymbol{p} = \frac{\hbar}{i}\nabla$, and the kinetic energy operator as $K = \frac{\boldsymbol{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$. Unfortunately, these statements are correct only in Cartesian coordinates. For a general coordinate system $x^j$, one should define a conjugate momentm as a non-hermitian operator with components $p_j = \frac{\hbar}{i}\frac{\partial}{\partial x^j}$, a physical momentum as a hermitian operator $P_j = \frac{1}{2m}\left(p_j + p_j^+\right)$, and the kinetic energy as a hermitian scalar operator $K = \frac{1}{2m} p_j^+ g^{jk} p_k = -\frac{\hbar^2}{2m}\nabla^2$, where $g_{jk}$ is the metric tensor of the configuration space.

## Theory

Ref: Any textbook on differential geometry, e.g., M.Fecko, “Differential Geometry & Lie Groups for Physicists”, Cambridge Univ. Press (2006).

In an 1-particle Hilbert space, the inner product between states $\psi$ & $\phi$ is defined as

$$\langle \psi \mid \phi \rangle = \int d\tau\, \psi^* \phi = \langle \phi \mid \psi \rangle^*$$

where $d\tau$ is the volume element of an $n$-D configuration space, which is assumed to be a differentiable manifold. In terms of local coordinates $x^j$, we have

$$d\tau = \sqrt{|g|} \prod_{j=1}^{n} dx^j = \sqrt{|g|}\, d^n x$$

where $|g| = \det g_{jk}$ and $g_{jk}$ is the metric tensor defined via the line element $dl$ as

$$dl^2 = g_{jk}\, dx^j\, dx^k$$

Summation over repeated indices is understood.

The matrix element of operator $A$ between states $\psi$ & $\phi$ is defined as

$$\langle \psi \mid A \mid \phi \rangle = \int d\tau\, \psi^* A \phi = \langle \psi \mid A \phi \rangle$$

$$= \langle A^+ \psi \mid \phi \rangle = \int d\tau\, (A^+ \psi)^* \phi$$

where $A^+$ is called the adjoint of $A$.

In terms of the coordinates, we have

$$\langle \psi \mid A \mid \phi \rangle = \int d^n x \sqrt{|g|}\; \psi^* A \phi$$

$$= \int d^n x \sqrt{|g|}\; (A^+ \psi)^* \phi$$

For the coordinate $x^j$, it is straightforward to verify that a solution to the quantization condition

$$\left[ x^j, \; p_k \right] = i \hbar\, \delta^j_k$$

is

$$p_j = \frac{\hbar}{i} \frac{\partial}{\partial x^j}$$

We'll call $p_j$ the canonical momentum conjugate to $x^j$.

Assuming the surface term vanishes, the adjoint of $p_j$ can be obtained by taking a partial integration as follows

$$\begin{aligned}\langle \psi \mid p_j \mid \phi \rangle &= \int d^n x \sqrt{\mid g \mid}\ \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x^j} \phi \\ &= -\int d^n x \left( \frac{\hbar}{i} \frac{\partial}{\partial x^j} \sqrt{\mid g \mid}\ \psi^* \right) \phi \\ &= \int d^n x \sqrt{\mid g \mid} \left( \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \frac{\partial}{\partial x^j} \sqrt{\mid g \mid}\ \psi \right)^* \phi\end{aligned}$$

since $g_{jk}$ is real.

Hence,

$$p_j^+ \psi = \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \frac{\partial}{\partial x^j} \left( \sqrt{\mid g \mid}\ \psi \right)$$

so that

$$\begin{aligned}p_j^+ &= \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \frac{\partial}{\partial x^j} \sqrt{\mid g \mid} \\ &= \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \left( \frac{\partial \sqrt{\mid g \mid}}{\partial x^j} + \sqrt{\mid g \mid} \frac{\partial}{\partial x^j} \right) \\ &= \frac{\hbar}{i} \left( \frac{\partial \ln \sqrt{\mid g \mid}}{\partial x^j} + \frac{\partial}{\partial x^j} \right)\end{aligned}$$

Hence, $p_j$ is not hermitian ( & hence not an observable ) unless $\mid g \mid$ is independent of $x^j$, e.g., the Cartesian coordinates.

For example, $p_\phi = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$ is hermitian & represents the angular momentum operator for rotations about the $z$-axis. However, $p_r = \frac{\hbar}{i} \frac{\partial}{\partial r}$ & $p_\theta = \frac{\hbar}{i} \frac{\partial}{\partial \theta}$ are not hermitian so that they cannot be the physical momentum operators.

Now,

$$\begin{aligned}\left[ x^j, p_k^+ \right] \psi &= x^j \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \frac{\partial}{\partial x^k} \left( \sqrt{\mid g \mid}\ \psi \right) - \frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \frac{\partial}{\partial x^k} \left( \sqrt{\mid g \mid}\ x^j \psi \right) \\ &= -\frac{\hbar}{i} \frac{1}{\sqrt{\mid g \mid}} \left( \sqrt{\mid g \mid}\ \delta^j_k \psi \right) \\ &= i \hbar \delta^j_k \psi\end{aligned}$$

so that $p_k^+$ also satisfies the quantization condition.

We can therefore define the physical momentum operator $P_j$ conjugate to $x^j$ as

$$P_j = \frac{1}{2} \left( p_j + p_j^+ \right)$$

$$= \frac{\hbar}{i}\left(\frac{\partial}{\partial x^j} + \frac{1}{2}\frac{\partial \ln\sqrt{|g|}}{\partial x^j}\right)$$

with

$$\left[x^j,\ P_k\right] = i\hbar\,\delta^j_k$$

Thus, the physical radial momentum operators are

$$P_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{2r}\right) \qquad (\ E^2 \text{ space. })$$

$$P_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \qquad (\ E^3 \text{ space. })$$

The classical kinetic energy is a scalar given by

$$K = \frac{1}{2m} p^j p_j = \frac{1}{2m} g^{jk} p_j p_k = \frac{1}{2m} p_j p^j$$

where $g^{jk}$ is the inverse of $g_{jk}$ so that

$$g^{jk} g_{kl} = \delta^j_l$$

We therefore define the kinetic energy operator as

$$\langle \psi \mid K \mid \phi \rangle = \frac{1}{2m}\left\langle p^j \psi \,\middle|\, p_j \phi \right\rangle$$
$$= \frac{1}{2m}\int d\tau\, \left(p^j \psi\right)^* (p_j \phi)$$
$$= \frac{1}{2m}\int d\tau\ \ g^{jk} (p_j \psi)^* (p_k \phi)$$
$$= \frac{1}{2m}\int d\tau\ \ \psi^* p_j^+ \left(g^{jk} p_k \phi\right)$$

Hence,

$$K = \frac{1}{2m} p_j^+ g^{jk} p_k$$
$$= -\frac{\hbar^2}{2m}\frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^j}\left(\sqrt{|g|}\ g^{jk}\frac{\partial}{\partial x^k}\right)$$
$$= -\frac{\hbar^2}{2m}\nabla^2$$

where the Laplace-Beltrami operator ( see Fecko, p.174. )

$$\nabla^2 = \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^j}\left(\sqrt{|g|}\ g^{jk}\frac{\partial}{\partial x^k}\right)$$

is just a generalization of the Laplacian to general coordinates.

The adjoint of $p^j = g^{jk} p_k$ can be obtained by taking a partial integration as follows

$$\left\langle \psi \mid p^j \mid \phi \right\rangle = \int d^n x \sqrt{|g|}\ \ \psi^* \frac{\hbar}{i} g^{jk}\frac{\partial}{\partial x^k}\phi$$
$$= -\int d^n x \left(\frac{\hbar}{i}\frac{\partial}{\partial x^k}\left(\sqrt{|g|}\ \ g^{jk}\psi^*\right)\right)\phi$$
$$= \int d^n x \sqrt{|g|}\left(\frac{\hbar}{i}\frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^k}\left(\sqrt{|g|}\ \ g^{jk}\psi\right)\right)^*\phi$$

Since $g^{jk}$ is symmetric, we have

$$p^{+j}\,\psi = \frac{\hbar}{i}\,\frac{1}{\sqrt{|\,g\,|}}\,\frac{\partial}{\partial x^k}\left(\sqrt{|\,g\,|}\;g^{kj}\,\psi\right)$$
$$= p_k^+\,g^{kj}\,\psi$$

Thus, $K$ can also be written as

$$K = \frac{1}{2\,m}\,p_j^+\,p^j = \frac{1}{2\,m}\,p^{+\,k}\,p_k$$

showing explicitly that it is a scalar hermitian operator.

## Examples

For the 2-D Euclidean plane $E^2$ described by the polar coordinates, we have

$$d\,l^2 = d\,r^2 + r^2\,d\,\phi^2$$

so that

$$g_{j\,k} = \text{diag}(1,\, r^2)$$
$$|\,g\,| = r^2$$
$$d\,\tau = r\,d\,r\,d\,\phi$$
$$g^{j\,k} = \text{diag}\left(1,\, \frac{1}{r^2}\right)$$
$$p_r = \frac{\hbar}{i}\,\frac{\partial}{\partial\,r} \qquad p_r^+ = \frac{\hbar}{i}\,\frac{1}{r}\,\frac{\partial}{\partial\,r}\,r$$
$$p_\phi = \frac{\hbar}{i}\,\frac{\partial}{\partial\,\phi} \qquad p_\phi^+ = \frac{\hbar}{i}\,\frac{\partial}{\partial\phi}$$
$$K = \frac{1}{2\,m}\left(p_r^+\,p_r + \frac{1}{r^2}\,p_\phi^2\right)$$
$$\nabla^2 = \frac{1}{r}\,\frac{\partial}{\partial\,r}\left(r\,\frac{\partial}{\partial\,r}\right) + \frac{1}{r}\,\frac{\partial}{\partial\theta}\left(r\,\frac{1}{r^2}\,\frac{\partial}{\partial\,\theta}\right)$$
$$= \frac{1}{r}\,\frac{\partial}{\partial\,r}\left(r\,\frac{\partial}{\partial\,r}\right) + \frac{1}{r^2}\,\frac{\partial^2}{\partial\,\theta^2}$$

For the 3-D Euclidean space $E^3$ described by the spherical coordinates, we have

$$d\,l^2 = d\,r^2 + r^2\,d\,\theta^2 + r^2\sin^2\theta\,d\,\phi^2$$

so that

$$g_{j\,k} = \text{diag}(1,\, r^2,\, r^2\sin^2\theta)$$
$$|\,g\,| = (r^2\sin\theta)^2$$
$$d\,\tau = r^2\sin\theta\,d\,r\,d\,\theta\,d\,\phi$$
$$g^{j\,k} = \text{diag}\left(1,\, \frac{1}{r^2},\, \frac{1}{r^2\sin^2\theta}\right)$$
$$p_r = \frac{\hbar}{i}\,\frac{\partial}{\partial\,r} \qquad p_r^+ = \frac{\hbar}{i}\,\frac{1}{r^2}\,\frac{\partial}{\partial\,r}\,r^2$$
$$p_\theta = \frac{\hbar}{i}\,\frac{\partial}{\partial\,\theta} \qquad p_\theta^+ = \frac{\hbar}{i}\,\frac{1}{\sin\theta}\,\frac{\partial}{\partial\,\theta}\sin\theta$$
$$p_\phi = \frac{\hbar}{i}\,\frac{\partial}{\partial\,\phi} \qquad p_\phi^+ = \frac{\hbar}{i}\,\frac{\partial}{\partial\phi}$$
$$K = \frac{1}{2\,m}\left[p_r^+\,p_r + \frac{1}{r^2}\left(p_\theta^+\,p_\theta + \frac{1}{\sin^2\theta}\,p_\phi^2\right)\right]$$

$$\nabla^2 = \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial r}\left(r^2 \sin\theta \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(r^2 \sin\theta \frac{1}{r^2} \frac{\partial}{\partial \theta}\right)$$
$$+ \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \phi}\left(r^2 \sin\theta \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi}\right)$$
$$= \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

In both cases, $\nabla^2$ reduces to the familiar Laplacian, as expected.