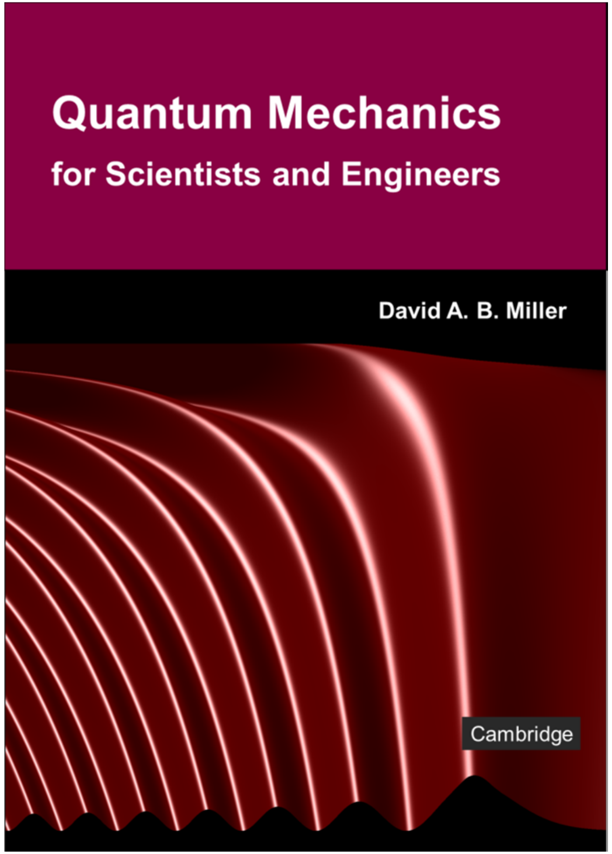
5.1 Uncertainty principle and particle current

Slides: Video 5.1.3 Particle current

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.14



Uncertainty principle and particle current

Particle current

Quantum mechanics for scientists and engineers

David Miller

The divergence of a vector

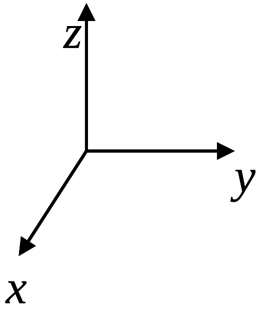
In Cartesian coordinates

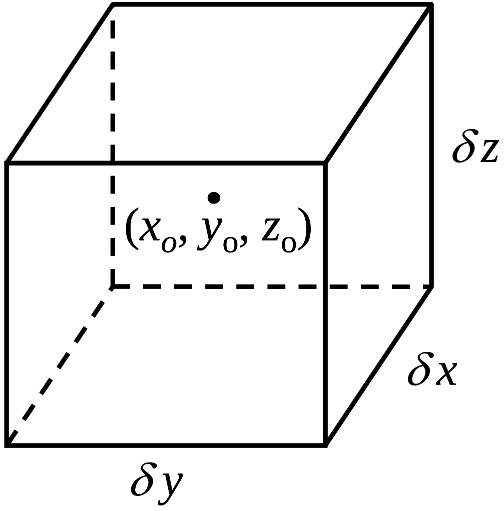
- the divergence of a vector $\mathbf{F}$ is

$$\operatorname{div}\mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

We can visualize this in terms of the flux $\mathbf{F}$ of some quantity

- such as mass or charge
  - through a small cuboidal box of sides δx, δy, and δz
    - centered at some point (x_o, y_o, z_o)





The divergence of a vector

Because $\mathbf{F}$ represents the flow of the quantity per unit area

an amount $F_x(x_o + \delta x/2, y_o, z_o)\delta y \delta z$

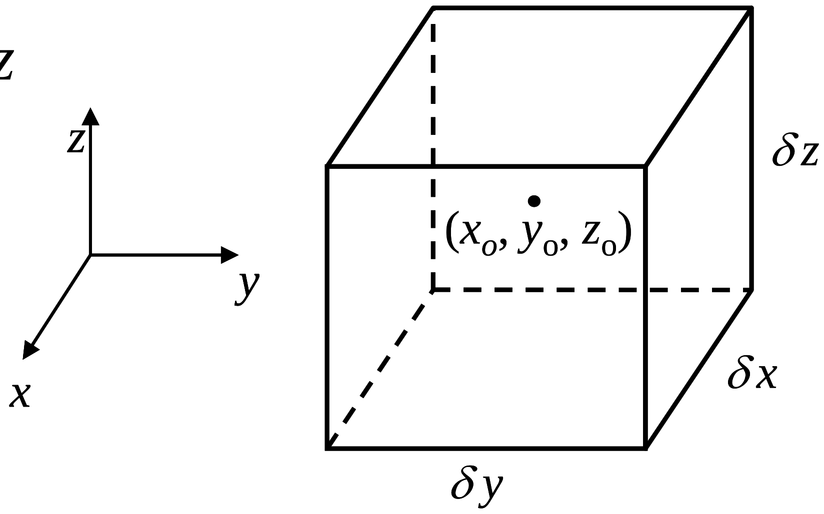
leaves the box at the front

(Note that the area of the front face of the box is $\delta y \delta z$)

This quantity

is the x-component of the flux

multiplied by the area perpendicular to the x-direction



The divergence of a vector

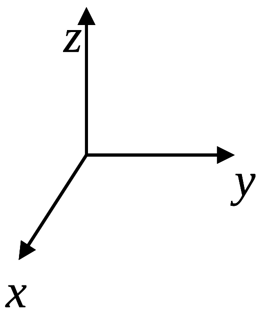
We can also think of this quantity as

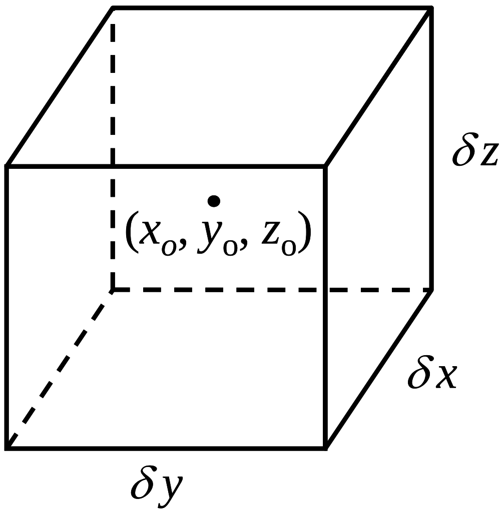
$$F_x\left(x_o+\frac{\delta x}{2},y_o,z_o\right)\delta y\delta z \equiv \mathbf{F}\left(x_o+\frac{\delta x}{2},y_o,z_o\right)\cdot\delta\mathbf{A}_{yz}$$

where $\delta\mathbf{A}_{yz}$ is a vector

whose magnitude is the area of the front surface of the box and

whose direction is outward from the box





The amount arriving into the box on the back face is similarly $F_x(x_o-\delta x/2,y_o,z_o)\delta y\delta z$

The divergence of a vector

Hence the net amount leaving the box through the front or back faces is

$$F_x\left(x_o+\frac{\delta x}{2},y_o,z_o\right)\delta y\delta z-F_x\left(x_o-\frac{\delta x}{2},y_o,z_o\right)\delta y\delta z$$

$$=\frac{F_x\left(x_o+\frac{\delta x}{2},y_o,z_o\right)-F_x\left(x_o-\frac{\delta x}{2},y_o,z_o\right)}{\delta x}\delta x\delta y\delta z$$

$$\simeq\frac{\partial F_x}{\partial x}\delta x\delta y\delta z$$

where we are assuming a very small box

The divergence of a vector

We can repeat this analysis for each of the other two pairs of faces

so, adding three such equations

we can write

for the total amount of flow leaving the small box

per unit volume of the box

i.e., dividing by $\delta V = \delta x \delta y \delta z$

$$\operatorname{div} \mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

Particle current

When we are thinking of flow of particles

to conserve particles

$$\frac{\partial s}{\partial t} = -\nabla . \mathbf{j}_p$$

where s is the particle density and

$\mathbf{j}_p$ is the particle current density

The minus sign is because the divergence of the flow or current

is the net amount *leaving* the volume

(Note: this is particle not electrical current)

Particle current and the wavefunction

In our quantum mechanical case

the particle density is $\left|\Psi(\mathbf{r},t)\right|^2$

so we are looking for a relation of the form

$$\frac{\partial s}{\partial t} = -\nabla.\mathbf{j}_p$$

but with $\left|\Psi(\mathbf{r},t)\right|^2$ instead of s

To do this requires a little algebra

and a clever substitution

Particle current and the wavefunction

We know that

$$\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = \frac{1}{i\hbar}\hat{H}\Psi(\mathbf{r},t)$$

which is simply Schrödinger's equation

We can also take the complex conjugate of both sides

$$\frac{\partial \Psi^*(\mathbf{r},t)}{\partial t} = -\frac{1}{i\hbar}\hat{H}^*\Psi^*(\mathbf{r},t)$$

Noting that

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right] = \Psi^*\frac{\partial \Psi}{\partial t} + \Psi\frac{\partial \Psi^*}{\partial t}$$

then we have

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right] + \frac{i}{\hbar}\left(\Psi^*\hat{H}\Psi - \Psi\hat{H}^*\Psi^*\right) = 0$$

Particle current and the wavefunction

Presuming the potential V is real and does not depend in time

and taking our Hamiltonian to be of the form

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

then

$$\Psi^*\hat{H}\Psi - \Psi\hat{H}^*\Psi^* = -\frac{\hbar^2}{2m}\left[\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right] + \Psi^* V\Psi - \Psi V\Psi^*$$

$$= -\frac{\hbar^2}{2m}\left[\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right]$$

Particle current and the wavefunction

So our equation

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]+\frac{i}{\hbar}\left(\Psi^*\hat{H}\Psi-\Psi\hat{H}^*\Psi^*\right)=0$$

becomes

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]-\frac{i\hbar}{2m}\left(\Psi^*\nabla^2\Psi-\Psi\nabla^2\Psi^*\right)=0$$

Now we use the following algebraic trick

$$\Psi\nabla^2\Psi^*-\Psi^*\nabla^2\Psi=\Psi\nabla^2\Psi^*+\nabla\Psi\nabla\Psi^*-\nabla\Psi\nabla\Psi^*-\Psi^*\nabla^2\Psi$$

$$=\nabla\cdot\left(\Psi\nabla\Psi^*-\Psi^*\nabla\Psi\right)$$

Particle current and the wavefunction

Hence we have $$\frac{\partial\left(\Psi^*\Psi\right)}{\partial t} = -\frac{i\hbar}{2m}\nabla\cdot\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)$$

which is an equation in the same form as $\frac{\partial s}{\partial t} = -\nabla.\mathbf{j}_p$

with $\left|\Psi\left(\mathbf{r},t\right)\right|^2$ instead of s

as desired

and

$$\boxed{\mathbf{j}_p = \frac{i\hbar}{2m}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)}$$

So we can calculate particle currents from the wavefunction when the potential does not depend on time

Particle current and stationary states

This expression applies also for an energy eigenstate

Suppose we are in the nth energy eigenstate

$$\Psi_n(\mathbf{r},t) = \exp\left(-i\frac{E_n}{\hbar}t\right)\psi_n(\mathbf{r})$$

Then

$$\mathbf{j}_{pn}(\mathbf{r},t) = \frac{i\hbar}{2m}\left(\Psi_n(\mathbf{r},t)\nabla\Psi_n^*(\mathbf{r},t) - \Psi_n^*(\mathbf{r},t)\nabla\Psi_n(\mathbf{r},t)\right)$$

Particle current and stationary states

In $\mathbf{j}_{pn}(\mathbf{r},t)=\frac{i\hbar}{2m}\left(\Psi_n(\mathbf{r},t)\nabla\Psi_n^*(\mathbf{r},t)-\Psi_n^*(\mathbf{r},t)\nabla\Psi_n(\mathbf{r},t)\right)$

the gradient has no effect on the time factor

so the time factors in each term can be factored to the front of the expression

and multiply to unity

$$\mathbf{j}_{pn}(\mathbf{r},t)=\frac{i\hbar}{2m}\exp\left(-i\frac{E_n}{\hbar}t\right)\exp\left(i\frac{E_n}{\hbar}t\right)\left(\psi_n(\mathbf{r})\nabla\psi_n^*(\mathbf{r})-\psi_n^*(\mathbf{r})\nabla\psi_n(\mathbf{r})\right)$$

$$=\frac{i\hbar}{2m}\left(\psi_n(\mathbf{r})\nabla\psi_n^*(\mathbf{r})-\psi_n^*(\mathbf{r})\nabla\psi_n(\mathbf{r})\right)$$

Particle current and stationary states

In $$\mathbf{j}_{pn}(\mathbf{r},t)=\frac{i\hbar}{2m}\left(\psi_n(\mathbf{r})\nabla\psi_n^*(\mathbf{r})-\psi_n^*(\mathbf{r})\nabla\psi_n(\mathbf{r})\right)$$

nothing on the right depends on time

so the particle current $\mathbf{j}_{pn}$ does not depend on time

That is, for any energy eigenstate n

$$\mathbf{j}_{pn}(\mathbf{r},t)=\mathbf{j}_{pn}(\mathbf{r})$$

Therefore

particle current is constant in any energy eigenstate

For real spatial eigenfunctions

particle current is actually zero