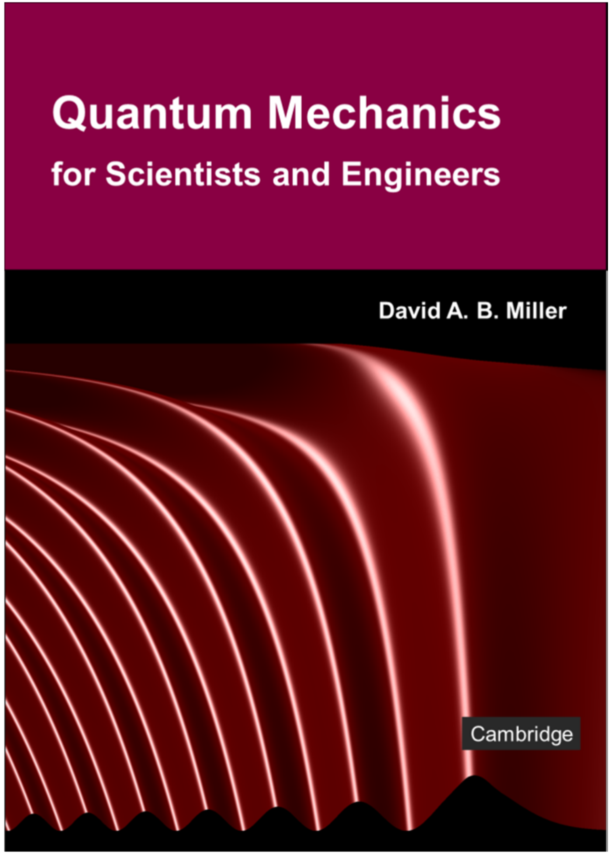
5.1 Uncertainty principle and particle current

Slides: Video 5.1.1 Momentum, position, and the uncertainty principle

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 3.12 – 3.13



Uncertainty principle and particle current

Momentum, position and the uncertainty principle

Quantum mechanics for scientists and engineers

David Miller

Momentum and the momentum operator

For momentum

we write an operator $\hat{p}$

We postulate this can be written as

$$\boxed{\hat{p} \equiv -i\hbar\nabla}$$

with

$$\nabla \equiv \mathbf{x}_o \frac{\partial}{\partial x} + \mathbf{y}_o \frac{\partial}{\partial y} + \mathbf{z}_o \frac{\partial}{\partial z}$$

where $\mathbf{x}_o$, $\mathbf{y}_o$, and $\mathbf{z}_o$ are unit vectors in the x, y, and z directions

Momentum and the momentum operator

With this postulated form $\hat{p} \equiv -i\hbar\nabla$ we find that

$$\frac{\hat{p}^2}{2m} \equiv -\frac{\hbar^2}{2m}\nabla^2$$

and we have a correspondence between the classical notion of the energy E

$$E = \frac{p^2}{2m} + V$$

and the corresponding Hamiltonian operator of the Schrödinger equation

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V = \frac{\hat{p}^2}{2m} + V$$

Momentum and the momentum operator

Note that

$$\hat{p}\exp(i\mathbf{k}\cdot\mathbf{r}) = -i\hbar\nabla\exp(i\mathbf{k}\cdot\mathbf{r}) = \hbar\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r})$$

This means the plane waves $\exp(i\mathbf{k}\cdot\mathbf{r})$ are the eigenfunctions of the operator $\hat{p}$

with eigenvalues $\hbar\mathbf{k}$

We can therefore say for these eigenstates that

the momentum is $\mathbf{p} = \hbar\mathbf{k}$

Note that $\mathbf{p}$ is a vector, with three components with scalar values

not an operator

Position and the position operator

For the position operator

- the postulated operator is almost trivial when we are working with functions of position
  - It is simply the position vector, $\mathbf{r}$, itself

At least when we are working in a representation that is in terms of position

- we therefore typically do not write $\hat{\mathbf{r}}$
  - though rigorously we should

The operator for the z-component of position would, for example, also simply be z itself

The uncertainty principle

Here we illustrate the position-momentum uncertainty principle by example

We have looked at a Gaussian wavepacket before

We could write this as a sum over waves of different k-values, with Gaussian weights

or we could take the limit of that process by using an integration

$$\Psi_G(z,t) \propto \int_k \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right] \exp\left\{-i\left[\omega(k)t - kz\right]\right\} dk$$

The uncertainty principle

We could rewrite

$$\Psi_G(z,t) \propto \int_k \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right] \exp\left\{-i\left[\omega(k)t - kz\right]\right\} dk$$

at time t = 0 as

$$\Psi(z,0) = \int_k \Psi_k(k) \exp(ikz)\, dk$$

where

$$\Psi_k(k) \propto \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right]$$

The uncertainty principle

In

$$\Psi_k(k) \propto \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right]$$

$\Psi_k(k)$ is the representation of the wavefunction in k space

$|\Psi_k(k)|^2$ is the probability P_k

strictly, the probability density

that if we measured the momentum of the particle

actually the z component of momentum

it would be found to have value $\hbar k$

The uncertainty principle

With

$$\Psi_k(k) \propto \exp\left[-\left(\frac{k-\bar{k}}{2\Delta k}\right)^2\right]$$

then this probability (density) of finding a value $\hbar k$ for the momentum would be

$$P_k = \left|\Psi_k(k)\right|^2 \propto \exp\left[-\frac{\left(k-\bar{k}\right)^2}{2\left(\Delta k\right)^2}\right]$$

This Gaussian corresponds to the statistical Gaussian probability distribution

with standard deviation Δk

The uncertainty principle

Note also that $\Psi(z,0) = \int\limits_k \Psi_k(k)\exp(ikz)\,dk$

is the Fourier transform of $\Psi_k(k)$

and, as is well known

the Fourier transform of a Gaussian is a Gaussian

specifically here

$$\Psi(z,0) \propto \exp\left[-(\Delta k)^2 z^2\right]$$

The uncertainty principle

If we want to rewrite

$$\left|\Psi(z,0)\right|^2 \propto \exp\left[-2(\Delta k)^2 z^2\right]$$

in the standard form

$$\left|\Psi(z,0)\right|^2 \propto \exp\left[-\frac{z^2}{2(\Delta z)^2}\right]$$

where the parameter Δz

would now be the standard deviation

in the probability distribution for z

then $\Delta k \Delta z = 1/2$

The uncertainty principle

From $\Delta k \Delta z = 1/2$

if we now multiply by $\hbar$ to get the standard deviation we would measure in momentum

we have

$$\Delta p \Delta z = \frac{\hbar}{2}$$

which is the relation between the standard deviations we would see in measurements of position and measurements of momentum

The uncertainty principle

This relation

$$\Delta p \Delta z = \frac{\hbar}{2}$$

is as good as we can get for a Gaussian

- For example
  - a Gaussian pulse will broaden in space as it propagates
    - even though the range of k values remains the same

The uncertainty principle

It also turns out that the Gaussian shape

is the one with the minimum possible

product of Δp and Δz

So quite generally

$$\boxed{\Delta p \Delta z \geq \frac{\hbar}{2}}$$

which is the uncertainty principle

for position and momentum in

one direction

The uncertainty principle in Fourier analysis

Uncertainty principles are well known in Fourier analysis

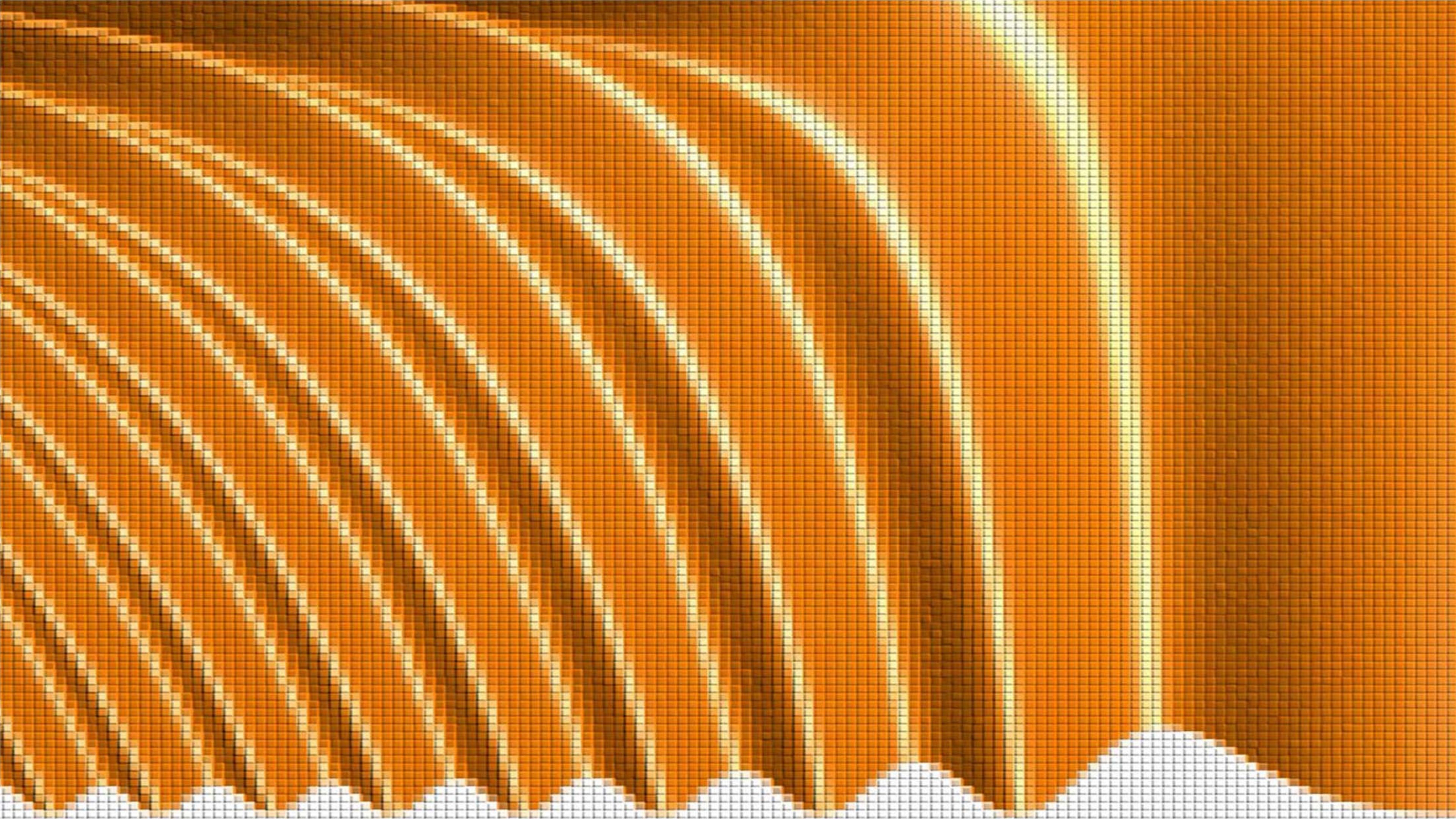
- One cannot simultaneously have both
  - a well defined frequency and
  - a well defined time

If a signal is a short pulse

- it is necessarily made up out of a range of frequencies

$$\Delta\omega \Delta t \geq \frac{1}{2}$$

  - The shorter the pulse is
    - the larger the range of frequencies

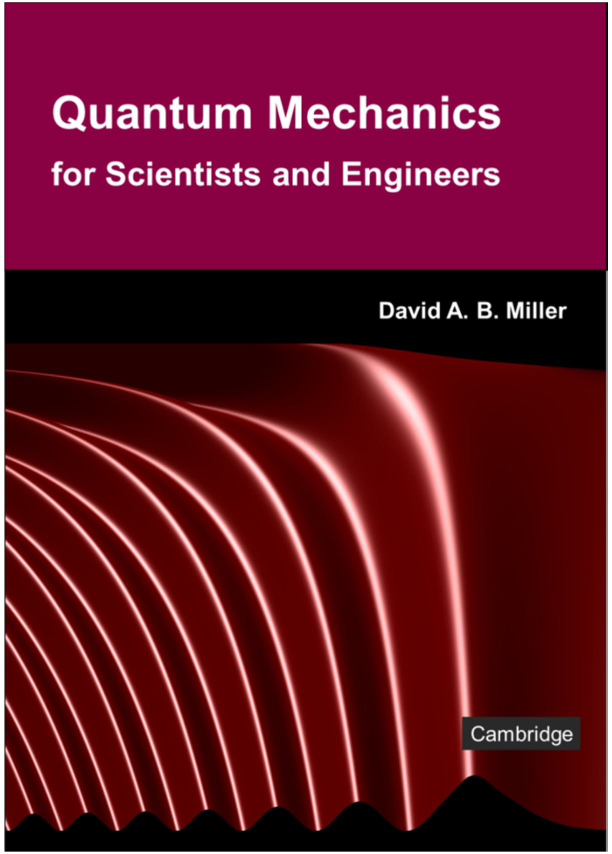


5.1 Uncertainty principle and particle current

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

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The divergence of a vector

In Cartesian coordinates

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

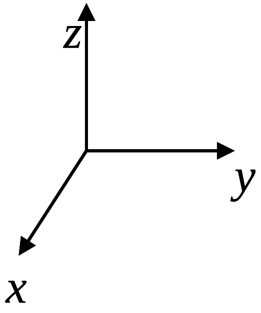
$$\operatorname{div}\mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

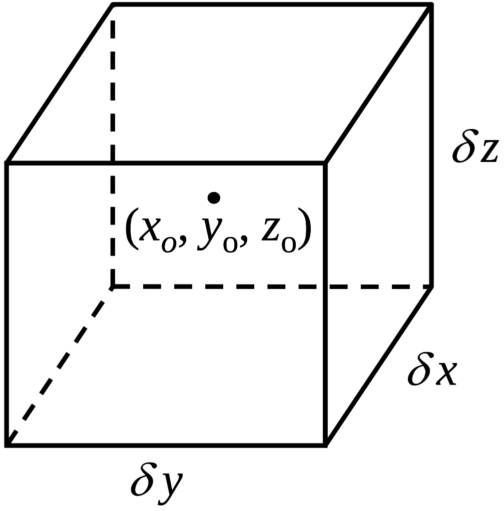
We can visualize this in terms of the flux $\mathbf{F}$ of some quantity

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)





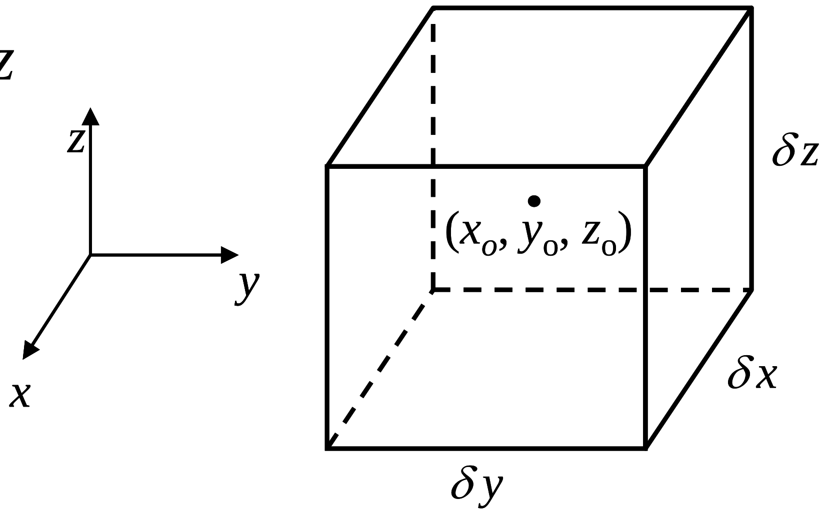
The divergence of a vector

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

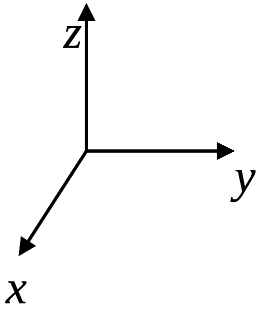
We can also think of this quantity as

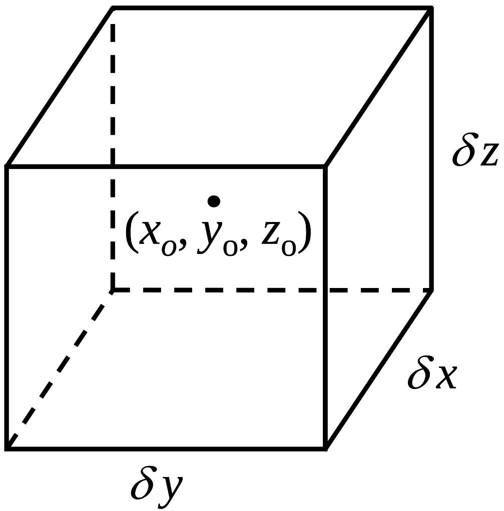
$$F_x\left(x_o+\frac{\delta x}{2},y_o,z_o\right)\delta y\delta z\equiv\mathbf{F}\left(x_o+\frac{\delta x}{2},y_o,z_o\right)\cdot\delta\mathbf{A}_{yz}$$

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

so we are looking for a relation of the form

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

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