

### H3: The Schrödinger equation

#### 3.1 the time-dependent Schrödinger equation

derivation the Schrödinger-eq

consider a particle of mass  $m$  moving non-relativistically in a field without potential energy  
 $\Psi$  has well-defined momentum  $\mathbf{p} = p_x \hat{x}$  with  $p = |\mathbf{p}_x|$  an energy  $E$   
 $\Psi$  is described by monochromatic plane wave with  $k = p_x/\hbar$  and  $\omega = E/\hbar$ , thus:

$$\begin{aligned}\Psi(x, t) &= Ae^{i(kx - \omega t)} \\ &= Ae^{i(p_x x - Et)/\hbar}\end{aligned}$$

but since  $\omega = \hbar k^2/2m$  we find the classical relation:

$$E = \frac{p_x^2}{2m}$$

connecting energy and momentum

If we differentiate once and twice we find two relations:

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi, \quad \frac{\partial^2 \Psi}{\partial x^2} = -\frac{p_x^2}{\hbar^2} \Psi.$$

Hence:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t).$$

$\Psi$  is linear and homogeneous

$\Psi(x, t)$  is satisfied by superposition of plane waves:

$$\Psi(x, t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i[p_x x - E(p_x)t]/\hbar} \phi(p_x) dp_x$$

quantum-mechanical E-p relation

Since we can represent the energy and momentum by the operators:

$$E_{\text{op}} = i\hbar \partial/\partial t, \quad (p_x)_{\text{op}} = -i\hbar \partial/\partial x$$

we find the relation:

$$E_{\text{op}} \Psi(x, t) = \frac{1}{2m} [(p_x)_{\text{op}}]^2 \Psi(x, t)$$

3D Schrödinger equation

We can define vector  $\mathbf{k}$ , for which we have the momentum vector  $\mathbf{p}$

$$\begin{aligned}\text{Now: } \Psi(\mathbf{r}, t) &= Ae^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \\ &= Ae^{i(\mathbf{p} \cdot \mathbf{r} - Et)/\hbar}\end{aligned}$$

we thus find the classical relation:  $E = \frac{\mathbf{p}^2}{2m}$

and thus the Schrödinger eq:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t)$$

where

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

3D E-p relation

We once again find operators for  $E$  and  $\mathbf{p}$ :

$$E_{\text{op}} = i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p}_{\text{op}} = -i\hbar \nabla$$

thus we find:

$$E_{\text{op}} \Psi(\mathbf{r}, t) = \frac{1}{2m} (\mathbf{p}_{\text{op}})^2 \Psi(\mathbf{r}, t)$$

in similar fashion we find for the kinetic energy  $T = \mathbf{p}^2/2m$ :

$$T = \frac{1}{2m} (\mathbf{p}_{\text{op}})^2 = -\frac{\hbar^2}{2m} \nabla^2$$

Schrödinger-eq for a particle in a potential energy field	<p>Consider the same particle moving in a field with potential energy &gt; the force acting on the particle is given by:</p> $\mathbf{F}(\mathbf{r}, t) = -\nabla V(\mathbf{r}, t)$ <p>for a classical particle the energy is given by:</p> $E = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t).$ <p>since <math>V</math> isn't dependent on <math>\mathbf{p}</math> or <math>E</math>, we can conclude:</p> $E_{\text{op}} \Psi(\mathbf{r}, t) = \left[ \frac{1}{2m} (\mathbf{p}_{\text{op}})^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$ <p>which:</p> $i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t).$
Schrödinger-eq and Hamiltonian	<p>We can find the Hamiltonian operator hiding in the Schrödinger-eq:</p> $H = -\frac{\hbar^2}{2m} \nabla^2 + V$ $= \frac{1}{2m} (\mathbf{p}_{\text{op}})^2 + V = T + V$ <p>thus we can rewrite:</p> $i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = H \Psi(\mathbf{r}, t).$
difference between classical and quantum $E$ and $\mathbf{p}$	<p>In a classical sense we know:</p> $E = H_{\text{cl}}(\mathbf{r}, \mathbf{p}, t)$ <p>where</p> $H_{\text{cl}}(\mathbf{r}, \mathbf{p}, t) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t).$ <p>however in quantum we find the Hamiltonian upon substitution <math>\mathbf{p} \rightarrow \mathbf{p}_{\text{op}} = -i\hbar \nabla</math></p> $H \equiv H_{\text{cl}}(\mathbf{r}, -i\hbar \nabla, t).$ <p>thus, the Schrödinger-eq can be found classically with substitutions:</p> $E \rightarrow E_{\text{op}} = i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow \mathbf{p}_{\text{op}} = -i\hbar \nabla$ <p>and applying the operators <math>E_{\text{op}}</math> and <math>H \equiv H_{\text{cl}}(\mathbf{r}, -i\hbar \nabla, t)</math> on both sides on <math>\Psi(\mathbf{r}, t)</math>.</p> <div style="background-color: #f0f0f0; padding: 10px; margin-top: 10px;"> <p>■ <b>Klassiek:</b> energie is een scalair en een functie van <math>\vec{r}, \vec{p}, t</math></p> <math display="block">E(\vec{r}, \vec{p}, t) \equiv H_{\text{cl}}(\vec{r}, \vec{p}, t)</math> <p><math>H_{\text{cl}}</math>: <b>Klassieke Hamiltoniaan van het deeltje = energie</b></p> <p>1 Vrij deeltje: <math>H_{\text{cl}} = \frac{\vec{p} \cdot \vec{p}}{2m}</math></p> <p>2 Harmonische oscillator: <math>H_{\text{cl}} = \frac{\vec{p} \cdot \vec{p}}{2m} + \frac{1}{2} k \vec{r} \cdot \vec{r}</math></p> <p>■ <b>Kwantummechanisch:</b> de Hamiltoniaan wordt een operator</p> <math display="block">E_{\text{op}}(\vec{r}_{\text{op}}, \vec{p}_{\text{op}}, t) \equiv H(\vec{r}, -i\hbar \vec{\nabla}, t)</math> <p><math>H</math>: <b>Kwantummechanische Hamiltoniaan = energie-operator</b></p> <p>1 Vrij deeltje: <math>H = \frac{-\hbar^2}{2m} \vec{\nabla} \cdot \vec{\nabla}</math></p> <p>2 Harmonische oscillator: <math>H = \frac{-\hbar^2}{2m} \vec{\nabla} \cdot \vec{\nabla} + \frac{1}{2} k \vec{r} \cdot \vec{r}</math></p> </div>

3.2 conservation of probability	
statistical interpretation of $\Psi$	<p>If a particle is described by a wave function <math>\Psi(\mathbf{r}, t)</math>  &gt; the probability of finding the particle at time <math>t</math> within volume <math>d\mathbf{r} = dx dy dz</math> is:</p> $P(\mathbf{r}, t) d\mathbf{r} =  \Psi(\mathbf{r}, t) ^2 d\mathbf{r}$ <p>Which is normalised by:</p> $\int  \Psi(\mathbf{r}, t) ^2 d\mathbf{r} = 1$ <p>&gt; if <math>\Psi</math> can be normalised its <i>square integrable</i></p>
change of $P(\mathbf{r}, t)$ over time	<p>Probability should be conserved over time  ie: once <math>\Psi</math> is normalised at a given time <math>t</math>, it must remain so at all times:</p> $\frac{\partial}{\partial t} \int P(\mathbf{r}, t) d\mathbf{r} = 0$
Conservation of probability	<p>We can find an expression that verifies that <math>P</math> stays normalised over time</p> <p>Consider:</p> $\int_V P(\mathbf{r}, t) d\mathbf{r} = \int_V  \Psi(\mathbf{r}, t) ^2 d\mathbf{r} \quad (3.30)$ <p>where the integrals extend over the volume <math>V</math>. The rate of change of this probability is</p> $\frac{\partial}{\partial t} \int_V P(\mathbf{r}, t) d\mathbf{r} = \int_V \left[ \Psi^* \left( \frac{\partial \Psi}{\partial t} \right) + \left( \frac{\partial \Psi^*}{\partial t} \right) \Psi \right] d\mathbf{r}. \quad (3.31)$ <p>Where, according to the Schrödinger equation:</p> $-i\hbar \frac{\partial}{\partial t} \Psi^*(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi^*(\mathbf{r}, t)$ <p>we find:</p> $\begin{aligned} \frac{\partial}{\partial t} \int_V P(\mathbf{r}, t) d\mathbf{r} &= \frac{i\hbar}{2m} \int_V [\Psi^* (\nabla^2 \Psi) - (\nabla^2 \Psi^*) \Psi] d\mathbf{r} \\ &= \frac{i\hbar}{2m} \int_V \nabla \cdot [\Psi^* (\nabla \Psi) - (\nabla \Psi^*) \Psi] d\mathbf{r} \\ &= - \int_V \nabla \cdot \mathbf{j} d\mathbf{r}. \end{aligned} \quad (3.33)$ <p>In the last line we have introduced the vector</p> $\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi} [\Psi^* (\nabla \Psi) - (\nabla \Psi^*) \Psi] \quad (3.34)$ <p>We can thus verify that <math>P</math> is normalised at all times if there is a <math>\mathbf{j}</math> for which:</p> $\frac{\partial}{\partial t} \int_V P(\mathbf{r}, t) d\mathbf{r} = - \int_S \mathbf{j} \cdot d\mathbf{S}$
3.2.1 probability conservation and the Hermiticity of the Hamiltonian	
probability conservations in terms of $H$	<p>Use the form of the Schrödinger eq. with the Hamiltonian:</p> $-i\hbar \frac{\partial}{\partial t} \Psi^*(\mathbf{r}, t) = [H \Psi(\mathbf{r}, t)]^*$ <p>we can write the left-hand side of (3.29) as</p> $\begin{aligned} \frac{\partial}{\partial t} \int P(\mathbf{r}, t) d\mathbf{r} &= \frac{\partial}{\partial t} \int  \Psi(\mathbf{r}, t) ^2 d\mathbf{r} \\ &= \int \left[ \Psi^* \left( \frac{\partial \Psi}{\partial t} \right) + \left( \frac{\partial \Psi^*}{\partial t} \right) \Psi \right] d\mathbf{r} \\ &= (i\hbar)^{-1} \int [\Psi^* (H \Psi) - (H \Psi)^* \Psi] d\mathbf{r} \end{aligned}$ <p>so that the condition (3.29) becomes</p> $\int \Psi^* (H \Psi) d\mathbf{r} = \int (H \Psi)^* \Psi d\mathbf{r}.$ <p>ie <math>H</math> should be a Hermitian when acting on square integrable wave functions</p>

### 3.2.2 probability current density

probability current density

=  $\mathbf{j}$  as defined by the equation:

$$\frac{\partial}{\partial t} P(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0$$

ie: rate of change of the probability of finding a particle in a volume  $V$   
= the probability flux passing through the surface  $S$  of bounding  $V$

properties of  $\mathbf{j}$

We can also express  $\mathbf{j}$  as:

$$\mathbf{j}(\mathbf{r}, t) = \text{Re} \left\{ \Psi^* \frac{\hbar}{im} \nabla \Psi \right\}.$$

- $\frac{\hbar}{im} \nabla$  represents the quantity  $\mathbf{p}/m$ 
  - > product of velocity and density
  - >  $\mathbf{j}$  is the current density
- if  $\Psi$  is real,  $\mathbf{j}$  vanishes
  - > complex  $\Psi$  is needed if we describe non-zero probability situations
- $\Psi$  and  $\nabla \Psi$  are continuous
  - >  $\mathbf{j}$  and  $P$  are also continuous

### 3.3 expectation values and operators

expectation value of a function

for a function  $f(\mathbf{r}, t)$  working on  $\Psi$  we define:

$$\begin{aligned} \langle f(\mathbf{r}, t) \rangle &= \int f(\mathbf{r}, t) P(\mathbf{r}, t) d\mathbf{r} \\ &= \int \Psi^*(\mathbf{r}, t) f(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r} \end{aligned}$$

for example:

$$\begin{aligned} \langle \mathbf{r} \rangle &= \int \mathbf{r} P(\mathbf{r}, t) d\mathbf{r} \\ &= \int \Psi^*(\mathbf{r}, t) \mathbf{r} \Psi(\mathbf{r}, t) d\mathbf{r}. \end{aligned}$$

and we can do the same for  $\mathbf{p}$  with  $\Pi(\mathbf{p}, t) d\mathbf{p} = \Phi^*(\mathbf{p}, t) \Phi(\mathbf{p}, t) d\mathbf{p}$

$$\begin{aligned} \langle \mathbf{p} \rangle &= \int \mathbf{p} \Pi(\mathbf{p}, t) d\mathbf{p} \\ &= \int \Phi^*(\mathbf{p}, t) \mathbf{p} \Phi(\mathbf{p}, t) d\mathbf{p} \end{aligned}$$

expectation value of  $\mathbf{p}$

We can rewrite  $\langle \mathbf{p} \rangle$  as:

$$\langle \mathbf{p} \rangle = \int \Psi^*(\mathbf{r}, t) (-i\hbar \nabla) \Psi(\mathbf{r}, t) d\mathbf{r}.$$

> proof: p92

expectation value of  $E$

Consider  $E(\mathbf{r}, \mathbf{p})$  a function in both  $\mathbf{r}$  and  $\mathbf{p}$ :

$$E = \mathbf{p}^2/2m + V(\mathbf{r}, t)$$

> define the expectation value as:

$$\langle E \rangle = \left\langle \frac{\mathbf{p}^2}{2m} \right\rangle + \langle V \rangle$$

or in operator form:

$$\left\langle i\hbar \frac{\partial}{\partial t} \right\rangle = \left\langle -\frac{\hbar^2}{2m} \nabla^2 \right\rangle + \langle V \rangle$$

> now  $\mathbf{p}$  isn't included in  $E$  anymore, thus we can just use  $\Psi$ :

$$\begin{aligned} \langle E \rangle &= \int \Psi^*(\mathbf{r}, t) \left( i\hbar \frac{\partial}{\partial t} \right) \Psi(\mathbf{r}, t) d\mathbf{r} \\ &= \int \Psi^*(\mathbf{r}, t) H \Psi(\mathbf{r}, t) d\mathbf{r} = \int \Psi^*(\mathbf{r}, t) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t) d\mathbf{r} \\ &= \langle H \rangle. \end{aligned} \tag{3}$$

<p>expectation value of functions in <math>\mathbf{r}</math> and <math>\mathbf{p}</math></p>	<p>Consider <math>A(\mathbf{r}, \mathbf{p}, t)</math> a function defined by <math>\Psi(\mathbf{r}, t)</math></p> <p>1: substitute variables by their operators:</p> $A(\mathbf{r}, -i\hbar \nabla, t)$ <p>2: calculate <math>\langle A \rangle</math> from the expression:</p> $\langle A \rangle = \int \Psi^*(\mathbf{r}, t) A(\mathbf{r}, -i\hbar \nabla, t) \Psi(\mathbf{r}, t) d\mathbf{r}.$ <p>&gt; if <math>A</math> isn't normalised, it should be replaced by:</p> $\langle A \rangle = \frac{\int \Psi^*(\mathbf{r}, t) A(\mathbf{r}, -i\hbar \nabla, t) \Psi(\mathbf{r}, t) d\mathbf{r}}{\int \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r}}.$																
<p>&gt; variables and their operators</p>	<table border="1"> <thead> <tr> <th>Physical quantity</th><th>Operator</th></tr> </thead> <tbody> <tr> <td>Position coordinate <math>x</math></td><td><math>x</math></td></tr> <tr> <td>Position vector <math>\mathbf{r}</math></td><td><math>\mathbf{r}</math></td></tr> <tr> <td><math>x</math> component of momentum <math>p_x</math></td><td><math>-i\hbar \frac{\partial}{\partial x}</math></td></tr> <tr> <td>Momentum <math>\mathbf{p}</math></td><td><math>-i\hbar \nabla</math></td></tr> <tr> <td>Kinetic energy <math>T = \frac{\mathbf{p}^2}{2m}</math></td><td><math>-\frac{\hbar^2}{2m} \nabla^2</math></td></tr> <tr> <td>Potential energy <math>V(\mathbf{r}, t)</math></td><td><math>V(\mathbf{r}, t)</math></td></tr> <tr> <td>Total energy <math>\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)</math></td><td><math>H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t)</math></td></tr> </tbody> </table> <p>&gt; say <math>A</math> is an operator associated with physical quantities <math>B</math></p> <p>&gt; expectation value <math>\langle A \rangle</math> must be real quantities</p> <p>&gt; for any wave function, it should hold:</p> $\int \Psi^* A \Psi d\mathbf{r} = \int (A \Psi)^* \Psi d\mathbf{r}$ <p>&gt; operator must be Hermitian</p>	Physical quantity	Operator	Position coordinate $x$	$x$	Position vector $\mathbf{r}$	$\mathbf{r}$	$x$ component of momentum $p_x$	$-i\hbar \frac{\partial}{\partial x}$	Momentum $\mathbf{p}$	$-i\hbar \nabla$	Kinetic energy $T = \frac{\mathbf{p}^2}{2m}$	$-\frac{\hbar^2}{2m} \nabla^2$	Potential energy $V(\mathbf{r}, t)$	$V(\mathbf{r}, t)$	Total energy $\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)$	$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t)$
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<p>commutator of operators</p>	<p>For <math>A</math> and <math>B</math> two operators</p> <p>&gt; define <math>[A, B] = AB - BA</math> the <i>commutator of <math>A</math> and <math>B</math></i></p> <p>&gt; if <math>[A, B] = 0</math> then <math>A</math> and <math>B</math> commute ie: <math>AB = BA</math></p> <p>&gt;&gt; not all operators commute</p>																

### 3.4 transition from quantum mechanics to classical mechanics: The Ehrenfest theorem

Ehrenfest theorem

Quantum mechanics should converge to classical mechanics for big enough scales  
> to test this, we need to prove two classical Newton formulas:

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m} \quad \text{and} \quad \frac{d\mathbf{p}}{dt} = -\nabla V$$

for expectation values of corresponding quantum operators  
for  $\Psi$  a square-integrable solution normalised to unity

1:  $dr/dt = p/m$

For the expectation value of  $x$ :

$$\begin{aligned} \frac{d}{dt}\langle x \rangle &= \frac{d}{dt} \int \Psi^*(\mathbf{r}, t) x \Psi(\mathbf{r}, t) d\mathbf{r} \\ &= \int \Psi^*(\mathbf{r}, t) x \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} d\mathbf{r} + \int \frac{\partial \Psi^*(\mathbf{r}, t)}{\partial t} x \Psi(\mathbf{r}, t) d\mathbf{r}. \end{aligned}$$

using the Schrödinger eq. for  $\Psi$  and  $\Psi^*$ :

$$\begin{aligned} \frac{d}{dt}\langle x \rangle &= (i\hbar)^{-1} \left[ \int \Psi^* x (H\Psi) d\mathbf{r} - \int (H\Psi)^* x \Psi d\mathbf{r} \right] \\ &= (i\hbar)^{-1} \left[ \int \Psi^* x \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \right) d\mathbf{r} \right. \\ &\quad \left. - \int \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \right) x \Psi d\mathbf{r} \right]. \end{aligned}$$

The terms involving the potential  $V$  cancel out, so that

$$\frac{d}{dt}\langle x \rangle = \frac{i\hbar}{2m} \int [\Psi^* x (\nabla^2 \Psi) - (\nabla^2 \Psi^*) x \Psi] d\mathbf{r}.$$

> Now Greens identity says:  $\int_V [u(\nabla^2 v) + (\nabla u) \cdot (\nabla v)] d\mathbf{r} = \int_S u(\nabla v) \cdot d\mathbf{S}$

Thus we could write:

$$\int (\nabla^2 \Psi^*) x \Psi d\mathbf{r} = \int_S x \Psi (\nabla \Psi^*) \cdot d\mathbf{S} - \int (\nabla \Psi^*) \cdot \nabla (x \Psi) d\mathbf{r}. \quad (3.84)$$

The first integral on the right is over the infinite bounding surface  $S$ , and hence is equal to zero because the wave function  $\Psi$  vanishes at large distances. Consequently, we have

$$\int (\nabla^2 \Psi^*) x \Psi d\mathbf{r} = - \int (\nabla \Psi^*) \cdot \nabla (x \Psi) d\mathbf{r}. \quad (3.85)$$

Using again Green's first identity, we have

$$- \int (\nabla \Psi^*) \cdot \nabla (x \Psi) d\mathbf{r} = - \int_S \Psi^* \nabla (x \Psi) \cdot d\mathbf{S} + \int \Psi^* \nabla^2 (x \Psi) d\mathbf{r}. \quad (3.86)$$

Again the surface integral vanishes, so that

$$\int (\nabla^2 \Psi^*) x \Psi d\mathbf{r} = \int \Psi^* \nabla^2 (x \Psi) d\mathbf{r}. \quad (3.87)$$

Which we can use to simplify the equation:

$$\begin{aligned} \frac{d}{dt}\langle x \rangle &= \frac{i\hbar}{2m} \int \Psi^* [x \nabla^2 \Psi - \nabla^2 (x \Psi)] d\mathbf{r} \\ &= -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} d\mathbf{r}. \end{aligned}$$

which is the expression:

$$\frac{d}{dt}\langle x \rangle = \frac{\langle p_x \rangle}{m}$$

$$2: dp/dt = -\nabla V$$

$$\begin{aligned}\frac{d}{dt}\langle p_x \rangle &= -i\hbar \frac{d}{dt} \int \Psi^* \frac{\partial \Psi}{\partial x} d\mathbf{r} \\ &= -i\hbar \left[ \int \Psi^* \frac{\partial}{\partial x} \frac{\partial \Psi}{\partial t} d\mathbf{r} + \int \frac{\partial \Psi^*}{\partial t} \frac{\partial \Psi}{\partial x} d\mathbf{r} \right].\end{aligned}$$

Replace  $\Psi$  and  $\Psi^*$  by their schrödinger eq.:

$$\begin{aligned}\frac{d}{dt}\langle p_x \rangle &= -\int \Psi^* \frac{\partial}{\partial x} \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \right) d\mathbf{r} + \int \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \right) \frac{\partial \Psi}{\partial x} d\mathbf{r} \\ &= \frac{\hbar^2}{2m} \int \left[ \Psi^* \left( \nabla^2 \frac{\partial \Psi}{\partial x} \right) - (\nabla^2 \Psi^*) \frac{\partial \Psi}{\partial x} \right] d\mathbf{r} \\ &\quad - \int \Psi^* \left[ \frac{\partial}{\partial x} (V\Psi) - V \frac{\partial \Psi}{\partial x} \right] d\mathbf{r}.\end{aligned}\quad (3.91)$$

Assuming that  $\partial \Psi / \partial x$ , as well as  $\Psi$ , vanishes at large distances, the first integral on the right of (3.91) is equal to zero by Green's second identity<sup>7</sup>, in which  $u = \Psi^*$  and  $v = \partial \Psi / \partial x$ . The second integral on the right of (3.91) is just

$$\begin{aligned}- \int \Psi^* \left[ \frac{\partial}{\partial x} (V\Psi) - V \frac{\partial \Psi}{\partial x} \right] d\mathbf{r} &= - \int \Psi^* \frac{\partial V}{\partial x} \Psi d\mathbf{r} \\ &= - \left\langle \frac{\partial V}{\partial x} \right\rangle\end{aligned}\quad (3.92)$$

so that

$$\frac{d}{dt}\langle p_x \rangle = - \left\langle \frac{\partial V}{\partial x} \right\rangle \quad (3.93)$$

### 3.5 the time-dependent Schrödinger equation. Stationary states

time independent Schrödinger eq.

Consider a potential  $V(\mathbf{r})$  independent from  $t$

> then  $H$  is also independent from  $t$ :  $H = -(\hbar^2/2m)\nabla^2 + V(\mathbf{r})$

For a solution of  $\Psi$  of the form:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r})f(t)$$

we can substitute in the TDSE to get:

$$i\hbar \psi(\mathbf{r}) \frac{df(t)}{dt} = \left[ -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) \right] f(t).$$

Dividing both sides of this equation by  $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})f(t)$ , we find that

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = \frac{1}{\psi(\mathbf{r})} \left[ -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) \right].$$

the left side is only dependent on  $t$

right side  $\mathbf{r}$

> both sides should be constant

> has the dimension of an energy  $E$ :

$$i\hbar \frac{d}{dt} f(t) = E f(t)$$

and

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r}).$$

The first equation can be immediately integrated to give

$$f(t) = C \exp(-iEt/\hbar)$$

Where we can take  $C=1$ , to find the solutions of the TISE given by:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp(-iEt/\hbar).$$

TISE as an eigenvalue problem	<p>Since <math>H = -(\hbar^2/2m)\nabla^2 + V(\mathbf{r})</math> we can simplify the TISE to:</p> $H\psi(\mathbf{r}) = E\psi(\mathbf{r})$ <p>where the eigenfunction <math>\psi(\mathbf{r})</math> corresponds to an eigenvalue <math>E</math></p> <p>And each solution of the TISE is also an eigenfunction of <math>H</math></p> $H\Psi = E\Psi.$ <p>which can be rewritten since <math>E_{\text{op}} = i\hbar\partial/\partial t</math> :</p> $i\hbar\frac{\partial}{\partial t}\Psi = E\Psi$
proof: E a real constant	<p>To prove that <math>E</math> is real, we can look at the probability density:</p> $P(\mathbf{r}, t) = \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)$ $= \psi^*(\mathbf{r})\psi(\mathbf{r})\exp\left[-\frac{i}{\hbar}(E - E^*)t\right].$ <p>since probability conservation we get:</p> $(E - E^*) \int \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d\mathbf{r} = 0$ <p>thus <math>E=E^*</math></p>
expectation value of $E$	<p>We can calculate <math>\langle E \rangle</math>:</p> $\langle E \rangle = \int \Psi^*(\mathbf{r}, t) \left( i\hbar \frac{\partial}{\partial t} \right) \Psi(\mathbf{r}, t) d\mathbf{r} = \int \Psi^*(\mathbf{r}, t) H \Psi(\mathbf{r}, t) d\mathbf{r}$ $= E$ <p>Which can be shown to be:</p> $E = \langle H \rangle = \langle T \rangle + \langle V \rangle.$ <p>More generally:</p> $\langle E^n \rangle = \int \Psi^*(\mathbf{r}, t) H^n \Psi(\mathbf{r}, t) d\mathbf{r} = E^n.$
expectation values of functions of $E$	<p>For a function <math>f()</math> that can be expanded around <math>E</math>:</p> $f(E) = \sum_n a_n E^n$ <p>its expectation value, in a state (3.100) normalised to unity, is given by</p> $\langle f(E) \rangle = \sum_n a_n \langle E^n \rangle = \sum_n a_n E^n = f(E)$
<b>3.5.1 stationary states</b>	
stationary state	<p>= <math>\psi()</math> that are not dependent on time</p> <p>ie: <math>\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp(-iEt/\hbar).</math></p> <p>then: - probability density is given by:</p> $P(\mathbf{r}) = \psi^*(\mathbf{r})\psi(\mathbf{r}) =  \psi(\mathbf{r}) ^2$ <p>&gt; constant over time</p> <p>- the probability current density is given by:</p> $\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2mi} \{ \psi^*(\mathbf{r})[\nabla\psi(\mathbf{r})] - [\nabla\psi^*(\mathbf{r})]\psi(\mathbf{r}) \}$ <p>and since <math>P</math> is time-independent, the continuity eq. reduce to:</p> $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0.$



### 3.6 energy quantisation

energy case study

consider a particle moving in 1D on a potential  $V(x)$

> stationary states:

$$\Psi(x, t) = \psi(x) \exp(-iEt/\hbar)$$

solutions of the TISE:

$$H\psi(x) \equiv -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

which we shall rewrite for convenience as

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E]\psi(x).$$

Where  $\psi(x)$  should be finite and single-valued everywhere

For a solution  $\psi(x)$ , we know that: - the real part of  $\psi(x)$  is also a solution:

$$[\psi(x) + \psi^*(x)]/2$$

- the imaginary part is also a solution:

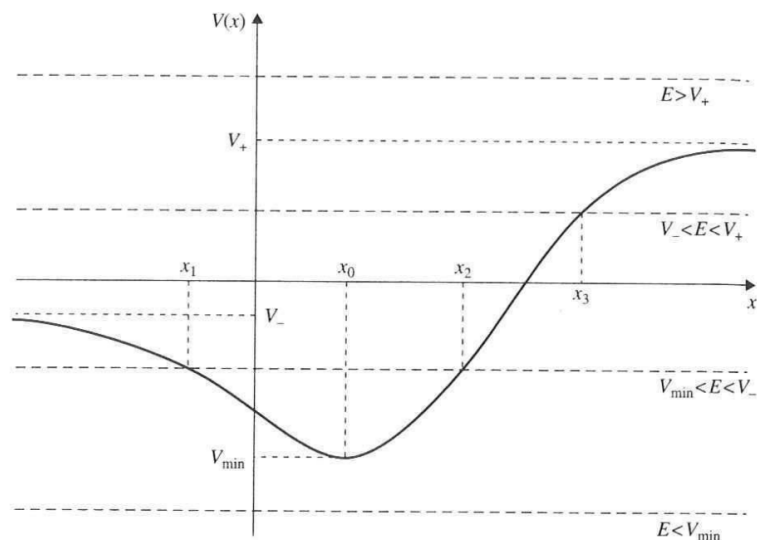
$$[\psi(x) - \psi^*(x)]/2i$$

which are both real functions

> we only need to analyse the real eigenfunctions to construct all eigenfunctions

>> we study 4 cases in a potential  $V(x)$  where:

- $V(x) = V_-$  for  $x \rightarrow -\infty$
- as  $x$  increases,  $V(x)$  decreases to  $V_{\min}$
- for  $x > x_0$   $V(x)$  increases until it becomes equal to  $V_+$



1:  $E < V_{\min}$

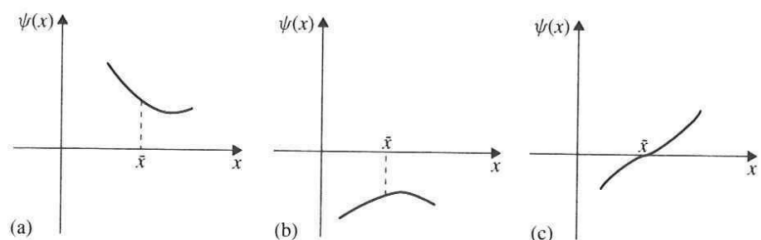
$V(x) - E$  is always positive

>  $d^2\psi/dx^2$  always has the same sign as  $\psi$

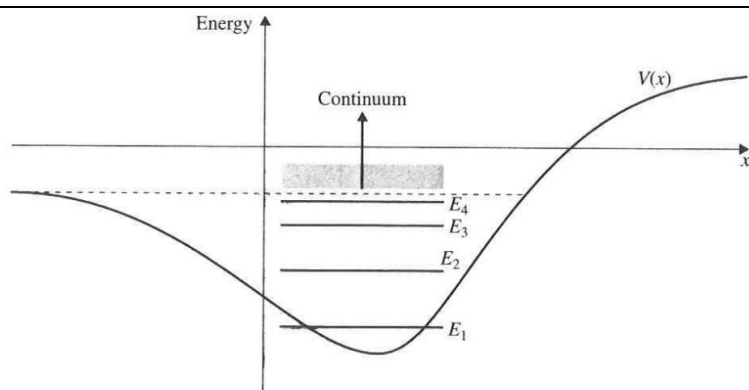
- > if: -  $\psi > 0$ , then the function curves upwards
- $\psi < 0$ , the function curves downwards
- $\psi = 0$ , the function escapes the x-axis

>> each solution will approach infinite values

> there is no physically acceptable solution



<p>2: <math>V_{\min} &lt; E &lt; V_{\infty}</math></p>	<p>There are two points <math>x_1</math> and <math>x_2</math> for which <math>E = V(x)</math>  &gt; these are <i>turning points</i></p> <p>a) For <math>x_1 &lt; x &lt; x_2</math>, <math>V(x) - E</math> is negative  &gt; <math>d^2\psi/dx^2</math> has opposite sign as <math>\psi</math>  &gt; for:     - <math>\psi &gt; 0</math>, the function curves downwards                - <math>\psi &lt; 0</math>, the function curves upwards                - <math>\psi = 0</math>, the function escapes the x-axis  &gt; =oscillatory behaviour</p> <p>b) For <math>x &lt; x_1</math> and <math>x &gt; x_2</math>, <math>V(x) - E</math> is positive  &gt; <math>d^2\psi/dx^2</math> has same sign as <math>\psi</math>  &gt; same as case study one</p> <p>we can find energies for which <math>\psi \rightarrow 0</math> as <math>x \rightarrow \pm\infty</math>  &gt; there are certain, discrete energies for which <math>\psi \rightarrow 0</math>  &gt; only these solutions are physically acceptable</p> <div data-bbox="786 674 1476 1176"> </div> <p>&gt; quantisation of bound state energies  &gt; result of eigenvalue problem in TISE</p> <p>We can prove that for a certain <math>E</math>, there is only one <math>\psi</math></p>
<p>3: <math>V_{\infty}^- &lt; E &lt; V_{\infty}^+</math></p>	<p>There is only one turning point <math>x_3</math>  &gt; only the unique solution for which <math>\psi \rightarrow 0</math> for <math>x \rightarrow +\infty</math> for a certain <math>E</math> is physically acceptable</p> <p>however for <math>x &lt; x_3</math> there is permanent oscillatory behaviour  &gt; <math>\psi</math> isn't square integrable</p> <p>These solutions are called <i>unbound</i>  &gt; continuum</p> <div data-bbox="1129 1395 1497 1585"> </div>
<p>4: <math>E &gt; V_{\infty}^+</math></p>	<p>permanent oscillatory behaviour  &gt; for each <math>E</math>, there are two physically acceptable solutions  &gt; non square integrable</p> <p>&gt;&gt; unbound solutions</p> <div data-bbox="1173 1601 1497 1796"> </div>



3.7: properties of the energy eigenfunctions	
Integrability of unbound solutions	<p>We have seen that unbound solutions aren't square integrable</p> <p>Solution: enclose the system in a box with impenetrable walls          &gt; entire eigenvalue spectrum becomes discrete          &gt; for volumes V of the box large enough this doesn't effect the outcome</p>
orthogonality relations	<p>Let <math>\psi_E(x)</math> be the eigenfunction for an energy E          &gt; for V the volume of a large box, the eigenfunction can be normalised:</p> $\int_V \psi_E^*(\mathbf{r})\psi_E(\mathbf{r})d\mathbf{r} = 1$ <p>we can prove the orthogonality of two eigenfunctions <math>\psi_E</math> and <math>\psi_{E'}</math> for E and E':</p> $\int \psi_{E'}^*(\mathbf{r})\psi_E(\mathbf{r})d\mathbf{r} = 0, \quad E \neq E'.$ <p>which can be combined to form orthogonality relations:</p> $\int \psi_{E'}^*(\mathbf{r})\psi_E(\mathbf{r})d\mathbf{r} = \delta_{EE'}$ <p>where <math>\delta_{EE'}</math> is the Kronecker <math>\delta</math>-symbol, such that</p> $\delta_{EE'} = \begin{cases} 1 & \text{if } E = E' \\ 0 & \text{if } E \neq E' \end{cases}$
proof: orthogonality	<p>Since <math>H\psi_E = E\psi_E</math> we can multiply both sides by <math>\psi_{E'}^*</math>:</p> $\psi_{E'}^*(H\psi_E) = E\psi_{E'}^*\psi_E$ <p>But we also have that <math>H\psi_{E'} = E'\psi_{E'}</math>, so taking the complex conjugate:</p> $(H\psi_{E'})^* = E'\psi_{E'}^*$ <p>and multiplying both sides by <math>\psi_E</math> gives us:</p> $(H\psi_{E'})^*\psi_E = E'\psi_{E'}^*\psi_E.$ <p>subtract the two and integrate over volume V:</p> $(E - E') \int \psi_{E'}^*\psi_E d\mathbf{r} = \int [\psi_{E'}^*(H\psi_E) - (H\psi_{E'})^*\psi_E] d\mathbf{r} = 0$
general solution of $\Psi(\mathbf{r},t)$	<p>For a given potential V(x) independent from t</p> <p>&gt; the solution of <math>\Psi(\mathbf{r},t)</math> is a superposition of all the eigenfunctions of the TISE:</p> $\Psi(\mathbf{r}, t) = \sum_E C_E(t)\psi_E(\mathbf{r})$ <p>with expansion coefficients dependent on time</p>
calculating $C_E(t)$	<p>We can easily see:</p> $\begin{aligned} \int \psi_{E'}^*(\mathbf{r})\Psi(\mathbf{r}, t)d\mathbf{r} &= \sum_E C_E(t) \int \psi_{E'}^*(\mathbf{r})\psi_E(\mathbf{r})d\mathbf{r} \\ &= \sum_E C_E(t)\delta_{EE'} \\ &= C_{E'}(t). \end{aligned}$
oscillation theorem	<p>For bound states of one-dimensional systems</p> <p>For bound state eigenfunctions <math>\psi_1, \psi_2, \dots, \psi_n, \dots</math> for energies <math>E_1 &lt; E_2 &lt; \dots &lt; E_n &lt; \dots</math></p> <p>&gt; the nth eigenfunction will have (n-1) zeros for finite values of x          and          between two consecutive zeros of <math>\psi_n</math> the following eigenvalues will have at least 1 zero</p>

### 3.8 general solution of the time-dependent Schrödinger equation for a time-independent potential

expansion of  $\Psi(\mathbf{r}, t)$

We know that  $\Psi$  can be expanded in terms of eigenfunctions:

$$\Psi(\mathbf{r}, t) = \sum_E C_E(t) \psi_E(\mathbf{r})$$

we can simplify the right-hand of the equation by multiplying by  $H$ :

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \sum_E C_E(t) \psi_E(\mathbf{r}) &= H \sum_E C_E(t) \psi_E(\mathbf{r}) \\ &= \sum_E C_E(t) H \psi_E(\mathbf{r}) \\ &= \sum_E C_E(t) E \psi_E(\mathbf{r}). \end{aligned}$$

multiply by  $\psi_{E'}^*$  and integrate over a box with volume  $V$ :

$$i\hbar \frac{\partial}{\partial t} \sum_E C_E(t) \int \psi_{E'}^*(\mathbf{r}) \psi_E(\mathbf{r}) d\mathbf{r} = \sum_E C_E(t) E \int \psi_{E'}^*(\mathbf{r}) \psi_E(\mathbf{r}) d\mathbf{r}.$$

which, due to orthogonality, reduces to:

$$i\hbar \frac{d}{dt} C_E(t) = E C_E(t)$$

integration leaves us with the result:

$$C_E(t) = C_E(t_0) \exp[-iE(t - t_0)/\hbar].$$

Thus we have a solution for the TDSE:

$$\Psi(\mathbf{r}, t) = \sum_E C_E(t_0) \exp[-iE(t - t_0)/\hbar] \psi_E(\mathbf{r})$$

or:

$$\Psi(\mathbf{r}, t) = \sum_E c_E \psi_E(\mathbf{r}) \exp(-iEt/\hbar)$$

where the constants  $c_E$  are given by

$$c_E = C_E(t_0) \exp(iEt_0/\hbar).$$

propagator  $K(\mathbf{r}, t; \mathbf{r}', t_0)$

At any particular time  $t_0$ , the constants  $c_E$  can be evaluated by knowledge of  $\Psi$ :

$$c_E = \exp(iEt_0/\hbar) \int \psi_E^*(\mathbf{r}) \Psi(\mathbf{r}, t_0) d\mathbf{r} \quad (3.154)$$

so that the general solution (3.152) may be written as

$$\Psi(\mathbf{r}, t) = \sum_E \left[ \int \psi_E^*(\mathbf{r}') \Psi(\mathbf{r}', t_0) d\mathbf{r}' \right] \exp[-iE(t - t_0)/\hbar] \psi_E(\mathbf{r}). \quad (3.155)$$

This expression gives  $\Psi(\mathbf{r}, t)$  at any time, once it is known at the time  $t = t_0$ . If we define the function

$$K(\mathbf{r}, t; \mathbf{r}', t_0) = \sum_E \psi_E^*(\mathbf{r}') \psi_E(\mathbf{r}) \exp[-iE(t - t_0)/\hbar] \quad (3.156)$$

we see that we may recast (3.155) in the simpler form

$$\Psi(\mathbf{r}, t) = \int K(\mathbf{r}, t; \mathbf{r}', t_0) \Psi(\mathbf{r}', t_0) d\mathbf{r}'. \quad (3.157)$$

normalization condition in $c_E$	<p>The complex conjugate of <math>\Psi</math> is:</p> $\Psi^*(\mathbf{r}, t) = \sum_{E'} c_{E'}^* \psi_{E'}^*(\mathbf{r}) \exp(iE't/\hbar)$ <p>Where we must have:</p> $\int \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r} = \sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] \int \psi_{E'}^*(\mathbf{r}) \psi_E(\mathbf{r}) d\mathbf{r}$ $= 1 \quad (3.159)$ <p>since the energy eigenfunctions are orthogonal, we have:</p> $\sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] \int \psi_{E'}^*(\mathbf{r}) \psi_E(\mathbf{r}) d\mathbf{r}$ $= \sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] \delta_{EE'}$ $= \sum_E  c_E ^2$ <p>thus we can simplify the normalization condition to be: <math>\sum_E  c_E ^2 = 1.</math></p>
expectation value of E	<p>For a general wave function:</p> $\langle E \rangle = \langle H \rangle = \int \Psi^*(\mathbf{r}, t) H \Psi(\mathbf{r}, t) d\mathbf{r}$ $= \sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] \int \psi_{E'}^*(\mathbf{r}) H \psi_E(\mathbf{r}) d\mathbf{r}$ $= \sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] E \int \psi_{E'}^*(\mathbf{r}) \psi_E(\mathbf{r}) d\mathbf{r}$ $= \sum_E \sum_{E'} c_{E'}^* c_E \exp[-i(E - E')t/\hbar] E \delta_{EE'}$ $= \sum_E  c_E ^2 E$
TDSE outside the box	<p>Until now we have enclosed the system in a box with volume V</p> <ul style="list-style-type: none"> <li>&gt; system without box: partly discrete and partly continuous</li> <li>&gt; general solution of TDSE will be a sum of infinite eigenfunctions</li> <li>ie: take an integral instead of a sum for the continuous part</li> </ul>
<b>3.9: Schrödinger equation in momentum space</b>	
Momentum space TDSE	<p>Insert the equation for <math>\phi</math> in the TDSE and we find:</p> $i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{p}, t) = \frac{\mathbf{p}^2}{2m} \Phi(\mathbf{p}, t) + (2\pi\hbar)^{-3/2} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} V(\mathbf{r}, t) \Psi(\mathbf{r}, t) d\mathbf{r}.$ <p>using the convolution theorem we can simplify this to:</p> $i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{p}, t) = \frac{\mathbf{p}^2}{2m} \Phi(\mathbf{p}, t) + \int \tilde{V}(\mathbf{p} - \mathbf{p}', t) \Phi(\mathbf{p}', t) d\mathbf{p}'$ <p>where</p> $\tilde{V}(\mathbf{p} - \mathbf{p}', t) = (2\pi\hbar)^{-3} \int e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} V(\mathbf{r}, t) d\mathbf{r}.$ <p>&gt;&gt; more complicated than the TDSE</p> <ul style="list-style-type: none"> <li>&gt; not used very much</li> </ul>

### 3.9.1 expectation values

expectation value of  $\mathbf{r}$

for the x-component of  $\mathbf{r}$ , we find  $\langle x \rangle$  by using  $\psi$  and expressing this in terms of  $\phi$ :

$$\langle x \rangle = \int \Phi^*(\mathbf{p}, t) \left( i\hbar \frac{\partial}{\partial p_x} \right) \Phi(\mathbf{p}, t) d\mathbf{p}$$

Thus we find for  $\mathbf{r}$ :

$$\langle \mathbf{r} \rangle = \int \Phi^*(\mathbf{p}, t) (i\hbar \nabla_{\mathbf{p}}) \Phi(\mathbf{p}, t) d\mathbf{p}$$

thus  $\mathbf{r}$  is represented in momentum space as the operator:

$$\mathbf{r}_{\text{op}} = i\hbar \nabla_{\mathbf{p}}$$

expectation values in momentum space

We can find any expectation value by following the same rules as in configuration space:

1: For a dynamical variable  $A(\mathbf{r}, \mathbf{p}, t)$  substitute position vars with their operators:

$$A(i\hbar \nabla_{\mathbf{p}}, \mathbf{p}, t)$$

2: the expectation value is then given by

$$\langle A \rangle = \int \Phi^*(\mathbf{p}, t) A(i\hbar \nabla_{\mathbf{p}}, \mathbf{p}, t) \Phi(\mathbf{p}, t) d\mathbf{p}. \quad (3.179)$$

If the wave function  $\Phi(\mathbf{p}, t)$  is not normalised to unity, the above expression must be replaced by

$$\langle A \rangle = \frac{\int \Phi^*(\mathbf{p}, t) A(i\hbar \nabla_{\mathbf{p}}, \mathbf{p}, t) \Phi(\mathbf{p}, t) d\mathbf{p}}{\int \Phi^*(\mathbf{p}, t) \Phi(\mathbf{p}, t) d\mathbf{p}}. \quad (3.180)$$

variables and their operators

Physical quantity	Operator
Position coordinate $x$	$i\hbar \frac{\partial}{\partial p_x}$
Position vector $\mathbf{r}$	$i\hbar \nabla_{\mathbf{p}}$
x-component of momentum $p_x$	$p_x$
Momentum $\mathbf{p}$	$\mathbf{p}$
Kinetic energy $T = \frac{\mathbf{p}^2}{2m}$	$\frac{\mathbf{p}^2}{2m}$
Potential energy $V(\mathbf{r}, t)$	$V(i\hbar \nabla_{\mathbf{p}}, t)$
Total energy $\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)$	$H = \frac{\mathbf{p}^2}{2m} + V(i\hbar \nabla_{\mathbf{p}}, t)$

### 3.9.2 stationary states

separable form of  $\phi$

For  $V$  and time-independent potential energy, we find:

$$\Phi(\mathbf{p}, t) = \phi(\mathbf{p}) \exp(-iEt/\hbar)$$

with a probability density constant in time:

$$\Pi(\mathbf{p}) = |\phi(\mathbf{p})|^2 = \phi^*(\mathbf{p})\phi(\mathbf{p})$$

we clearly see that  $\phi$  is the Fourier-transform of  $\psi$

> eigenfunctions for momentum space can be found by Fourier-transforming:

$$\phi(\mathbf{p}) = (2\pi\hbar)^{-3/2} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \psi(\mathbf{r}) d\mathbf{r},$$

$$\psi(\mathbf{r}) = (2\pi\hbar)^{-3/2} \int e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \phi(\mathbf{p}) d\mathbf{p}.$$

TISE for momentum space

We can find:

$$\frac{\mathbf{p}^2}{2m} \phi(\mathbf{p}) + \int \tilde{V}(\mathbf{p} - \mathbf{p}') \phi(\mathbf{p}') d\mathbf{p}' = E \phi(\mathbf{p})$$

where

$$\tilde{V}(\mathbf{p} - \mathbf{p}') = (2\pi\hbar)^{-3} \int e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} V(\mathbf{r}) d\mathbf{r}.$$