Lesson 3: The interpretation of matter waves

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$\Psi(\vec{r}, t)$

- complex
- not measurable quantities

Connection between $\Psi(\vec{r}, t)$ and associated particle behavior

$$\Downarrow$$

PROBABILITY DENSITY

$$P(\vec{r}, t) \;=\; |\Psi(\vec{r}, t)|^2$$

probability per unit volume of finding the particle in the neighborhood of $\vec{r}$ at time t (is real and positive)
in one dimension $P(x, t) \;=\; |\Psi(x, t)|^2 \;\rightarrow$ prob. per unit length .... x. .. t

PROBABILITY

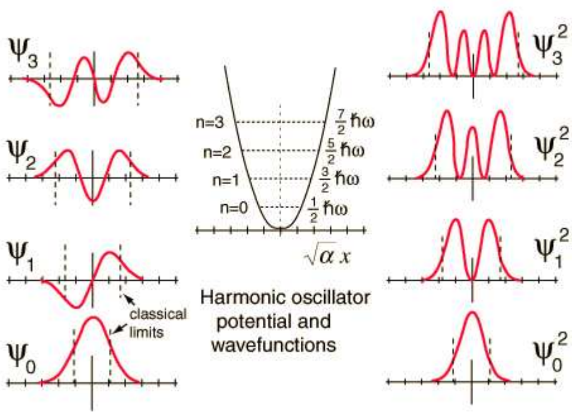
$$P(\vec{r}, t)\; d^3\vec{r}$$

probability of finding the particle in a volume $d^3\vec{r}$ around $\vec{r}$ at time t
(in one dimension $P(x, t)\; dx$ probab.....in length dx.... x....t)

We demand the normalization of the wave function

$$\int_{all\;\; space} P(\vec{r}, t)\; d^3\vec{r} \;=\; 1$$

(the probability of finding the particle in all space is $100\;\%$)



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In one dimension, the probability of finding the particle between $x = a$ and $x = b$, $P(a \leq x \leq b)$:

$$\int_a^b P(x,t)\,dx$$

In three dimensions, the probability of finding the particle in a volume V

$$\int_V P(\vec{r},t)\,d^3\vec{r}$$

Quantum predictions do not give the position of the particle in a time (classical), they give the probability of being in a volume (or length)

they are statistical predictions

It is Born's interpretation of the wave function

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Characteristic position of a particle with wave function $\Psi(\vec{r}, t)$ can be its mean or expected value

$$< \vec{r} > \; = \bar{\vec{r}} = \frac{\int \vec{r} P(\vec{r}, t) \; d^3\vec{r}}{\int P(\vec{r}, t) \; d^3\vec{r}} = \frac{\int \Psi^*(\vec{r}, t) \; \vec{r} \; \Psi(\vec{r}, t) \; d^3\vec{r}}{\int \Psi^*(\vec{r}, t)\Psi(\vec{r}, t) \; d^3\vec{r}}$$

For a problem in one dimension

$$< x > \; = \bar{x} = \frac{\int_{-\infty}^{\infty} \Psi^*(x, t) \; x \; \Psi(x, t) \; dx}{\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t) \; dx}$$

Expected value of $f(x)$

$$< f(x) > \; = \frac{\int_{-\infty}^{\infty} \Psi^*(x, t) \; f(x) \; \Psi(x, t) \; dx}{\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t) \; dx}$$

analogue in three dimensions

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Expected value of $f(x, t)$

$$< f(x, t) > \; = \frac{\int_{-\infty}^{\infty} \Psi^*(x, t) \; f(x, t) \; \Psi(x, t) \; dx}{\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t) \; dx}$$

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With functions $\neq f(\vec{r}, t)$. How do you calculate mean values?

$$\Downarrow$$

operators must be associated

- For example $\vec{p} \neq f(\vec{r})$
  Let's consider the plane wave $\Psi(\vec{r}, t) \;=\; e^{i(\vec{k}\cdot\vec{r}-\omega t)}$

$$\frac{\partial \Psi(\vec{r}, t)}{\partial x_j} \;=\; i\, k_j\, \Psi(\vec{r}, t) \;= i\, \frac{p_j}{\hbar}\, \Psi(\vec{r}, t)\ ;\ j = 1, 2, 3$$

$$\vec{p}\, \Psi(\vec{r}, t) \;=\; -\, i\hbar \vec{\nabla} \Psi(\vec{r}, t)$$

  we associate $\vec{p} \rightarrow -i\hbar\vec{\nabla}$ (differential operator)

- For the energy

$$\frac{\partial \Psi(\vec{r}, t)}{\partial t} \;=\; -\, i\, \omega\, \Psi(\vec{r}, t) \;=\; -\, i\, \frac{E}{\hbar}\, \Psi(\vec{r}, t)$$

$$E\, \Psi(\vec{r}, t) \;=\; i\, \hbar\, \frac{\partial \Psi(\vec{r}, t)}{\partial t}$$

  we associate $E \rightarrow i\, \hbar\, \frac{\partial}{\partial t}$ (differential operator)

- If the particle is not free

$$\frac{p^2}{2m} \;+\; V(\vec{r}, t) \;=\; E$$

  we substitute the associated operators

$$-\frac{\hbar^2}{2m}\, \nabla^2 \;+\; V(\vec{r}, t) \;=\; i\, \hbar\, \frac{\partial}{\partial t} \;=\; H$$

We obtain the operator equation
We call **Hamiltonian** the operator associated with the energy, H

Therefore

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

SCHRÖDINGER EQUATION

ASSOCIATED OPERATORS ARE COMPATIBLE WITH SCHRÖDINGER EQUATION

If we assume a normalized $\Psi(\vec{r},t)$s $\rightarrow \int |\Psi(\vec{r},t)|^2\ d^3\vec{r}\ =\ 1$

$$\begin{aligned} <\vec{p}> &= \int d^3\vec{r}\ \Psi^*(\vec{r},t)\left(-i\hbar\vec{\nabla}\right)\Psi(\vec{r},t) \\ &= -i\hbar\int d^3\vec{r}\ \Psi^*(\vec{r},t)\vec{\nabla}\Psi(\vec{r},t) \end{aligned}$$

Important: you have to respect the order of the definition of mean value (because there appear differential operators)

$$\begin{aligned} <H> &= \int d^3\vec{r}\ \Psi^*(\vec{r},t)\left(i\hbar\frac{\partial}{\partial t}\right)\Psi(\vec{r},t) \\ &= i\hbar\int d^3\vec{r}\ \Psi^*(\vec{r},t)\frac{\partial\Psi(\vec{r},t)}{\partial t} \\ <H> &= \int d^3\vec{r}\ \Psi^*(\vec{r},t)\left(\frac{-\hbar^2}{2m}\nabla^2\ +\ V(\vec{r},t)\right)\Psi(\vec{r},t) \end{aligned}$$

The wave function has information of expected values of any dynamic quantity

$$< f(\vec{r},\vec{p},t) > \;=\; \int d^3\vec{r}\;\Psi^*(\vec{r},t)\;f(\vec{r},-i\hbar\vec{\nabla},t)\;\Psi(\vec{r},t)$$

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Probability current

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We study the propagation of the probability density over time for a particle moving under the influence of a potential V. We assume that $\Psi(\vec{r},t)$ is normalized for all t. We have

$$\left(-\frac{\hbar^2}{2m}\nabla^2 \;+\; V(\vec{r},t)\right)\Psi(\vec{r},t) \;=\; i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \tag{1}$$

(Schrödinger eq.)

We take complex conjugates in (1). We assume

$$V \;=\; V^* \;\; (real)$$
$$V \;=\; V(\vec{r},t)$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 \;+\; V(\vec{r},t)\right)\Psi^*(\vec{r},t) \;=\; -\,i\hbar\frac{\partial\Psi^*(\vec{r},t)}{\partial t}$$

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The time variation of $|\Psi(\vec{r},t)|^2$

$$\begin{aligned}
\frac{\partial|\Psi|^2}{\partial t} &= \frac{\partial\left(\Psi^*\Psi\right)}{\partial t} = \frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t} \\
&= \frac{i\hbar}{2m}\left(\Psi^*\Delta\Psi - \Psi\Delta\Psi^*\right) \\
&\quad -\frac{1}{i\hbar}\left(V\Psi^*\right)\Psi + \Psi^*\frac{1}{i\hbar}V\Psi \\
&\quad \Delta = \nabla^2
\end{aligned}$$

As $V = V(\vec{r},t) \rightarrow \left(V\Psi^*\right)\Psi = \Psi^*V\Psi$ (it is a product, V does not involve derivatives)

$$\frac{\partial|\Psi|^2}{\partial t} = \frac{i\hbar}{2m}\left(\Psi^*\Delta\Psi - \Psi\Delta\Psi^*\right)$$

We define **probability current (vector)**

$$\begin{aligned}
\vec{J}(\vec{r},t) &= \frac{i\hbar}{2m}\left(\Psi(\nabla\Psi^*) - \Psi^*(\nabla\Psi)\right) \\
&= \frac{\hbar}{m}\,Re\left(\frac{1}{i}\Psi^*(\nabla\Psi)\right) \\
\vec{\nabla}\cdot\vec{J} &= \frac{i\hbar}{2m}\left(\Psi\Delta\Psi^* - \Psi^*\Delta\Psi\right)
\end{aligned}$$

a We used

$$\begin{aligned}
\vec{\nabla}\cdot\left(\phi\vec{A}\right) &= \vec{\nabla}\phi\cdot\vec{A} + \phi\,\vec{\nabla}\cdot\vec{A} \\
&and \\
a - a^* &= \frac{2}{i}Re\left(\frac{a^*}{i}\right)
\end{aligned}$$

Therefore (**continuity equation)**

$$\frac{\partial|\Psi|^2}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0$$

Analogy with fluids $\frac{\partial\rho}{\partial t} = -\vec{\nabla} \cdot \vec{\jmath}$

$$|\Psi|^2 \rightarrow \rho$$

$$\vec{J} \rightarrow \vec{\jmath}$$

In one dimension $J \rightarrow$ **probability current**

$$J = \frac{\hbar}{2mi}\left[\phi^*\frac{\partial\phi}{\partial x} - \phi\frac{\partial\phi^*}{\partial x}\right]$$

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If we integrate over all space the continuity equation

$$\int_{all\ space} \frac{\partial|\Psi|^2}{\partial t}\, d\tau = -\int_{all\ space} \vec{\nabla} \cdot \vec{J}\, d\tau$$

By the theorem of Gauss

$$\frac{d}{dt}\int_{all\ space} |\Psi|^2\, d\tau = -\oint_S \vec{J} \cdot d\vec{S}$$

But $\oint_S \vec{J} \cdot d\vec{S} = 0$ as the flow of $\vec{J}$ through the surface surrounding the entire space is zero,

$$\frac{d}{dt}\int_{all\ space} |\Psi|^2\, d\tau = 0$$

Therefore, the normalization of the wave function is the same at all times

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Variation of probability in a volume V (over time) $\rightarrow$ due to flow of $\vec{J}$ through its surface (conservation of probability)

In 1D

$$\frac{d}{dt}\int_a^b dx P(x,t) \ = \ -\int_a^b dx \frac{\partial J(x,t)}{\partial x} \ = J(a,t) - J(b,t)$$

A change of prob. in a region is compensated by a net change of flow in the same region

The fact that $\int |\Psi|^2 \, d\tau$ extended to the entire space remains constant at all times does not mean that $|\Psi|^2$ should be independent of t at each point

The situation is equivalent to that given in **electromagnetism**. If, in an isolated system, there is charge distributed in the space with volume density $\rho(\vec{r},t)$, the total charge (the integral of $\rho(\vec{r},t)$ extended to all space) is conserved in the time. However, in the system, the spatial distribution of this charge can vary, resulting in charge currents.

If the charge contained within a fixed volume V varies over time, closed surface S which surround V must be traversed by a electric current The variation dQ in time dt of the charge

contained in V is equal to $-I \, dt$, where I is the intensity of the current through S , ie, the flow of current density vector $J(\vec{r},t)$ that leaves S

ANALOGY $|\Psi|^2$ $\rho(\vec{r}, t)$

probability **charge**

1 dim.: $[\phi] \rightarrow L^{-\frac{1}{2}}$ $[J] \rightarrow T^{-1}$

3 dim.: $[\Psi] \rightarrow L^{-\frac{3}{2}}$ $[\vec{J}] \rightarrow L^{-2}T^{-1}$

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