Coordinate Representation and Applications

In this and the next section, we make a specific representation of $|\psi\rangle$. In the coordinate representation we expand $|\psi\rangle$ as

$$|\psi\rangle = \sum \underbrace{\langle x|\psi\rangle}_{\text{call this the wavefunction } \psi(x).} \, |x\rangle$$

The action of an operator acting on $\psi(x)$ is then

$$\hat{A}\,\psi(x) = \langle x|\hat{A}|\psi\rangle$$

$$a|\psi'\rangle = \hat{A}|\psi\rangle$$
$$a\langle x|\psi'\rangle = \langle x|\hat{A}|\psi\rangle$$
$$a\underbrace{\psi'(x)}_{\hat{A}\psi(x)} = \langle x|\hat{A}|\psi\rangle.$$

In particular, the position operator gives $\hat{Q}\,\psi(x) = \langle x|\hat{Q}|\psi\rangle$
$= x\,\langle x|\psi\rangle$

Let's now find representations for the operators. We know that the generator of displacements gives (specialize to one dimension for notational simplicity):

$$e^{-ia\hat{P}/\hbar}\,|x\rangle = |x+a\rangle$$

$$\Rightarrow \quad \langle x+a|\psi\rangle = \langle x|e^{+ia\hat{P}/\hbar}|\psi\rangle$$

$$= \langle x|\mathbb{1} + ia\hat{P}/\hbar + \mathcal{O}(a^2)|\psi\rangle$$

$$= \psi(x) + \frac{ia\hat{P}}{\hbar}\psi(x) + \mathcal{O}(a^2)$$

If we compare this with a Taylor series for $\psi(x+a)$:

$$\psi(x+a) = \psi(x) + a\frac{d}{dx}\psi(x) + \cdots$$

then $\quad \dfrac{i\hat{P}}{\hbar} = \dfrac{d}{dx} \quad \Rightarrow \quad \hat{P} = -i\hbar\dfrac{d}{dx}.$

For 3-dimensions, $\hat{\vec{P}} = -i\hbar\vec{\nabla} \quad$ or $\quad \hat{P}_\alpha = -i\hbar\dfrac{\partial}{\partial x_\alpha}.$

[It is not in general true that, $\hat{P} = -i\hbar \frac{d}{dq}$ for conjugate coordinates $\hat{P}$ and $\hat{q}$.]

We already have a representation, in a sense, for $\hat{H}$ from the discussion of time displacements:

$$\hat{H}\,|\psi(t)\rangle = i\hbar \frac{d}{\partial t}|\psi(t)\rangle$$

For $\hat{H} = \frac{\hat{P}^2}{2M} + \underline{W}(x)$, then this equation becomes the Schrodinger equation

scalar potential

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + W(x)\right]\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t).$$

We often think of ψ as a "real" wave: i.e. it represents a physical wave propagating in space. While this picture is sometimes intuitively helpful, it is not strictly correct. For example, a many-particle system is also described by a single $|\psi\rangle$:

$$\psi(x_1, x_2 \cdots) = \langle x_1, x_2, \cdots|\psi\rangle.$$

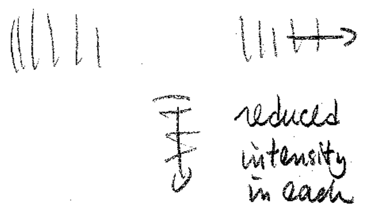
and Schrodinger's equation does <u>not</u> break up into N separate equations.

Further, the interpretation of $|\psi|^2$ as a probability density follows from the form $\rho = |\psi\rangle\langle\psi|$ of the density matrix. The probability should be interpreted as follows:

Suppose we have a preparation procedure which produces one particle at a time. This "ψ" is then split by a beam splitter into 2 detectors

Depending on how one thinks of ψ one could imagine 3 scenarios for this experiment.

i) like water wave

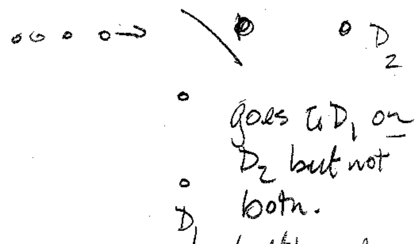


reduced intensity in each direction

ii) mix of i) and iii)

sometimes D_1
sometimes D_2
sometimes $D_1 + D_2$.

iii) like a particle:



goes to D_1 or D_2 but not both.
(although may exhibit diffraction).

Experimentally, it's iii) which is observed in Clausser, Phys. Rev. D9, 853 (1974)

Galilean Invariance

We have used Galilei transformations in Sec. 3 to derive the forms of quantum operators, so we should not be surprised that Schrodinger's Eq. is invariant under Galilei transformations. Still, the proof can be used to examine another transformation property (namely, where does the deBroglie wavelength come from?) so we examine the proof in some detail:

The transformation is $\quad x = x' + vt' \qquad t' = t \qquad$ or $x' = x - vt$
where frame F' is moving with velocity v w.r.t. frame F.

The potential energy W satisfies $\quad W'(x', t') = W(x, t)$
and S.E. appears as, in 1 dimension:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x'^2} \psi' + W'(x') \psi'(x', t') = i\hbar \frac{\partial}{\partial t'} \psi'(x', t').$$

Now, the operators transform like:

$$\frac{\partial}{\partial x'} = \frac{\partial x}{\partial x'}\frac{\partial}{\partial x} = \frac{\partial}{\partial x} \qquad \frac{\partial}{\partial t'} = \frac{\partial x}{\partial t'}\frac{\partial}{\partial x} + \frac{\partial t}{\partial t'}\frac{\partial}{\partial t} = v\frac{\partial}{\partial x} + \frac{\partial}{\partial t}.$$

Suppose we write $\psi(x,t) = e^{if}\psi'(x',t')$, since all that we demand physically is $|\psi(x,t)|^2 = |\psi'(x',t')|^2$. Then, subbing for ψ' etc.

$$-\frac{\hbar^2}{2M}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}e^{-if}\psi\right) + W e^{-if}\psi = i\hbar\left(v\frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right)e^{-if}\psi$$

$$-\frac{\hbar^2}{2M}\left[\frac{\partial}{\partial x}\left(\left(-i\frac{\partial f}{\partial x}\right)e^{-if}\psi + e^{-if}\frac{\partial}{\partial x}\psi\right)\right] + We^{-if}\psi = i\hbar\Big[v\left(-i\frac{\partial f}{\partial x}\right)e^{-if}\psi + ve^{-if}\frac{\partial \psi}{\partial x} - i\left(\frac{\partial f}{\partial t}\right)e^{-if}\psi + e^{-if}\frac{\partial \psi}{\partial t}\Big]$$

$$-\frac{\hbar^2}{2M}\left[-i\left(\frac{\partial^2 f}{\partial x^2}\psi + \frac{\partial f}{\partial x}\left(-i\frac{\partial f}{\partial x}\right)\psi + \frac{\partial f}{\partial x}\frac{\partial \psi}{\partial x}\right) - i\frac{\partial f}{\partial x}\frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi}{\partial x^2}\right]e^{-if} + We^{-if}\psi$$
$$-\hbar v\frac{\partial f}{\partial x}\psi e^{-if} - i\hbar v e^{-if}\frac{\partial \psi}{\partial x} - \hbar\frac{\partial f}{\partial t}e^{-if}\psi = i\hbar e^{-if}\frac{\partial \psi}{\partial t}$$

$$-\frac{\hbar^2}{2M}\frac{\partial^2 \psi}{\partial x^2} + W\psi + \left(-\frac{\hbar^2}{2M}(-i)2\frac{\partial f}{\partial x} - i\hbar v\right)\frac{\partial \psi}{\partial x} + \Big[\underbrace{-i\frac{\partial^2 f}{\partial x^2}\frac{\hbar^2}{2M}}_{\text{pure imaginary}} + \underbrace{\frac{\hbar^2}{2M}\left(\frac{\partial f}{\partial x}\right)^2 - \hbar v\frac{\partial f}{\partial x} - \hbar\frac{\partial f}{\partial t}}_{\text{pure real}}\Big]\psi = i\hbar\frac{\partial \psi}{\partial t}$$

To be equivalent to $-\frac{\hbar^2}{2M}\frac{\partial^2 \psi}{\partial x^2} + W\psi = i\hbar\frac{\partial \psi}{\partial t}$, we require

$$\frac{\hbar}{M}\frac{\partial f}{\partial x} - v = 0 \qquad \underbrace{\frac{\partial^2 f}{\partial x^2} = 0}_{\text{imaginary must vanish}} \qquad \frac{\hbar^2}{2M}\left(\frac{\partial f}{\partial x}\right)^2 - \hbar v\frac{\partial f}{\partial x} - \hbar\frac{\partial f}{\partial t} = 0$$

These equations can be satisfied by $f(x,t) = \frac{Mvx - Mv^2t/2}{\hbar}$.

So, there exists a function f ($\neq 0$) which allows the S.E. to be Galilei invariant.

Suppose we take $W = 0$, so that the solution for ψ' looks like

From $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\psi' = \frac{\hbar^2 k'^2}{2m}\psi'$

$\frac{\partial}{\partial t'}\psi' = \frac{i}{\hbar}\hat{H}'\psi'$

$$\psi'(x',t') = e^{i(k'x' - \omega' t')}$$

$p' = \hbar k'$

$E' = \hbar\omega' = \hbar^2 k'^2 / 2M$.

If we interpret k as $\frac{\hbar}{\lambda}$,

Then λ is frame-independent in a Galilei frame and therefore k and p should be frame independent.

This gives rise to a minor problem of interpreting λ as a wavelength from de Broglie.

$$\text{But} \quad e^{if}\psi' = e^{i\left(\frac{Mvx}{\hbar} - \frac{Mv^2t}{2\hbar} + k'(x - vt) - \omega' t\right)}$$

$$= e^{i\left[\left(k' + \frac{Mv}{\hbar}\right)x - \left(\omega' + kv + \frac{Mv^2}{2\hbar}\right)t\right]}$$

$$\hookrightarrow \frac{\hbar^2 k'^2}{2M\hbar} + k'v + \frac{Mv^2}{2\hbar} = \frac{1}{2M\hbar}\left(\hbar^2 k'^2 + 2Mk'v\hbar + M^2v^2\right)$$

$$= e^{i\left[\left(k' + \frac{Mv}{\hbar}\right)x - (\hbar k' + Mv)^2 \frac{t}{2M\hbar}\right]}.$$

In other words, the momentum transforms as expected $\hbar k' \to \hbar k + Mv$. However, the "de Broglie" wavelength λ does not remain invariant like a classical wave. It changes according to $p = \frac{2\pi\hbar}{\lambda}$.

Probability Flux

The last topic which we wish to touch in the coordinate representation is probability flux. For a single-particle state with wavefunction $\psi(x,t)$ we interpret $|\psi|^2$ as the probability density. This arises from $|\psi\rangle = \sum \langle x|\psi\rangle |x\rangle$ — $|\langle x|\psi\rangle|^2$ = prob. of system having coord. x

Then the probability of finding the particle within a coordinate space volume Ω is $\int_\Omega |\psi|^2 d^3x$. How does this probability change with time?

$$\frac{\partial}{\partial t}\int_\Omega \psi^*\psi\, d^3x = \int_\Omega \left(\psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}\right)d^3x$$

$$= \frac{i\hbar}{2M}\int_\Omega \left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)d^3x$$

$$= \frac{i\hbar}{2M}\int_\Omega \vec{\nabla}\cdot\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)d^3x$$

Since this equation is valid for any Ω, then it is valid for the integrands as well.

$$\frac{\partial}{\partial t}|\psi|^2 + \vec{\nabla}\cdot\vec{J} = 0 \quad \text{or} \quad \frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{J} = 0.$$

Where

$$\vec{J} \equiv -\frac{i\hbar}{2M}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) = \frac{\hbar}{M}\,\mathrm{Im}\left(\psi^*\vec{\nabla}\psi\right).$$

and $\vec{J}$ behaves like a conserved current obeying a continuity equation in coordinate space. We can recast this using

$$\hat{\vec{V}} = \frac{\hat{\vec{P}}}{M} = -\frac{i\hbar}{M}\vec{\nabla}$$

$$\Rightarrow \quad \vec{J} = \mathrm{Re}\left(\psi^*\vec{V}\psi\right).$$

Other topics in this chapter which we assume to have covered elsewhere:

i) boundary conditions on ψ
ii) eigenstates $e^{i(kx-\omega t)}$ for free particles
iii) tunnelling in 1 dimension through a square barrier.