Coordinate Representation

Suppose that we have an infinite set of states $|r\rangle$ covering coordinate space. Then

$$\hat{r}|r\rangle = r|r\rangle .$$

Since the states are continuous, the usual Kronecker delta ~~etc~~. won't work. A continuous function analogous to the discrete delta is the Dirac delta function:

$$\langle r'|r\rangle = \delta(r-r')$$

which has the properties

$$\delta(r-r') = \infty \qquad r=r'$$
$$= 0 \qquad r\neq r'$$
$$\int \delta(r-r')dr = 1$$
$$\int \delta(r-r')f(r)\,dr = f(r').$$

Now, we said previously that we could expand a state in terms of a basis set $|\alpha_i\rangle$ via

$$|\beta\rangle = \sum_i |\alpha_i\rangle\langle\alpha_i|\beta\rangle.$$

The same applies with the coordinate representation

$$|\beta,t\rangle = \sum_{\substack{\text{all}\\\text{space}}} |r_i\rangle\langle r_i|\beta,t\rangle \rightarrow \int dr\, \underbrace{\langle r|\beta,t\rangle}_{\substack{\text{This is Schrodingers}\\\text{wavefunction } \psi_\beta(r,t)}} |r\rangle .$$

Using postulate 4, the probability for finding the state in a volume element $d\vec{r}$ around $\vec{r}$ must then be [we move now to 3 dimensions].

$$|\langle \vec{r} \,|\, \beta, t\rangle|^2 d\vec{r} \qquad \text{(just as before with Postulate \#4)}$$

$$= \underline{\underline{|\psi_\beta(\vec{r}, t)|^2}} d\vec{r}$$

This [including the square] must be a probability density

Suppose now we look at the inner product of the state vectors:

$$\langle \alpha|\beta\rangle = \left\{ \int \langle \vec{r}\,'| \langle \alpha|\vec{r}\,'\rangle d\vec{r}\,' \right\} \left\{ \int \langle \vec{r}|\beta\rangle |\vec{r}\rangle d\vec{r} \right\}$$

$$= \int \langle \vec{r}\,'| \psi_\alpha^*(\vec{r}\,') d\vec{r}\,' \cdot \int \psi_\beta(\vec{r}) |\vec{r}\rangle d\vec{r}$$

$$= \int \psi_\alpha^*(\vec{r}\,') \psi_\beta(\vec{r}) \, \delta(\vec{r} - \vec{r}\,') d\vec{r}\,' d\vec{r}$$

$$= \int \psi_\alpha^*(\vec{r}) \psi_\beta(\vec{r}) dr.$$

In other words, it is just as convenient to use $\psi_\alpha(\vec{r})$ [an <u>eigenfunction</u>] as it is to use $|\alpha\rangle$ [an <u>eigenvector</u> of $\hat{A}$].

The choice of working in the $|\vec{r}\rangle$ basis is not unique. One could equivalently working in the momentum basis $|\vec{p}\rangle$ and this is frequently done in particle physics.

Operator form of $\hat{p}$:

Suppose that we have a matrix element of the form [consider 1-Dim only, for now]

$$\langle x | \hat{p}_x | a_i \rangle$$

coordinate basis set. — momentum in the x-direction — an eigenvector

We begin by finding the effect of

$$\underbrace{\hat{1}}_{\text{unit operator}} + \frac{\hat{p}_x \, dx}{i\hbar} \quad \text{has on} \quad |x\rangle$$

$$\hat{x}\left[\left(\hat{1} + \frac{\hat{p}_x \, dx}{i\hbar}\right)|x\rangle\right] \quad \text{compared to} \quad \hat{x}\,|x\rangle$$

Q: does this shift x?

$$= \left(\hat{x} + \hat{x}\hat{p}_x \frac{dx}{i\hbar}\right)|x\rangle$$

$$= \left(\hat{x} + \underbrace{(i\hbar\hat{1} + \hat{p}_x\hat{x})}_{\text{by commutation relation}}\frac{dx}{i\hbar}\right)|x\rangle$$

$$= \left(\hat{x} + \hat{1}\,dx + \hat{p}_x\hat{x}\frac{dx}{i\hbar}\right)|x\rangle$$

$$= \left(x + dx + \frac{x\,dx}{i\hbar}\hat{p}_x\right)|x\rangle \quad \leftarrow \text{after operating.}$$

$$= \left((x + dx) + \overbrace{(x + dx)\frac{dx\,\hat{p}_x}{i\hbar} - dx^2\frac{\hat{p}_x}{i\hbar}}^{\text{add and subtract}}\right)|x\rangle$$

In other words, to 1[st] order in dx [the other terms ultimately work as well, if one starts with $U_{p_x}(x) = \exp(-i\hat{p}_x x/\hbar)$ instead of the infinitesimal form] the effect of

$$\hat{1} + \frac{\hat{p}_x dx}{i\hbar}$$

is to shift $|x\rangle$ to $|x+dx\rangle$.

* We say that $\hat{p}_x$ is the generator of infinitesimal translations along the x-axis.

$$\therefore \ |x+dx\rangle = \left(\hat{1} + \frac{\hat{p}_x dx}{i\hbar}\right)|x\rangle = |x\rangle + \left(\frac{dx}{i\hbar}\right)\hat{p}_x |x\rangle$$

$$\Rightarrow \frac{|x+dx\rangle - |x\rangle}{dx} i\hbar = \hat{p}_x |x\rangle .$$

Similarly $\quad \langle x|\hat{p}_x = -i\hbar \dfrac{\langle x+dx| - \langle x|}{dx}$

$$\therefore \ \langle x|\hat{p}_x|a_i\rangle = -\frac{i\hbar}{dx}\left(\langle x+dx|a_i\rangle - \langle x|a_i\rangle\right)$$

$$= -\frac{i\hbar}{dx}\left[\psi_{a_i}(x+dx) - \psi_{a_i}(x)\right]$$

$$= -i\hbar \frac{d}{dx}\psi_{a_i}(x).$$

This can be generalized to 3-D and any power of $\hat{p}$:

$$\langle \vec{r}\,|\,\underbrace{\hat{G}(\hat{p})}_{\text{function of } \hat{p}}\,|a_i\rangle = \hat{G}\left(-i\hbar\vec{\nabla}\right)\psi_{a_i}$$

In other words, in going from the eigenvector to eigenfunction basis, we find the transformation

$$\langle \vec{r} \,|\, \hat{A}(\hat{p}, \hat{r}) \,|\, a_i \rangle = \hat{A}(-i\hbar\vec{\nabla}, \vec{r})\, \psi_{a_i}(\vec{r})$$

$$= a_i\, \psi_{a_i}(\vec{r})$$

Further, using the closure relation $\int |\vec{r}\rangle\langle\vec{r}|\, d\vec{r} = \hat{1}$.

$$\langle \alpha | \hat{A} | \beta \rangle = \int \langle \alpha | \vec{r} \rangle \langle \vec{r} | \hat{A} | \beta \rangle\, d\vec{r}$$
$$= \int \psi_\alpha^*(\vec{r})\, \hat{A}(-i\hbar\vec{\nabla}, \vec{r})\, \psi_\beta(\vec{r})\, d\vec{r} .$$

To summarize, in the coordinate representation $\hat{\vec{r}} \to \vec{r}$, $\vec{p} \to -i\hbar\vec{\nabla}$

$$\langle r | \alpha \rangle = \psi_\alpha(\vec{r})$$

$$\langle \alpha | \beta \rangle = \int \psi_\alpha^*(\vec{r})\, \psi_\beta(\vec{r})\, dr$$

$$\langle \alpha | \hat{A} | \beta \rangle = \int \psi_\alpha^*(\vec{r})\, \hat{A}(-i\hbar\vec{\nabla}, \vec{r})\, \psi_\beta(\vec{r})\, d\vec{r}$$

One could equally well use the momentum representation $\hat{p} \to \vec{p}$.

The picture we have developed here is referred to as the Schrodinger picture : $|\alpha, \underline{\underline{t}}\rangle$ $\quad \hat{A}$ no t

Heisenberg picture : $|\alpha\rangle$ $\quad \hat{A}(\underline{\underline{t}})$

Interaction picture : time dependence in both $|\alpha\rangle$, $\hat{A}$.

Schrodinger Equ.

We have now shown how to introduce, and work in, the coordinate space representation. Let's now derive the equation governing the time evolution of ψ:
From Ehrenfest's Thm.

$$\hat{\mathcal{H}} |\beta, t\rangle = i\hbar \frac{\partial}{\partial t} |\beta, t\rangle$$

$$\Rightarrow \quad \langle \vec{r} | \hat{\mathcal{H}} | \beta, t \rangle = i\hbar \langle r | \frac{\partial}{\partial t} | \beta, t \rangle = i\hbar \frac{\partial}{\partial t} \langle \vec{r} | \beta, t \rangle .$$

$$\Rightarrow \quad \hat{\mathcal{H}}(-i\hbar \vec{\nabla}, \vec{r}) \psi_\beta(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi_\beta(\vec{r}, t)$$

But if $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\vec{r}) \Rightarrow \hat{\mathcal{H}}(-i\hbar \vec{\nabla}, \vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$

and we have the Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial}{\partial t} \psi$$

One approach to solving the time evolution problem is to specify $\psi(\vec{r}, t=0)$ and then use:

$$|\beta, t\rangle = \hat{U}(t, t_0) |\beta, t_0\rangle$$

$$\Rightarrow \quad \underbrace{\langle r | \beta, t \rangle}_{\psi} = \langle r | \hat{U}(t, t_0) | \beta, t_0 \rangle$$

insert $\hat{1} = \int dr' |r'\rangle\langle r'|$

$$\Rightarrow \quad \psi_\beta(\vec{r}, t) = \int dr' \underbrace{\langle r | \hat{U}(t, t_0) | r' \rangle}_{} \psi_\beta(r', t_0)$$

This is referred to as the propagation kernel or propagator $\equiv G(r, r', t, t')$.

Schroedinger Eqn. and Probability Flow

The interpretation of $\Psi^*\Psi$ as a probability flow can be taken a step further. Suppose for now that $V(\vec{r})$ is real:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial}{\partial t}\Psi \qquad (1)$$

and c.c. gives

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

$$\Psi^* \times (1) \Rightarrow -\frac{\hbar^2}{2m}\Psi^*\nabla^2\Psi + V\Psi^*\Psi = i\hbar\Psi^*\frac{\partial}{\partial t}\Psi \qquad (3)$$

$$\Psi + (2) \Rightarrow -\frac{\hbar^2}{2m}\Psi\nabla^2\Psi^* + V\Psi^*\Psi = -i\hbar\Psi\frac{\partial}{\partial t}\Psi^* \qquad (4)$$

$$(3) - (4) \Rightarrow -\frac{\hbar^2}{2m}\left(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right) = i\hbar\left(\Psi^*\frac{\partial}{\partial t}\Psi + \Psi\frac{\partial}{\partial t}\Psi^*\right).$$

$$\Rightarrow -\frac{\hbar^2}{2m}\vec{\nabla}\cdot\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right) = i\hbar\frac{\partial}{\partial t}|\Psi|^2.$$

or

$$\vec{\nabla}\cdot\underbrace{\frac{i\hbar}{2m}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right)}_{\text{looks like }(-)\text{ probability flux } \equiv -\vec{J}} = \underbrace{\frac{\partial}{\partial t}|\Psi|^2}_{\text{probability density } \equiv \rho}$$

$$\text{ie. } \vec{\nabla}\cdot\vec{J} = -\frac{\partial}{\partial t}\rho.$$ ← (need this for scattering flux, pg. 9-4).

This is in the form of the equation of continuity.
This leads us to Postulate #7:
A state function and its derivatives representing a real physical system must be everywhere finite, continuous* and single valued. (*assume V is continuous).