QM states : abstract & in specific bases

In QM one begins by learning about a wavefunction $\psi(\vec{x},t)$, which is the amplitude to find a particle at a position $\vec{x}$ at time t, given that it is a state ψ.

Since the probability density $\rho(\vec{x}) = \psi^*(\vec{x},t)\,\psi(\vec{x},t)$, the chance that the particle is somewhere, unity, implies that

$$1 = \int d\vec{x}\; \psi^*(\vec{x},t)\,\psi(\vec{x},t)$$

The wavefunction $\psi(\vec{x},t)$ actually follows from the choice of a specific set of basis states of particles with definite positions, $\{|\vec{x}\rangle\}$, and the wfn is the overlap of the abstract state the particle is in $|\psi(t)\rangle$ (at time t) with a state of definite position $\vec{x}$,

$$\underline{\psi(\vec{x},t) \equiv \langle \vec{x}|\psi(t)\rangle} \qquad\qquad \psi^*(\vec{x},t) = \langle\psi(t)|\vec{x}\rangle$$

The norm of these position eigenstates is usually chosen to be a Dirac δ-function, since $\vec{x}$ is a continuous label:

$$\langle \vec{x}'|\vec{x}\rangle = \delta(\vec{x}-\vec{x}')$$

Note the usual discrete-state identity operator

$$I = \sum_n |n\rangle\langle n|$$

generalizes to

$$I = \int d^3x\; |\vec{x}\rangle\langle\vec{x}|$$

check: $$I\,|\vec{x}'\rangle \stackrel{?}{=} \int d^3x\; |\vec{x}\rangle\underbrace{\langle\vec{x}|\vec{x}'\rangle}_{\delta(\vec{x}-\vec{x}')} = |\vec{x}'\rangle \checkmark$$

also $I^2 = I$.

To take matrix elements between such basis states, which are not normalized to unity, one should use

$$\langle O \rangle \underset{\text{generalize to}}{\longrightarrow} \frac{\langle \vec{x}' | O | \vec{x} \rangle}{\langle \vec{x}' | \vec{x} \rangle} \quad \text{or} \quad \frac{\langle \vec{x} | O | \vec{x} \rangle}{\langle \vec{x} | 1 | \vec{x} \rangle}$$

for diagonal m.e.s

One simple operator on this basis is the position operator $\vec{X}_{op}$, which just returns the position vector $\vec{x}$ on this basis

$$\vec{X}_{op} \, |\vec{x}\rangle = \vec{x} \, |\vec{x}\rangle$$

The expected value of $\vec{X}_{op}$ is

$$\frac{\langle \vec{x} | \vec{X}_{op} | \vec{x} \rangle}{\langle \vec{x} | \vec{x} \rangle} = \frac{\delta(\overrightarrow{x-x}) \; \vec{x}}{\delta(\overrightarrow{x-x})} = \vec{x} \;\checkmark \quad \text{(plausible)}$$

A more interesting 'delocalized' state might have the particle in two positions with equal amplitude,

$$\underline{|\psi\rangle} = \underline{\frac{1}{\sqrt{2}} \left(|\vec{x}_1\rangle + |\vec{x}_2\rangle \right)}$$

and the expected position (mean of many measurements) is

$$\underbrace{\frac{\langle \psi | \vec{X}_{op} | \psi \rangle}{\langle \psi | \psi \rangle}} = \frac{\frac{1}{2}\left(\langle \vec{x}_1 | \vec{X}_{op} | \vec{x}_1 \rangle + \langle \vec{x}_2 | \vec{X}_{op} | \vec{x}_2 \rangle \right)}{\frac{1}{2}\left(\langle \vec{x}_1 | \vec{x}_1 \rangle + \langle \vec{x}_2 | \vec{x}_2 \rangle \right)}$$

(assume $\vec{x}_1 \neq \vec{x}_2$ so cross terms $\propto \delta(\overrightarrow{x_1 - x_2})$ vanish)

$$= \frac{\frac{1}{2}\left[\vec{x}_1 \, \delta(\overrightarrow{x_1 - x_1}) + \vec{x}_2 \, \delta(\overrightarrow{x_2 - x_2}) \right]}{\frac{1}{2}\left[\delta(\overrightarrow{x_1 - x_1}) + \delta(\overrightarrow{x_2 - x_2}) \right]} = \underbrace{\frac{1}{2}\left(\overrightarrow{x_1 + x_2} \right)}$$

Momentum basis $|\vec{p}\rangle$

There is nothing "magic" about the choice of basis $\{|\vec{x}\rangle\}$, as always one may replace a basis by any linear combination related by a unitary transformation

$$\hat{e}_i' = U_{ij}\hat{e}_j \quad (\text{vectors}) \qquad U^\dagger = U^{-1}$$
$$(\textstyle\sum_j \text{ implicit})$$

or for QM

$$|m\rangle = U_{mn}|n\rangle$$
$$(\textstyle\sum_n \text{ implicit})$$

A familiar choice is the set of momentum eigenstates $\{|\vec{p}\rangle\}$, in which the particle is in an eigenstate of momentum

$$\vec{P}_{op}|\vec{p}\rangle = \vec{p}\,|\vec{p}\rangle$$

In a general state $|\psi\rangle$, we can determine the "momentum space wavefunction" $\phi(\vec{p})$ by calculating the overlap of $|\psi\rangle$ with a momentum eigenstate $|\vec{p}\rangle$,

$$\phi(\vec{p}) = \langle\vec{p}|\psi\rangle \qquad (\text{and } \phi^*(\vec{p}) = \langle\psi|\vec{p}\rangle)$$

These momentum eigenstates are similarly normed as

$$\langle\vec{p}\,'|\vec{p}\rangle = \delta(\vec{p}-\vec{p}\,')$$

and the identity operator is

$$I = \int d\vec{p}\; |\vec{p}\rangle\langle\vec{p}|$$

How is the momentum-space wfn $\phi(\vec{p})$ related to the familiar coordinate-space wfn $\psi(\vec{x})$?

we can work this out by inserting the identity, $I = \int d\vec{x}\, |\vec{x}\rangle\langle\vec{x}|$:

$$\phi(\vec{p}) = \langle\vec{p}|\psi\rangle = \int d\vec{x}\, \underbrace{\langle\vec{p}|\vec{x}\rangle}_{\substack{\text{what is} \\ \text{this?}}} \underbrace{\langle\vec{x}|\psi\rangle}_{\psi(\vec{x})}$$

note $\langle\vec{x}|\vec{p}\rangle$ is the spatial wavefunction $\psi_{\vec{p}}(\vec{x})$ for a particle in a momentum eigenstate, which is a plane wave:

$$\psi_{\vec{p}}(\vec{x}) = \eta e^{i\vec{p}\cdot\vec{x}}$$

$\eta = \frac{1}{(2\pi)^{3/2}}$ for continuum norm states in 3D.

so,

$$\langle\vec{p}|\vec{x}\rangle = \underbrace{\frac{1}{(2\pi)^{3/2}}}_{\text{we will specialize to 3D}} e^{-i\vec{p}\cdot\vec{x}}$$

(this is the momentum-space wavefunction of a particle with definite position, $\phi_{\vec{x}}(\vec{p})$) (!)

and thus

$$\phi(\vec{p}) = \underbrace{\frac{1}{(2\pi)^{3/2}}}_{1/(2\pi)^{D/2} \text{ in D space dimensions}} \int d\vec{x}\, e^{-i\vec{p}\cdot\vec{x}}\, \psi(\vec{x})$$

$\left(\text{and } \psi(\vec{x}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{p}\, e^{i\vec{p}\cdot\vec{x}}\, \phi(\vec{p})\right)$

aha! The momentum- and coordinate-space wfns are Fourier transforms of each other.

n.b. $\int d\vec{p}\, |\phi(\vec{p})|^2 = \int d\vec{x}\, |\psi(\vec{x})|^2$, so a normed $\psi(\vec{x})$ gives a normed $\phi(\vec{p})$

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e.g. Given a spatial wfn for a particle with momentum $\vec{p}_1$, $\psi_{\vec{p}_1}(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{p}_1\cdot\vec{x}}$, what is the corresponding momentum-space wfn?

$$\phi(\vec{p}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{x}\, e^{-i\vec{p}\cdot\vec{x}}\, \psi(\vec{x}) = \frac{1}{(2\pi)^3} \underbrace{\int d\vec{x}\, e^{-i\vec{p}\cdot\vec{x}}\, e^{i\vec{p}_1\cdot\vec{x}}}_{(2\pi)^3 \delta(p-\vec{p}_1)}$$

$$= \delta(p-\vec{p}_1)$$

no $\vec{p}$ present except $\vec{p}_1$ ✓

Reconstructing the abstract state $|\psi\rangle$.

We are basically finding the coefficients $\{c_n\}$ in an expansion of the quantum state $|\psi\rangle$ in a basis $\{|n\rangle\}$,

$$|\psi\rangle = \sum_n c_n |n\rangle$$

$$\langle n'|\psi\rangle = \sum_n c_n \underbrace{\langle n'|n\rangle}_{\delta_{nn'}} = c_{n'}$$

compare

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

so the "wavefunction" is the set of coefficients in the expansion of the state in a given basis.

We may back up and write the state as

(an ∞ # of other bases $\exists$)

$$\underline{|\psi\rangle} = \overbrace{\underline{\int d\vec{x}\ \underbrace{\psi(\vec{x})}_{\substack{\text{coeffs.}\\ \text{"}\\ \text{wavefunction}}}\ \underbrace{|\vec{x}\rangle}_{\substack{\text{basis}\\ (\vec{x})}}}}^{\text{one basis}} = \overbrace{\underline{\int d\vec{p}\ \underbrace{\phi(\vec{p})}_{\substack{\text{coeffs.}\\ \text{"}\\ \text{mom-space}\\ \text{wfn}}}\ \underbrace{|\vec{p}\rangle}_{\substack{\text{basis}\\ (\vec{p})}}}}^{\text{another basis}} = \ldots$$