B7.3 Further quantum theory lecture 2

In this lecture, want to introduce a notational device due to Dirac that is widely used in Q.M. and is particularly well-adapted to treatment of "continuum states".

We will then see an application in the study of the free particle: propagator.

Bra-Ket notation [P.A.M. Dirac, "The Principles of Quantum Mechanics" (1930)]

To a state vector $\psi \in \mathcal{H}$, associate the "ket" $|\psi\rangle$

$$\psi \longleftrightarrow |\psi\rangle$$

To a state vector, can also associate an element φ_ψ of the dual space $\mathcal{H}^*$

Here, in ∞-dim's we mean the "continuous dual".

$$\varphi_\psi : \mathcal{H} \to \mathbb{C}$$
$$\tilde{\psi} \mapsto (\psi, \tilde{\psi})$$

This map is $\mathbb{C}$-antilinear (conjugate linear) due to antilinearity of inner product in first entry.
We represent φ_ψ by a "bra"

$$\varphi_\psi \longleftrightarrow \langle\psi|$$

Riesz-Fréchet rep^n theorem: every element of $\mathcal{H}^*$ can be written as $\langle\psi|$ for some $\psi \in \mathcal{H}$.

Now the inner product (ϕ, ψ) is expressed as a "bra(c)ket"

$$(\phi, \psi) \longleftrightarrow \langle\phi|\psi\rangle$$

For operators $A : \mathcal{H} \to \mathcal{H}$, we write $|A\psi\rangle \equiv A|\psi\rangle$, so we also have

$$\langle\phi|A|\psi\rangle = (\phi, A\psi) = (A^*\phi, \psi) = \langle A^*\phi|\psi\rangle$$

so we can write $\langle\phi|A = \langle A^*\phi|$ (self-adjoint ops act as A to left and right).

The outer product of $|\alpha\rangle$ and $\langle\beta|$ is the operator

$$|\alpha\rangle\langle\beta| : |\psi\rangle \longmapsto |\alpha\rangle\langle\beta|\psi\rangle = (\beta,\psi)\,|\alpha\rangle \quad , \quad \left(|\alpha\rangle\langle\beta|\right)^* = |\beta\rangle\langle\alpha|$$

Concatenation of bra's & ket's works as suggested visually.

Let $\{|i\rangle, i\in I\}$ be a complete, orthonormal basis: $\langle i|j\rangle = \langle j|i\rangle = \delta_{ij}$.

we can write an arbitrary state in this basis as $|\psi\rangle = \sum_{i\in I} c_i |i\rangle$.

Then we can measure components as $c_i = \langle i|\psi\rangle$, and project onto $|i\rangle$ w/ $|i\rangle\langle i|$.

Can write orthogonal projection onto subspace w/ O.N. basis $\{|i\rangle, i\in\tilde{I}\}$

"resolution of the identity"
or
"completeness relation"
↓

$$P_{\tilde{I}} = \sum_{i\in\tilde{I}} |i\rangle\langle i|$$

In particular, for $\tilde{I}\equiv I$, this is just the identity operator $P_I \equiv \mathbb{1}_{\mathcal{H}} = \sum_{i\in I} |i\rangle\langle i|$.

Consider an operator A: define the matrix elements $A_{ij} = \langle i|A|j\rangle$. We have

$$A = \mathbb{1}_{\mathcal{H}} A\, \mathbb{1}_{\mathcal{H}} = \sum_{i,j\in I} |i\rangle\langle i|A|j\rangle\langle j| = \sum_{i,j\in I} A_{ij}\, |i\rangle\langle j|$$

In finite-dimensional setting, in basis $|i\rangle$, A_{ij} is $(i,j)^{th}$ entry in matrix representation.

Consider expectation value of an operator A with eigenvectors $A|i\rangle = a_i|i\rangle$, $i\in I$ in state ψ:

$$\begin{aligned} E_\psi(A) = \langle\psi|A|\psi\rangle &= \sum_{i\in I} \langle\psi|A|i\rangle\langle i|\psi\rangle \\ &= \sum_{i\in I} a_i\, |\langle i|\psi\rangle|^2 \\ &= \sum_{\substack{\text{possible}\\ \text{outcomes}}} (\text{outcome})\times(\text{Probability of outcome}). \end{aligned}$$

Clarifies that quantum mechanical "expectation value" matches statistical notion of expected value for associated random variable. Same for, e.g., dispersion and standard deviation.

We've said that observables admit orthonormal basis of eigenvectors, but in ∞-dim'l setting there can be a subtlety.

Consider free particle in $\mathbb{R}$ $\left(\mathcal{H} \cong L^2(\mathbb{R})\right)$.

Position observable X acts on wave functions $\Psi(x)$ according to

$$X : \Psi(x) \longmapsto x\Psi(x)$$

Introduce generalized eigenstate $|\xi\rangle$ of X operator $\forall \xi \in \mathbb{R}$ obeying

$$X|\xi\rangle = \quad |\xi\rangle$$

$|\xi\rangle$ is a state w/definite position ξ, so we have

$$\langle \xi | \Psi \rangle = \left\{ \begin{matrix} \text{amplitude to find particle} \\ \text{in state } \Psi \text{ at } x = \xi \end{matrix} \right\} = \Psi(\xi)$$

To represent $|\xi\rangle$ with a wave function, should have

$$\int_{-\infty}^{\infty} dx \, \Psi^*_{|\xi\rangle}(x) \Psi(x) \, dx = \Psi(\xi) \longrightarrow \Psi^*_{|\xi\rangle}(x) \overset{\dagger}{=} \delta(x-\xi) = \Psi_{|\xi\rangle}(x)$$

In particular, this gives us "continuum normalization condition

$$\langle \xi | \xi' \rangle = \Psi_{|\xi'\rangle}(\xi) = \delta(\xi - \xi')$$

† Dirac "δ-function" is the distribution obeying $\int_{-\infty}^{\infty} \delta(x-a) f(x) \, dx = f(a)$. Can think of this as limit $\epsilon \to 0$ of increasingly sharply peaked Gaussians

$$\frac{1}{\epsilon\sqrt{\pi}} \exp\left(-\frac{(x-a)^2}{\epsilon^2}\right) \xrightarrow[\epsilon \to 0]{} \delta(x-a)$$

Momentum observable P acts on wave functions $\Psi(x)$ according to

$$P : \Psi(x) \longmapsto -i\hbar \Psi'(x)$$

What is the basis of eigenfunctions?

$$P|p\rangle = p|p\rangle \quad (p \in \mathbb{R})$$

$$\frac{d}{dx}\Psi_{|p\rangle}(x) = \frac{i}{\hbar} p \Psi_{|p\rangle}(x)$$

$$\Psi_{|p\rangle}(x) = \underbrace{\mathcal{N} e^{\frac{ipx}{\hbar}}}_{} \text{ for some constant } \mathcal{N}.$$

not square-normalizable for any value of $\mathcal{N}$, so not really in $\mathcal{H}$!

So we have the overlap b/w momentum & position states:

$$\langle x | p \rangle = \Psi_{|p\rangle}(x) = \mathcal{N} e^{\frac{ipx}{\hbar}}$$

Momentum eigenstates should also obey some continuum normalization, compute overlap

$$\langle p | p' \rangle = \mathcal{N}^2 \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} e^{\frac{ip'x}{\hbar}} dx = \frac{\mathcal{N}^2}{2\pi\hbar} \int_{-\infty}^{\infty} e^{2\pi i (p-p')s} ds = \frac{\mathcal{N}^2}{2\pi\hbar} \delta(p-p')$$

integral representation of δ-function (Fourier transform of constant function)

So we choose $\mathcal{N} = (2\pi\hbar)^{1/2}$ to give canonical continuum normalization.

To recap:

$$\langle x | x' \rangle = \delta(x-x') \qquad \langle p | p' \rangle = \delta(p-p')$$

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \qquad \langle p | x \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{-ipx}{\hbar}}$$

a state of definite momentum is equally likely to be at any position.

a state of definite position is equally likely to have any momentum.

Resolution of identity (continuum)

$$\mathbb{1} = \int_{-\infty}^{\infty} dx \, |x\rangle\langle x| \qquad \mathbb{1} = \int_{-\infty}^{\infty} dp \, |p\rangle\langle p|$$

Gives new perspective on wave function of a state vector:

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle dx = \int_{-\infty}^{\infty} \psi(x)\,|x\rangle \, dx, \qquad \langle x|\psi\rangle = \psi(x)$$

$$|\psi\rangle = \int_{-\infty}^{\infty} |p\rangle\langle p|\psi\rangle dx = \int_{-\infty}^{\infty} \hat{\psi}(p)\,|p\rangle \, dp, \qquad \langle p|\psi\rangle = \hat{\psi}(p)$$

How are these related?

$$\hat{\psi}(p) = \langle p|\psi\rangle \qquad \psi(x) = \langle x|\psi\rangle$$

$$= \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|\psi\rangle \qquad = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle$$

$$= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} e^{-\frac{ipx}{\hbar}} \psi(x)\, dx \qquad = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \hat{\psi}(p)\, dp$$

Thus $\psi(x)$ & $\hat{\psi}(p)$ are related by Fourier transform and its inverse.

Indeed the Fourier transform is a unitary map $L^2(\mathbb{R}) \to L^2(\mathbb{R})$ (Plancherel theorem), so this preserves norms, overlaps. Just a "change of basis".

Given an (abstract) state vector $|\psi\rangle \in \mathcal{H} \cong L^2(\mathbb{R})$, can consider both its position-space and momentum-space representations. Completely equivalent.

Can now define an important & intuitively useful object, the propagator.

Intuitively, propagator tells you: given particle was at position x_0 at time t_0, what is the amplitude for it to be at position x_1 at time t_1?

$$\mathcal{U}(x_1,t_1;x_0,t_0) = \langle x_1 | \mathcal{U}(t_1,t_0) | x_0 \rangle$$

Suppose we consider the free particle w/ Hamiltonian $H = \frac{P^2}{2m}$. Energy eigenstates are just momentum eigenstates:

$$H_{free}|p\rangle = E_p|p\rangle = \frac{p^2}{2m}|p\rangle$$

$$\mathcal{U}_{free}(t_1,t_0)|p\rangle = e^{\frac{-iE_p\Delta t}{\hbar}}|p\rangle = e^{\frac{-ip^2\Delta t}{2m\hbar}}|p\rangle$$

Can determine propagator by inserting resolution of the identity next to $\mathcal{U}(t_1,t_0)$

$$\begin{aligned}\mathcal{U}(x_1,t_1;x_0,t_0) &= \int dp\, \langle x_1|\mathcal{U}(t_1,t_0)|p\rangle\langle p|x_0\rangle \\ &= \int dp\, \langle x_1|e^{\frac{-ip^2\Delta t}{2m\hbar}}|p\rangle\langle p|x_0\rangle \\ &= \int dp\, e^{\frac{-ip^2\Delta t}{2m\hbar}} \times \frac{1}{2\pi\hbar} \times e^{\frac{ip\Delta x}{\hbar}} \\ &= \frac{1}{2\pi\hbar}\int dp\, e^{\frac{i}{2}\left(-\frac{\Delta t}{m\hbar}\right)p^2 + i\left(\frac{\Delta x}{\hbar}\right)p}\end{aligned}$$

Integral can be computed using results for Fresnel integrals (or as an oscillatory Gaussian).

$$\boxed{\int dx\, e^{\frac{i}{2}ax^2 + ibx} = \left(\frac{2\pi i}{a}\right)^{1/2} e^{\frac{-ib^2}{2a}}}$$

$$\mathcal{U}(x_1,t_1;x_0,t_0) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} \exp\left(\frac{-m(\Delta x)^2}{2i\hbar\Delta t}\right)$$

Note that immediately after time t_0, amplitude is non-zero for arbitrarily large Δx. This reflects infinite uncertainty in momentum given certainty in position @ start.

However phase oscillates very fast at large $\left(\frac{m(\Delta x)^2}{\hbar\Delta t}\right)$, so averaging over positions leads to cancellations.

Using the propagator:

Can use propagator to give integral expression for time evolution of arbitrary wave function.

At $t=0$, wave function $\langle x|\psi\rangle = \psi(x)$

At $t>0$, wave function $\langle x|U(t,0)|\psi\rangle = \int dy\, \langle x|U(t,0)|y\rangle\langle y|\psi\rangle$

$$= \int dy\, U(x,t;y,0)\,\psi(y)$$

$$= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \int dy \left(\psi(y)\, e^{\frac{im(x-y)^2}{2\hbar t}}\right)$$

In problem sheet, will try this out w/ Gaussian initial wavefunction.