Dirac Notation: Vectors + Wavefunctions

How do we relate the vectorspace quantum mechanics to wavefunctions?

- Infinite Dimensional Vector Spaces
  - In the 1920s, there were 2 competing versions of quantum mechanics
    - Schrödinger's wave function formalism, based on the idea of wave-particle duality
    - Heisenberg matrix mechanics, inspired by ideas of quantization
    - Previous classes probably followed Schrödinger, but we've mostly followed Heisenberg
    - Dirac showed the connection between the two
  - Function Spaces
    - Sets of functions (including some types of b.c.) follow the rules for vector spaces (2 functions add to a function, etc)
    - The L^2 functions satisfy

$$\int d^n x \, |\psi|^2 \text{ finite}, \text{ so they can be normalized.}$$

These have inner product (for $|\psi\rangle \simeq \psi(x)$, $|\phi\rangle \simeq \phi(x)$)

$$\langle\psi|\phi\rangle = \int d^n x \; \psi^*(x)\,\phi(x)$$

    - The mathematical field of <u>functional analysis</u> is about these infinite-dimensional spaces (+ related ones)
    - Operators include multiplication by functions + differential operators
    - In many cases, there is a discrete basis of functions
  - Example: Periodic functions / Functions on a circle
    - Let's take functions satisfying $\psi(x) = \psi(x+2\pi R)$ using the L^2 inner product
    - The complex exponentials $|e_n\rangle \simeq \frac{1}{\sqrt{2\pi R}}\, e^{inx/R}$, $n \in \mathbb{Z}$

make an orthonormal set $\langle e_n | e_m \rangle = \delta_{nm}$. Theorems about Fourier series show this is a basis

$$\psi(x) = \sum_n \frac{\psi_n}{\sqrt{2\pi R}} e^{inx/R} \Longleftrightarrow |\psi\rangle = \sum_n \psi_n |e_n\rangle$$

+ We might think the $|e_n\rangle$ are e'states of a Hermitian operator. We define a momentum operator p s.t. $p|e_n\rangle = (\hbar n/R)|e_n\rangle$
  This means $p|\psi\rangle \simeq -i\hbar\, d\psi/dx$, or $p \simeq -i\hbar\, d/dx$
+ Can also have a position operator x s.t. $x|\psi\rangle \simeq (x\psi(x))$

- Example: Angular Momentum / Spherical harmonics
  + Recall that angular momentum s has $2s+1$ states, so we represent these states w/ $2s+1$ dim vectors

$$\begin{array}{cccc} [1], & \left\{\begin{bmatrix}1\\0\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix}\right\}, & \left\{\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\end{bmatrix}\right\}, & \text{etc} \\ |0,0\rangle & |\tfrac12,\tfrac12\rangle \; |\tfrac12,-\tfrac12\rangle & s=|1,1\rangle, |1,0\rangle, |1,-1\rangle & \end{array}$$

  + We can describe all the (spin) angular momentum states with an infinite dim vector
$$\begin{array}{c} s=0 \\ s=\tfrac12 \\ s=1 \end{array} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

  + Then the spin operators also fit in ∞ matrices

$$S_z \simeq [0], \frac{\hbar}{2}\begin{bmatrix}1&0\\0&-1\end{bmatrix}, \hbar\begin{bmatrix}1&0\\0&0\\&&-1\end{bmatrix}, \ldots \longrightarrow S_z \simeq \hbar \begin{array}{c} \left[\begin{matrix} 0 & & & \\ & \tfrac12 & & \\ & & -\tfrac12 & \\ & & & 1 \; 0 \; -1 \; \ldots \end{matrix}\right] \end{array} \begin{array}{l} \}s=0 \\ \}s=\tfrac12 \\ \}s=1 \end{array}$$

$$\& \quad S^2 \simeq \hbar^2 \begin{bmatrix} 0 & & & \\ & \tfrac34 & & \\ & & \tfrac34 & \\ & & & 2 \; 2 \; 2 \ldots \end{bmatrix}$$

with S_x, S_y, they are all block diagonal (b/c they don't change s)

  + If we limit to orbital angular momentum with $s \to l = 0, 1, 2, \ldots$, we know we can also represent the $|l,m\rangle$ states by spherical harmonic wavefunctions (on angular variables)!

So

$$|l,m\rangle \simeq \begin{array}{c} l=0 \\ l=1 \\ \\ \\ \\ \end{array} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \end{bmatrix} \begin{array}{c} \\ \\ \\ \\ \\ \\ \leftarrow l,m \\ \\ \end{array} \simeq Y_l^m(\theta, \phi)$$

  + The angular momentum operators convert to differential operators acting on angular functions

$L_z = -i\hbar \frac{\partial}{\partial\phi}$ and $L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

- Dirac-Normalized Basis Vectors
  - What are eigenstates of position operator x?
    - + Position should be observable, so e'states $|x\rangle$ of different e'values should be orthogonal.
    - + But ~~for~~ continuous e'values x, normalization $\langle x|x\rangle = 1$ is not useful
    - + Instead $\langle x'|x\rangle = \delta(x-x')$ and $x\cdot|x\rangle = x|x\rangle$ (Note the use of $\cdot$ for operator action for clarity.)
    - + We call this Dirac normalized or delta-function normalized
    - + We can treat $\{|x\rangle\}$ like a basis. In analogy to $|\psi\rangle = \sum \psi_n|e_n\rangle$ for orthonormal basis, say
$$|\psi\rangle = \int dx\, \psi(x)|x\rangle \quad \text{for } \psi(x) \text{ the wavefunction}$$
Then
$$\langle x|\psi\rangle = \int dx'\, \psi(x')\langle x|x'\rangle = \int dx'\, \psi(x')\delta(x'-x) = \psi(x)$$
like $\psi_n = \langle e_n|\psi\rangle$.

~~+ Dirac normalized vect~~

  - General properties
    - + A Dirac normalized set acts like an orthonormal basis in terms of finding "components" by inner products
    - + Similarly, there is a completeness relation
$$1 = \int dx\, |x\rangle\langle x| \qquad \text{etc}$$
    - + But delta-normalized kets are not physical states b/c they can't be normalized to one. They are the limit of normalized states (like Gaussian wavefunctions for $|x\rangle$)
    - + Wavefunction gives probability density $P(x, x+\Delta x) = \int_x^{x+\Delta x} dx' |\langle x'|\psi\rangle|^2 = \int_x^{x+\Delta x} dx' |\psi(x')|^2$
  - Momentum basis
    - + We've seen momentum e'states for periodic space as complex exponentials. For infinite range $(-\infty < x < \infty)$, we can switch to Dirac normalized $|p\rangle \simeq \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

+ This definition means we have inner product $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

+ We can write $|\psi\rangle$ as a superposition in either basis

$$|\psi\rangle = \int dx\, \psi(x)\,|x\rangle = \int dp\, \tilde{\psi}(p)\,|p\rangle$$

and convert via inner products

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int dx\, \psi(x)\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dx\, \psi(x)e^{-ipx/\hbar}$$

which is a Fourier transform (and vice versa)

+ We can also see that

$$\langle x|p|\psi\rangle = \int dp\, \tilde{\psi}(p)\langle x|p|p\rangle = \left(1/\sqrt{2\pi\hbar}\right)\int dp\, p\,\tilde{\psi}(p)e^{ipx/\hbar}$$

$$= -i\hbar\frac{d}{dx}\left(\frac{1}{\sqrt{2\pi\hbar}}\int dp\, \tilde{\psi}(p)e^{ipx/\hbar}\right) = -i\hbar\frac{d\psi}{dx}$$

This demonstrates

$$p \simeq -i\hbar\, d/dx$$

- Bound States vs Scattering States
  + Mostly we are interested in stationary states where the wavefunction is normalizable, ie, it drops off quickly for large distance.
  + These states are bound to a potential. They have a discrete spectrum of energies
  + But there are also states with energies above the potential V (unless $V \to \infty$ at large distance).
  + The exact energy e'states (scattering states) are delta-function normalizable, so physical scattering states (wavepackets) are not definite energy. (Think free particle)
  + In this case, the completeness relation must include a sum over bound state dyads & an integral over scattering state dyads.

- Note: In 3D, promote $x \to \vec{x}$ = vector of operators. The relation with $\vec{p}$ eigenstates is $\langle \vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}/\hbar}$ and $\vec{p} \simeq -i\hbar\vec{\nabla}$

- Review / Examples to Remember
  - The free particle: energy e'states are momentum e'states. All are scattering states
  - Infinite square well $V(x) = 0$ inside, $\to \infty$ at boundaries
    - Imposes Dirichlet b.c. at $x = \pm a$
    - Energy e'values are
      $$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2$$
      with
      $$\psi_n(x) = \langle x | E_n \rangle = \begin{cases} \cos(n\pi x/2a)/\sqrt{a}, & n \text{ odd} \\ \sin(n\pi x/2a)/\sqrt{a}, & n \text{ even} \end{cases}$$
  - Harmonic Oscillator $H = p^2/2m + m\omega^2 x^2/2$
    - Energy e'states labeled by $n = 0, 1, 2, \ldots$, denoted $|n\rangle$
      $$E_n = \hbar\omega(n + 1/2), \quad \langle x | n \rangle = \psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$
      where $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ and H_n = Hermite polynomial
    - More cleanly, define
      $$a = \sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{ip}{\sqrt{2\hbar m\omega}}$$
      and it's adjoint $a^\dagger$
    - Then $[a, a^\dagger] = 1$, $H = \hbar\omega(a^\dagger a + 1/2)$, $[H, a] = -\hbar\omega a$, $[H, a^\dagger] = \hbar\omega a$
    - This means a is the lowering operator
      $$a|n\rangle = \sqrt{n}\, |n-1\rangle$$
      and $a^\dagger$ is the raising operator
      $$a^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \Rightarrow |n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$$
    - Almost all the time, it's easier to use this operator notation than wavefunctions.
  - Coulomb Potential (1st Approx. of Hydrogen Atom)
    - Wavefunctions are best described in spherical coordinates, defined by n = principal quantum #, l, m = orbital angular momentum quantum numbers, s, m_s = spin quantum numbers. Write states as $|n, l, m; s = 1/2, m_s\rangle$
    - Wavefunctions are (spin factorizes out here)
      $$\langle \vec{x} | n, l, m \rangle = \psi_{nlm}(x) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}\, e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na}\right) Y_l^m(\theta, \phi)$$

where L^{2l+1}_{n-l-1} are associated Laguerre polynomials
and Y_l^m are spherical harmonics (as usual)
+ Tady, $a = 4\pi\epsilon_0\hbar^2/me^2$ = Bohr radius

+ Energy depends only on principal quantum number

$$E_n = \frac{-\hbar^2}{2ma^2}\frac{1}{n^2} = \frac{-m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{1}{n^2}$$

+ Since the energies don't depend on angular momentum, it can be advantageous to pick different e'states with definite total angular momentum quantum numbers j, m_j (and l, s), so we have $|n, j, m_j; l, s = \frac{1}{2}\rangle$