Today in Physics 237: observables and Hermitian operators

- Eigenfunctions of a Hermitian operator
    - Discrete spectra
    - Continuous spectra, which gets quite abstract; sorry about that
- Generalized statistical interpretation
- Generalized uncertainty principle; incompatible and compatible observables

$$\begin{aligned}
\langle f\,|\,g\rangle &= \left\langle \left(\hat{A}-\langle A\rangle\right)\Psi \middle\| \left(\hat{B}-\langle B\rangle\right)\Psi \right\rangle \\
&= \left\langle \Psi \middle| \left(\hat{A}-\langle A\rangle\right)\left(\hat{B}-\langle B\rangle\right) \middle| \Psi \right\rangle \\
&= \left\langle \Psi \middle| \left(\hat{A}\hat{B}-\hat{A}\langle B\rangle-\hat{B}\langle A\rangle+\langle A\rangle\langle B\rangle\right) \middle| \Psi \right\rangle \\
&= \langle \Psi\,|\,\hat{A}\hat{B}\Psi\rangle-\langle B\rangle\langle \Psi\,|\,\hat{A}\Psi\rangle-\langle A\rangle\langle \Psi\,|\,\hat{B}\Psi\rangle+\langle A\rangle\langle B\rangle\langle \Psi\,|\,\Psi\rangle \\
&= \left\langle \hat{A}\hat{B}\right\rangle-\langle B\rangle\langle A\rangle-\cancel{\langle A\rangle\langle B\rangle}+\cancel{\langle A\rangle\langle B\rangle} \\
&= \left\langle \hat{A}\hat{B}\right\rangle-\langle B\rangle\langle A\rangle \quad .
\end{aligned}$$

Eigenfunctions of a Hermitian operator

- Two little theorems first:

  1. The eigenvalues of Hermitian operators are real.

     - Suppose $\hat{Q}$ is Hermitian and $\hat{Q}f = qf$; then $\langle f|\hat{Q}f\rangle = \langle f\hat{Q}|f\rangle \quad \Rightarrow \quad q\langle f|f\rangle = q^*\langle f|f\rangle \quad \Rightarrow \boxed{q = q^*}$, as long as $\langle f|f\rangle$ exists and is nonzero.

     - It does exist, by definition of Hilbert space, q.e.d.

  2. Eigenfunctions of Hermitian operators which belong to distinct eigenvalues are orthogonal.

     - Suppose $\hat{Q}$ is Hermitian, $\hat{Q}f = qf$, and $\hat{Q}g = q'g$. Then $\langle f|\hat{Q}g\rangle = \langle f\hat{Q}|g\rangle \quad \Rightarrow \quad q'\langle f|g\rangle = q^*\langle f|g\rangle$.

     - By the first theorem, $q^* = q \neq q'$, so $\boxed{\langle f|g\rangle = 0}$, q.e.d.

- And an axiom, which is necessary for quantum mechanics but has only been proven for **finite**-dimensional Hilbert spaces:

  3. The eigenfunctions of a Hermitian operator are a **complete** set.

Eigenfunctions of a Hermitian operator (continued)

- Theorem 2 does not cover degenerate states: unique states which have the same eigenvalue for some given operator. Are they orthogonal too?
  - Not necessarily, but even if not, there is always a set of orthogonal linear combinations, which can be used in the basis set instead of the originals. For example, though not of a discrete spectrum (G&S problem 3.7):

a. Suppose that $f(x)$ and $g(x)$ are two eigenfunctions of an operator $\hat{Q}$, with eigenvalue q. Show that any linear combination of f and g is itself an eigenfunction of $\hat{Q}$, with eigenvalue q.

b. Check that $f(x)=e^{x}$ and $g(x)=e^{-x}$ are eigenfunctions of the operator d^2/dx^2, with the same eigenvalue. Construct two linear combinations of f and g that are orthogonal eigenfunctions, on the interval (-1,1).

a. Let $h(x)=af(x)+bg(x)$; then $\hat{Q}h=\hat{Q}(af+bg)=aqf+bqg=q(af+bg)=qh$, $\boxed{\text{q.e.d.}}$

b. All derivatives of e^{x} are also e^{x}. And even-numbered derivatives of e^{-x} are equal to e^{-x}, e.g.

$$\frac{d^2}{dx^2}e^{-x}=-\frac{d}{dx}e^{-x}=e^{-x}.$$

Eigenfunctions of a Hermitian operator (continued)

So both e^x and e^{-x} are eigenstates of $d^2\big/dx^2$, and are degenerate with eigenvalue 1. They are not orthogonal on the interval (-1,1):

$$\langle f\,|\,g\rangle = \int_{-1}^{1} e^x e^{-x} dx = 2,\ \text{not zero.}$$

With a little trial and error, though, one can find two linear combinations of *f* and *g* which are. Consider the simplest of such combinations, $\boxed{h(x) = e^x + e^{-x} \text{ and } j(x) = e^x - e^{-x}:}$

$$\langle h\,|\,j\rangle = \int_{-1}^{1} \left(e^x + e^{-x}\right)\left(e^x - e^{-x}\right) dx = \frac{1}{2}\left[e^{2x} + e^{-2x}\right]_{-1}^{1} = \frac{1}{2}e^2 + \frac{1}{2}e^{-2} - \frac{1}{2}e^{-2} - \frac{1}{2}e^2 = 0 \quad .$$

They are orthogonal. Note that you know these functions: $h(x) = 2\cosh x$ and $j(x) = 2\sinh x$.

- One can always construct such functions to substitute for non-orthogonal degenerate wavefunctions. The process is called **Gram-Schmidt orthogonalization**. See G&S Appendix A for details.

Eigenfunctions of a Hermitian operator (continued)

- These wavefunctions, though now orthogonal, are not normalizable, any more than the originals. Try it.
- Non-normalizability of eigenfunctions is characteristic of continuous spectra like these. We have encountered this before, with the separation solutions for free particles.
- A way around this is can be called "Dirac orthonormality." Show by example (Example 3.2 in G&S):

  Find the eigenfunctions and eigenvalues of the momentum operator $\hat{p}$, on the interval $-\infty < x < \infty$.

  - Call the momentum eigenvalue p: if $f_p(x)$ is an eigenstate, then $\hat{p}f_p(x) = -i\hbar\frac{d}{dx}f_p(x) = pf_p(x)$. f_p also has to be a Schrödinger equation solution, of course.
  - But the eigenvalue equation is directly integrable: move f_p to the LHS, integrate both sides over x, use the chain rule:

$$\int\frac{df_p}{f_p} = \frac{ip}{\hbar}\int dx \quad\Rightarrow\quad \ln f_p = \frac{ipx}{\hbar} + A' \quad\Rightarrow\quad \boxed{f_p(x) = Ae^{ipx/\hbar}} \; .$$

Eigenfunctions of $\hat{p}$, with eigenvalues p.

Eigenfunctions of a Hermitian operator (continued)

- So are we done? No; these wavefunctions are not square-integrable – can't live in a Hilbert space – any more than the free-quantum separation solutions were. (**Watch carefully,** here comes the abstract part.)
- What about the inner products? $\langle f_{p'} | f_p \rangle = \int f_{p'}^* f_p dx = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx \xrightarrow[p \to p']{} \infty$.
- So $\langle f_{p'} | f_p \rangle$ doesn't exist. However, it doesn't exist in the same way that the δ function doesn't. The Fourier transform of $\delta(x)$, which we may call $D(k)$, is

$$D(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \quad .$$

Fourier components of the delta function

- Inverse Fourier-transforming this expression gives us back an integral representation of the δ function:

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} D(k) e^{ikx} dk = \boxed{\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk} \quad .$$

Fourier spectrum of the delta function

Eigenfunctions of a Hermitian operator (continued)

- Use in $\langle f_{p'} | f_p \rangle$: **take p and p' to be real**. Then change names: the dummy variable x to $\hbar k$, and $p - p'$ to x.

$$\Rightarrow \boxed{\begin{aligned} \langle f_{p'} | f_p \rangle &= 2\pi\hbar |A|^2 \delta(p - p') \\ &= \delta(p - p') \quad . \end{aligned}}$$

Choose $A = 1/\sqrt{2\pi\hbar}$

"Dirac orthonormality"

- $\langle f_{p'} | f_p \rangle$ for real p and p' is almost like those for eigenfunctions in Hilbert space, except with the delta function playing the role of the Kronecker delta.

- And since any square-integrable function $f(x)$ can be written as Fourier integral,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{ikx} dk = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} dp = \int_{-\infty}^{\infty} c(p) f_p(x) dp \quad ,$$

it is in important ways as though the real-eigenvalue subset of $f_p(x)$ is a complete orthonormal set.

- This can be made more rigorous but it will do for now: the real-p are close to being a complete orthonormal set in Hilbert space, to which we can grant status similar to our infinite square well, or δ-function potential.

The generalized statistical interpretation of the wavefunction

The Copenhagen interpretation of the wavefunction can now be generalized, and cast in Dirac operator-algebra language to give us some interesting new tools. In 1-D:

- Measurement of an observable $Q(x,p)$ on a quantum in state $\Psi(x,t)$ is certain to yield one of the eigenvalues of the Hermitian operator $\hat{Q}(x,-i\hbar d/dx)$.

- If the spectrum of $\hat{Q}$ is discrete, the probability of getting the particular eigenvalue q_n associated with the orthonormalized eigenfunction $f_n(x)$ is $|c_n|^2$, where $c_n = \langle f_n|\Psi\rangle$.

- If the spectrum is continuous in z, with real eigenvalues $q(z)$ and associated (Dirac-orthonormalized) eigenfunctions $f_z(x)$, the probability of getting a result in the range z to $z + dz$ is $|c(z)|^2 dz$, where $c(z) = \langle f_z|\Psi\rangle$.

- Upon measurement, the wavefunction collapses to the corresponding eigenstate.

Generalized statistical interpretation (continued)

- Summary of the equations which go with the generalized statistical interpretation for a discrete spectrum:

$$\Psi(x,t)=\sum_n c_n(t) f_n(x) \qquad c_n=\langle f_n|\Psi\rangle=\int f_n^*(x)\Psi(x,t)dx$$

$$\sum_n |c_n|^2=1 \qquad \langle Q\rangle=\sum_n q_n|c_n|^2$$

- And introducing the **momentum-space wavefunction** $\Phi(p,t)$, in analogy with the momentum eigenfunctions discussed above (pp. 5-7), as the Fourier transform of the usual position-space wavefunction $\Psi(x,t)$:

$$\Phi(p,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\Psi(x,t)e^{-ipx/\hbar}dx \quad , \quad \Psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\Phi(p,t)e^{ipx/\hbar}dp \quad .$$

The probability of measuring momentum between p and $p + dp$ is $|\Phi(p,t)|^2\,dp$.

Generalized statistical interpretation (continued)

Connection of momentum-space functions and our trusty old position-space functions (G&S problem 3.12):

Find $\Phi(p,t)$ for the free quantum in terms of that quantum's Fourier amplitudes $\varphi(k)$. Show that, for the free quantum, $|\Phi(p,t)|^2$ is independent of time. (The time independence of this probability density is a manifestation of **momentum conservation** for the free quantum.)

- As we have seen (e.g. in Lecture 7), a free quantum can be represented by a wavepacket, normalized but composed of individually non-normalizable separation solutions. Letting $k = p/\hbar$ and $\omega = \hbar k^2/2m$,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{i\left(kx - \hbar k^2 t/2m\hbar\right)} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi\left(\frac{p}{\hbar}\right) e^{i\left(px/\hbar - p^2 t/2m\hbar\right)} \frac{dp}{\hbar} \quad .$$

- Compare to the expression on page 9. Evidently,

$$\boxed{\Phi(p,t) = \frac{1}{\hbar}\varphi\left(\frac{p}{\hbar}\right) e^{-ip^2 t/2m\hbar}} \quad , \quad \text{whence} \quad |\Phi(p,t)|^2 = \frac{1}{\hbar^2}\left|\varphi\left(\frac{p}{\hbar}\right)\right|^2 \quad \boxed{\text{, independent of } t.}$$

The generalized uncertainty principle

Let us now prove the uncertainty principle.

- For any observable *A*, the difference between measurement and expectation value is $\left|f\right\rangle = \left(\hat{A} - \left\langle A\right\rangle\right)\left|\Psi\right\rangle$, and the variance of measurements of *A* on an ensemble is

$$\sigma_A^2 = \langle f \,|\, f\rangle = \langle\Psi\left(\hat{A} - \left\langle A\right\rangle\right) | \left(\hat{A} - \left\langle A\right\rangle\right)\Psi\rangle$$

because $\hat{A}$ is Hermitian
and $\left\langle A\right\rangle$ is a real number

- Similarly, for a different observable *B*, $\sigma_B^2 = \langle g \,|\, g\rangle = \langle\Psi\left(\hat{B} - \left\langle B\right\rangle\right) | \left(\hat{B} - \left\langle B\right\rangle\right)\Psi\rangle$.
- Therefore, by the Schwartz inequality (Lecture 9, p. 7 and the green pages), $\sigma_A^2\sigma_B^2 = \langle f \,|\, f\rangle\langle g \,|\, g\rangle \geq \left|\langle f \,|\, g\rangle\right|^2$.
- We can write the square modulus of any complex number *z* as $\left|z\right|^2 = (\mathrm{Re}\, z)^2 + (\mathrm{Im}\, z)^2 \geq (\mathrm{Im}\, z)^2 = \left[\frac{1}{2i}\left(z - z^*\right)\right]^2$.
- Let $z = \langle f \,|\, g\rangle$, and we obtain $\sigma_A^2\sigma_B^2 \geq \left|\langle f \,|\, g\rangle\right|^2 = \left[\frac{1}{2i}\left(\langle f \,|\, g\rangle - \langle g \,|\, f\rangle\right)\right]^2$.

The generalized uncertainty principle (continued)

- Now put $\left|f\right\rangle = \left(\hat{A} - \langle A\rangle\right)\left|\Psi\right\rangle$ and $\left|g\right\rangle = \left(\hat{B} - \langle B\rangle\right)\left|\Psi\right\rangle$ into this last, simpler expression; keep in mind that the operators are Hermitian and the expectation values are ordinary real numbers; and simplify:

$$\langle f\,|\,g\rangle = \left\langle\left(\hat{A}-\langle A\rangle\right)\Psi\middle|\left(\hat{B}-\langle B\rangle\right)\Psi\right\rangle = \left\langle\Psi\middle|\left(\hat{A}-\langle A\rangle\right)\left(\hat{B}-\langle B\rangle\right)\middle|\Psi\right\rangle = \left\langle\Psi\middle|\left(\hat{A}\hat{B}-\hat{A}\langle B\rangle-\hat{B}\langle A\rangle+\langle A\rangle\langle B\rangle\right)\middle|\Psi\right\rangle$$

$$= \langle\Psi\,|\,\hat{A}\hat{B}\Psi\rangle - \langle B\rangle\langle\Psi\,|\,\hat{A}\Psi\rangle - \langle A\rangle\langle\Psi\,|\,\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\langle\Psi\,|\,\Psi\rangle = \left\langle\hat{A}\hat{B}\right\rangle - \langle B\rangle\langle A\rangle - \cancel{\langle A\rangle\langle B\rangle} + \cancel{\langle A\rangle\langle B\rangle}$$

$$= \left\langle\hat{A}\hat{B}\right\rangle - \langle B\rangle\langle A\rangle \quad .$$

- Do the same for $\langle g\,|\,f\rangle$, which just involves switching *A* and *B* everywhere in the previous expressions:

$$\langle g\,|\,f\rangle = \left\langle\hat{B}\hat{A}\right\rangle - \langle A\rangle\langle B\rangle \quad .$$

- The difference between these two results is the expectation value of the commutator of $\hat{A}$ and $\hat{B}$:

$$\langle f\,|g\rangle - \langle g\,|\,f\rangle = \left\langle\hat{A}\hat{B}\right\rangle + \cancel{\langle B\rangle\langle A\rangle} - \left\langle\hat{B}\hat{A}\right\rangle - \cancel{\langle A\rangle\langle B\rangle} = \left\langle\left[\hat{A},\hat{B}\right]\right\rangle \quad .$$

The generalized uncertainty principle (continued)

- Finally, combine the last expression on page 11 with the last expression on page 12:

$$\sigma_A^2\sigma_B^2 \geq \left[\frac{1}{2i}\left(\langle f\,|\,g\rangle - \langle g\,|\,f\rangle\right)\right]^2$$

$$\boxed{\geq \left(\frac{1}{2i}\left\langle[\hat{A},\hat{B}]\right\rangle\right)^2} \;. \qquad \textbf{Generalized uncertainty principle}$$

- From this we can recover the Heisenberg uncertainty principle, first seen in Lecture 2, p. 16:

$$\sigma_x^2\sigma_p^2 \geq \left(\frac{1}{2i}\left\langle[\hat{x},\hat{p}]\right\rangle\right)^2 = \left(\frac{1}{2i}i\hbar\right)^2 = \frac{\hbar^2}{4} \quad\Rightarrow\quad \boxed{\sigma_x\sigma_p \geq \frac{\hbar}{2}} \;.$$

The generalized uncertainty principle (continued)

- But there’s more to it than that: **any** two observables that do not commute give rise to their own uncertainty principle.

- We call such pairs **incompatible observables**.

  - Measurement of one of the pair collapses the wavefunction into an eigenstate of that operator.

  - Subsequent measurement of the other collapses the wavefunction again, into an eigenstate of the other operator. Consecutive measurements of the pair collapse consecutively to two different wavefunctions.

- The opposite: **compatible** observables commute. Consecutive measurements on the pair refer to the same wavefunction; the second measurement does not disturb the wavefunction to which the first collapsed.

  - For example, $\hat{p}$ and $\hat{H} = -\frac{\hat{p}^2}{2m} + V$ are compatible; see Quiz 2 parts b and c, for example.

- Finally we can note that the Heisenberg uncertainty principle is not an axiom. If our fundamental axiom is the statistical interpretation of the wavefunction, as generalized above, the Heisenberg uncertainty principle is a **consequence** of that axiom.