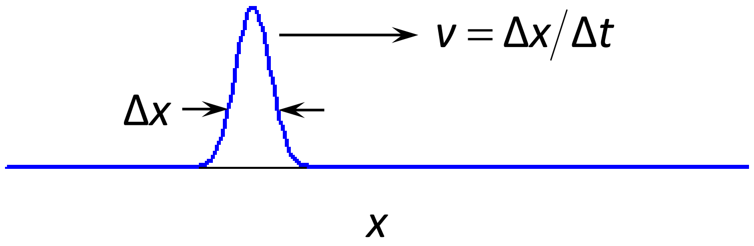
Today in Physics 237: full Dirac notation for state vectors

- Minimum-uncertainty wavepackets
- The generalized Ehrenfest theorem
- The energy-time uncertainty principle
- New (Dirac) notation for vectors and operators
- Bras and kets as dual vector spaces

$$H\Psi(x,t) = E\Psi(x,t); \quad E = p^2 / 2m$$



Minimum uncertainty wavefunctions are Gaussians

- We have noted a few instances of wavefunctions which give the minimum uncertainty product for *x* and *p*, e.g. the ground state of the quantum simple harmonic oscillator (Lecture 5), which has the form of a Gaussian:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \quad ; \quad \Psi(x,t) = \psi_0(x)e^{-i\omega t} \quad .$$

- We can find more **minimum-uncertainty** wavefunctions like this (G&S problem 3.17), by using
  - the wavefunctions and operators we defined last time (Lecture 10): $|f\rangle = \left(\hat{A} - \langle A\rangle\right)|\Psi\rangle$ and $|g\rangle = \left(\hat{B} - \langle B\rangle\right)|\Psi\rangle$
  - and the Schwartz inequality $|f||g| \geq |\langle f\,|g\rangle|$ in its minimum, “equality” limit, which is obtained when *f* and *g* are linearly dependent, i.e. $g = cf$ (Lecture 9, green pages);
  - returning to our use of $|\langle f\,|g\rangle|^2 = \mathrm{Re}\left(\langle f\,|g\rangle^2\right) + \mathrm{Im}\left(\langle f\,|g\rangle^2\right) \geq \mathrm{Im}\left(\langle f\,|g\rangle^2\right)$, for which the minimum, “equality” limit has $\mathrm{Re}\langle f|g\rangle = 0$:

$$\mathrm{Re}\left(c\langle f|f\rangle\right) = \mathrm{Re}(c) = 0 \quad \Rightarrow \quad c = ia \quad , \quad \text{with } a \text{ real} \quad \Rightarrow \quad g(x) = iaf(x) \quad .$$

Minimum uncertainty wavepackets are Gaussians (continued)

- Now take $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$: then $g(x) = iaf(x)$ becomes $\left(-i\hbar \frac{d}{dx} - \langle p \rangle\right)\Psi = ia\left(x - \langle x \rangle\right)\Psi$.
- This is a first-order differential equation, which can be solved for Ψ by separation, integration and chain rule:

$$\frac{d\Psi}{dx} = \frac{a}{\hbar}\left(-x + \langle x \rangle + \frac{i}{a}\langle p \rangle\right)\Psi \quad .$$

$$\int \frac{1}{\Psi}\frac{d\Psi}{dx}dx = \int \frac{d\Psi}{\Psi} = \frac{a}{\hbar}\int \left(-x + \langle x \rangle + i\langle p \rangle / a\right)dx$$

$$\ln\Psi = -\frac{a}{\hbar}\left(\frac{x^2}{2} - \langle x \rangle x\right) + i\frac{\langle p \rangle x}{\hbar} + C'' \quad .$$

- So this general minimum-uncertainty wavefunction is also a Gaussian. Before exponentiating, let's **complete the square** in the real part of the exponent, by reminding ourselves that $\langle x \rangle$ is constant, and letting

$$C'' = C' - \frac{a}{2\hbar}\langle x \rangle^2 \quad ;$$

Minimum uncertainty wavepackets are Gaussians (continued)

- then, $\ln\Psi = -\frac{a}{\hbar}\left(\frac{x^2}{2} - \langle x\rangle x + \frac{\langle x\rangle^2}{2}\right) + i\frac{\langle p\rangle x}{\hbar} + C' = -\frac{a}{2\hbar}\left(x - \langle x\rangle\right)^2 + i\frac{\langle p\rangle x}{\hbar} + C'$, and

$$\boxed{\Psi = Ce^{-a\left(x-\langle x\rangle\right)^2/2\hbar}e^{i\langle p\rangle x/\hbar}} \;.$$

- Thanks to the Gaussian form of the real part, this can be normalized, so it deserve the name of Wavepacket:

$$1 = \int_{-\infty}^{\infty}\Psi^*\Psi dx = |C|^2\int_{-\infty}^{\infty}e^{-a\left(x-\langle x\rangle\right)^2/\hbar}dx = |C|^2\sqrt{\frac{\hbar}{a}}\int_{-\infty}^{\infty}e^{-u^2}du = |C|^2\sqrt{\frac{\pi\hbar}{a}} \quad ,$$

$$\boxed{\Psi(x,0) = \left(\frac{a}{\pi\hbar}\right)^{1/4}e^{-a\left(x-\langle x\rangle\right)^2/2\hbar}e^{i\langle p\rangle x/\hbar}} \;.$$

Minimum-uncertainty
wavepackets are Gaussian

The (generalized) Ehrenfest theorem

- This refers to a theorem encountered in G&S chapter 1, otherwise unmentioned and unproven til now: that **expectation values obey the classical laws of physics**.

- Consider an operator $\hat{Q}$, and its expectation value $\langle Q\rangle$ given a wavefunction $\Psi(x,t)$. As we have seen before with wavefunctions which are superpositions of stationary states, $\langle Q\rangle$ can vary with time:

$$\frac{d}{dt}\langle Q\rangle=\frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle=\langle\partial\Psi/\partial t|\hat{Q}\Psi\rangle+\langle\Psi|\left(\partial\hat{Q}/\partial t\right)\Psi\rangle+\langle\Psi|\hat{Q}\partial\Psi/\partial t\rangle \quad .$$

- Use the Schrödinger equation, $i\hbar\partial\Psi/\partial t=\hat{H}\Psi$, to eliminate the time derivative of the wavefunction, noting that $\hat{H}$ is Hermitian so $\langle\hat{H}\Psi'|\Psi'\rangle=\langle\Psi'|\hat{H}\Psi'\rangle$:

$$\frac{d}{dt}\langle Q\rangle=\langle\hat{H}\Psi/(i\hbar)^{*}|\hat{Q}\Psi\rangle+\langle\Psi|\left(\partial\hat{Q}/\partial t\right)\Psi\rangle+\langle\Psi|\hat{Q}\hat{H}\Psi/i\hbar\rangle=\frac{i}{\hbar}\langle\Psi|\hat{H}\hat{Q}\Psi\rangle-\frac{i}{\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle+\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle \quad ;$$

$$\boxed{\frac{d}{dt}\langle Q\rangle=\frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle+\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle} \quad .$$

Generalized Ehrenfest theorem

Energy-time uncertainty

- Implications:
  - If $\hat{Q}$ does not depend explicitly on time – that is, if $\partial\hat{Q}/\partial t = 0$ – then $\left\langle d\hat{Q}/dt \right\rangle$ is determined by the commutator of $\hat{Q}$ with the Hamiltonian $\hat{H}$.
  - And if furthermore $\hat{Q}$ commutes with $\hat{H}$, then $\langle Q \rangle$ is constant, like the energy.
  - If $\hat{Q}$ does not commute with $\hat{H}$, the uncertainty in $\langle Q \rangle$ is governed by the generalized uncertainty principle we derived in Lecture 10 (p. 13), which, when combined with the generalized Ehrenfest theorem above, gives

$$\sigma_H \sigma_Q \geq \left| \frac{1}{2i} \left\langle \left[\hat{H}, \hat{Q}\right] \right\rangle \right| = \left| \frac{1}{2i} \frac{\hbar}{i} \frac{d}{dt} \langle Q \rangle \right| = \frac{\hbar}{2} \left| \frac{d}{dt} \langle Q \rangle \right| \quad .$$

- Now for a crude estimate. The uncertainty in energy ΔE is well enough determined: $\Delta E = \sigma_H$. For $\hat{Q}$ with given functional form we could calculate $\left[\hat{H}, \hat{Q}\right]$, thence σ_Q, but for the general expression we can do no better than to calculate the **characteristic time τ over which $\langle Q \rangle$ changes** relative to σ_Q, and approximate, for the uncertainty in time Δt,

$$\tau = \frac{\sigma_Q}{\left| d\langle Q \rangle / dt \right|} \approx \Delta t \quad \Rightarrow \boxed{\Delta E \Delta t \geq \frac{\hbar}{2}} \; .$$

Energy-time uncertainty principle

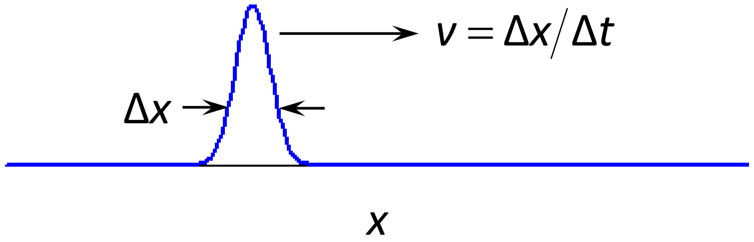
Energy-time uncertainty (continued)

- Here, τ is a characteristic of **systematic** change in $\langle Q \rangle$, rather than the statistical variance of $\langle Q \rangle$. So it's comforting to note that
  - (G&S Example 3.6) the time Δt it takes a free-quantum wavepacket to propagate by its width Δx, and the uncertainty ΔE in the packet's energy given its spread in momentum Δp, give the same answer as above:

$$\Delta E \Delta t = \Delta\left(\frac{p^2}{2m}\right)\frac{\Delta x}{v} = \frac{2p\Delta p}{2m}\frac{m\Delta x}{p} = \Delta p \Delta x \geq \frac{\hbar}{2} \quad .$$

  - explicit calculation of standard deviations of expectations for H and x also give the same answer (G&S problem 3.21, on this week's workshop/homework problems).

$$H\Psi(x,t) = E\Psi(x,t); \quad E = p^2/2m$$



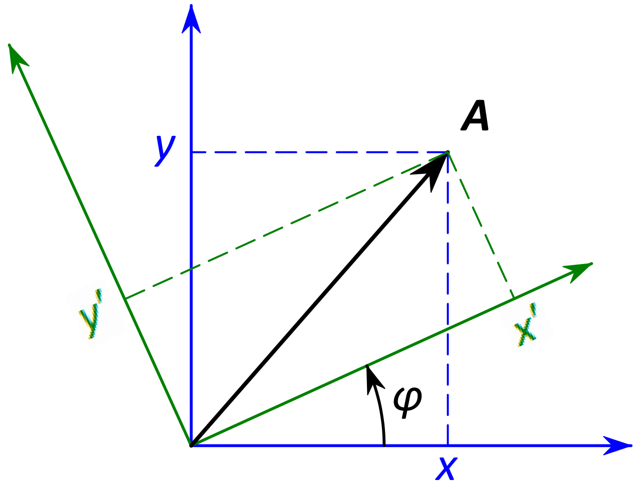
Dirac notation for vectors and operators **(more abstraction!)**

- Just as is the case for vectors in 3-D space, one always has a choice of bases in which to bookkeep a Hilbert-space vector's components.
    - And there are **unitary operators**, like the rotation matrix $\overleftrightarrow{\boldsymbol{R}}$ at right, which linearly transform vector components from one basis to another, while keeping the magnitude of the vector the same.
- For example, the state vector $|S(t)\rangle$ of a quantum can be expressed in different bases as a continuous function of position or momentum, or as a linear combination of discrete separation solutions/eigenstates of some operator:

$$\Psi(x,t)=\langle x|S(t)\rangle, \quad \Phi(p,t)=\langle p|S(t)\rangle, \quad c_\nu=\langle\psi_\nu(x)|S(t)\rangle \quad .$$

- And operators transform the state on which they operate – linearly, not necessarily unitarily – by changing their components:

$$|\beta\rangle=\hat{Q}|\alpha\rangle \quad .$$



$$\begin{bmatrix} A_{x'} \\ A_{y'} \\ A_{z'} \end{bmatrix} = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix}$$

$$= \overleftrightarrow{\boldsymbol{R}} \cdot \boldsymbol{A}$$

Dirac notation for vectors and operators (continued)

- Given a discrete orthonormal basis set, $|e_n\rangle$ with $\langle e_m|e_n\rangle = \delta_{mn}$, $|\alpha\rangle$ and $|\beta\rangle$ can be expressed as

$$|\alpha\rangle = \sum_n a_n |e_n\rangle = \sum_n \langle e_n|\alpha\rangle |e_n\rangle \quad , \quad |\beta\rangle = \sum_n b_n |e_n\rangle = \sum_n \langle e_n|\beta\rangle |e_n\rangle$$

- So we can express an operator $\hat{Q}$ by the **matrix elements** by which it transforms states in that basis. We have been dealing with scalar operators so far, but in general they have independent, basis-dependent components. So, **new notation**:

$$Q_{mn} = \langle e_m|\hat{Q}|e_n\rangle \quad .$$

  - If $\hat{Q}$ transforms $|\alpha\rangle$ into $|\beta\rangle$, then

$$|\beta\rangle = \sum_n b_n |e_n\rangle = \hat{Q}|\alpha\rangle = \sum_n a_n \hat{Q}|e_n\rangle \quad \Rightarrow \quad \langle e_m|\beta\rangle = \sum_n b_n \cancelto{\delta_{mn}}{\langle e_m|e_n\rangle} = b_m = \sum_n a_n \langle e_m|\hat{Q}|e_n\rangle = \sum_n Q_{mn} a_n \quad .$$

- **From now on**, we will leave the operator separate from the bra and ket in the inner product which gives the operator's matrix elements, as $Q_{mn} = \langle e_m|\hat{Q}|e_n\rangle$, rather than bundling it with the ket or bra, as $\langle e_m|\hat{Q}e_n\rangle$.

Dirac-notation definitions and rules

- As noted in Lecture 9, inner products of vectors take the form of multiplication of row and column matrices, and represent integrals of wavefunctions. Supposing both state vectors are expressed in basis $\left|e_n\right\rangle$,

$$\left\langle f\middle|g\right\rangle = \int_{-\infty}^{\infty} f^{*}g\,dx = \int_{-\infty}^{\infty} \begin{bmatrix} c_0^{*} & c_1^{*} & \ldots \end{bmatrix} \begin{bmatrix} d_0 \\ d_1 \\ \vdots \end{bmatrix} dx = \int_{-\infty}^{\infty} \sum_n c_n^{*} d_n\,dx \quad .$$

- The bras are represented by row vectors, with Fourier coefficients complex-conjugated, and the kets by columns:

$$\left\langle f\right| = \begin{bmatrix} c_0^{*} & c_1^{*} & \ldots \end{bmatrix} \quad , \quad \left|f\right\rangle = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \end{bmatrix} \quad .$$

- This makes the bras the **dual vector space** corresponding to the matching kets.

Dirac-notation definitions and rules (continued)

- The official definition of a dual vector space is: that complete orthonormal vector space $\langle e_m|$ such that

$$\langle e_m|e_n\rangle = \delta_{mn} \quad ,$$

where $|e_n\rangle$ is also a complete orthonormal set, and the inner product is used as shorthand for – that is, tacitly **understood** to involve – an integration over *x*:

$$\langle e_m|e_n\rangle \leftrightarrow \langle e_m|e_n\rangle = \int_{-\infty}^{\infty} e_m^*(x)e_n(x)dx = \delta_{mn} \quad .$$

- With this definition of bras and kets, one can move them around algebraically – and restore the integrals when necessary – to form other vector products which prove useful.
  - Like this **projection operator** $\hat{P}$, which picks out the component of one vector lying along another vector, and is formed by the **outer product** of vectors, this time $|f\rangle = \sum_n c_n|e_n\rangle$:

$$|g\rangle = \left(\langle f|g\rangle\right)|f\rangle = |f\rangle\langle f|g\rangle \equiv \hat{P}|g\rangle; \ \boxed{\hat{P} = |f\rangle\langle f|} \quad .$$

Dirac-notation definitions and rules (continued)

- Here, using $\left|f\right\rangle = \sum_m c_m \left|e_m\right\rangle$ and $\left\langle f\right| = \sum_n \left\langle e_n\right| c_n^*$,

$$\hat{P}_{mn} = c_m \left|e_m\right\rangle\left\langle e_n\right| c_n^* \leftrightarrow \begin{bmatrix} c_0 \\ c_1 \\ \vdots \end{bmatrix} \begin{bmatrix} c_0^* & c_1^* & \dots \end{bmatrix} = \begin{bmatrix} \left|c_0\right|^2 & c_0 c_1^* & \dots \\ c_1^* c_0 & \left|c_1\right|^2 & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad ;$$

$$\left|e_m\right\rangle\left\langle e_n\right| \leftrightarrow \begin{bmatrix} 0 & \dots & \dots & \dots \\ \vdots & \ddots & 1 & \\ \vdots & & \ddots & \\ \vdots & & & \ddots \end{bmatrix} \quad ;$$

Integral over *x* is understood

$$\sum_n \left|e_n\right\rangle\left\langle e_n\right| = 1 \leftrightarrow \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & & \\ \vdots & & \ddots & \\ 0 & & & 1 \end{bmatrix} \text{ (the identity matrix)} \quad .$$