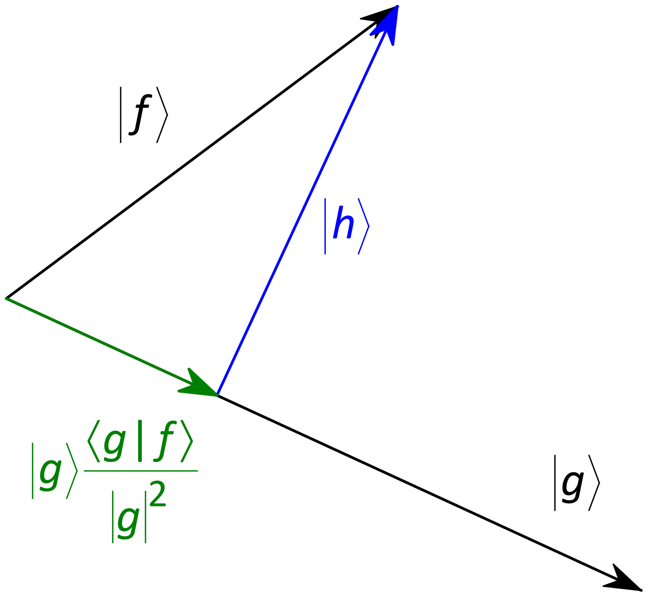
Today in Physics 237: state vectors and Hermitian operators

- State vectors, Hilbert space, and infinite-dimensional Hilbert space
- Observables and Hermitian operators
- The Schwartz inequality



Vectors

Familiar, fundamental properties of vectors:

- behavior under operations, prominently the rotation operator;
- the inner (scalar) product;
- the outer (dyadic, or tensor) product.

A vector like $\boldsymbol{E}$ has three components and finite magnitude $|E| = \sqrt{\boldsymbol{E} \cdot \boldsymbol{E}}$.

Coordinate-independent form	Matrix form, Cartesian coordinates	Compact Cartesian form
$\vec{\boldsymbol{R}} \cdot \boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}(\boldsymbol{r}')$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\vartheta & \sin\vartheta \\ 0 & -\sin\vartheta & \cos\vartheta \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \begin{bmatrix} E_{x'} \\ E_{y'} \\ E_{z'} \end{bmatrix}$, for example (rotation by +ϑ about *x*)	$\sum_{i=1}^{3}\sum_{j=1}^{3} R_{ij} E_j$
$\boldsymbol{E} \cdot \boldsymbol{B}$	$\begin{bmatrix} E_x & E_y & E_z \end{bmatrix} \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix} = E_x B_x + E_y B_y + E_z B_z$	$\sum_{i=1}^{3} E_i B_i$
$\boldsymbol{EB}$, a.k.a. $\boldsymbol{E} \otimes \boldsymbol{B}$	$\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \begin{bmatrix} B_x & B_y & B_z \end{bmatrix} = \begin{bmatrix} E_x B_x & E_x B_y & E_x B_z \\ E_y B_x & E_y B_y & E_y B_z \\ E_z B_x & E_z B_y & E_z B_z \end{bmatrix}$	$\sum_{i=1}^{3}\sum_{j=1}^{3} E_i B_j$

Vectors (continued)

Now you have seen general solutions to the Schrödinger equation, made from linear combinations of stationary, separation solutions, such as the quantum simple harmonic oscillator,

$$\Psi(x,t) = \sum_{v=0}^{\infty} A_v \psi_v(x) e^{-i\omega t} \quad ,$$

$$\psi_v(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{v!}} \left(\hat{a}_+\right)^v e^{-m\omega x^2/2\hbar} \quad ;$$

and the free-quantum wavepacket:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{-i\hbar k^2 t/2m} e^{ikx} dk \quad ,$$

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx \quad .$$

Vectors (continued)

These objects are also vectors. For example, a state of the quantum simple harmonic oscillator is represented by a vector with components $A_v \psi_v(x) e^{-i\omega t}$. (For simplicity, take the A_v to be constant here.)

- Such a vector can be transformed by operators:

$$\hat{a}_+ \Psi = \Psi' \quad \text{, or} \quad \hat{a}_+ \begin{bmatrix} A_0 \psi_0 e^{-i\omega_0 t} \\ A_1 \psi_1 e^{-i\omega_1 t} \\ \vdots \end{bmatrix} = \frac{1}{\sqrt{2m\hbar\omega}} \begin{bmatrix} A_0 \psi_1 e^{-i\omega_0 t} \\ \sqrt{2} A_1 \psi_2 e^{-i\omega_1 t} \\ \vdots \end{bmatrix} \quad \text{, or} \quad \hat{a}_+ |\Psi\rangle = |\Psi'\rangle \quad \text{, a.k.a. } |\hat{a}_+ \Psi\rangle$$

OK to write it either way.

- The vector participates in inner products with other vectors:

$$\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi'(x,t) dx \quad \text{, or} \quad \int_{-\infty}^{\infty} \left[A_0 \psi_0 e^{-i\omega t} \quad A_1 \psi_1 e^{-i\omega t} \quad \ldots \right]^* \begin{bmatrix} A_0' \psi_0 e^{-i\omega t} \\ A_1' \psi_1 e^{-i\omega t} \\ \vdots \end{bmatrix} dx = A_0^* A_0' + A_1^* A_1' + \ldots \quad \text{, or} \quad \langle \Psi | \Psi' \rangle \quad .$$

Vectors (continued)

- As we will see, such a vector also participates in outer products:

$$\Psi(x,t)\Psi'^*(x,t) \quad \text{, or} \quad \begin{bmatrix} A_0\psi_0 e^{-i\omega t} \\ A_1\psi_1 e^{-i\omega t} \\ \vdots \end{bmatrix} \begin{bmatrix} A_0'\psi_0 e^{-i\omega t} & A_1'\psi_1 e^{-i\omega t} & \dots \end{bmatrix}^* = \begin{bmatrix} |A_0 A_0'||\psi_0|^2 & \cdots \\ \vdots & \ddots \end{bmatrix} \quad \text{, or} \quad |\Psi\rangle\langle\Psi'|$$

- And of course it has a finite magnitude; that is, it is normalized: $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$, or $\langle\Psi|\Psi\rangle$.

- Our new compact expressions are in **Dirac bra-ket notation**. This will seem abstract at first, so keep in mind that there are equivalent expressions in our ordinary language of functions and their integrals, and in the language of explicit matrices and their algebra.

- Our new vectors, e.g. $|\Psi\rangle$, are called **state vectors**.

State and basis vectors (continued)

- The stationary states are the **basis vectors** which define the orthogonal “coordinates:” for example, $\left|\psi_v e^{-i(v+1/2)\omega t}\right\rangle$ is one of the “unit vectors” in the coordinate system of the simple harmonic oscillator.

- Each component of a state vector is a projection of the vector onto one of the orthogonal “coordinates” of the space in which the vector is defined. Just like $\hat{\boldsymbol{x}}\cdot\boldsymbol{E}=E_x$ is the x component of $\boldsymbol{E}$, $\langle\psi_v|\Psi\rangle=A_v$ is the v component of $\left|\Psi\right\rangle$.

- As we have noted all along, physical wavefunctions are normalizable: that is, square-integrable.

  - The name for a vector space like this is L^2 (mathematicians), or **Hilbert space** (physicists). We have been using the whole 1-D axis, $-\infty<x<\infty$, so it’s $L^2(-\infty,\infty)$.

  - The basis set for the simple harmonic oscillator thus occupies an **infinite-dimensional** Hilbert space. Don’t worry about the infinite dimensionality; this causes no additional problems compared to finite dimensions.

- So state vectors have importantly familiar properties, and represent a potential simplification in calculations: one can freely use all the techniques of linear algebra.

Vectors (continued)

Some useful properties of Hilbert space on the interval $(-\infty,\infty)$:

- If $|f(x)\rangle$ and $|g(x)\rangle$ belong to Hilbert space, then $\langle f(x)|g(x)\rangle = \int_{-\infty}^{\infty} f(x)^* g(x)dx$ exists and is finite.
  - In 2- or 3-D this is a consequence of the triangle inequality, e.g. $\boldsymbol{a}\cdot\boldsymbol{b} \le \sqrt{a^2 b^2}$. Here it is a consequence of the triangle inequality's generalization, the **Schwartz inequality** (see today's green pages): $|\langle f|g\rangle| \le \sqrt{|f|^2 |g|^2}$.
  - Thus $\boxed{\langle f|g\rangle = \langle g|f\rangle^* \quad .}$
- If $\{|f_v(x)\rangle\}$ is a complete orthonormal set, as the stationary states of the quantum simple harmonic oscillator are, then this set shares the useful properties of the QSHO:

$$\langle f_u | f_v\rangle = \delta_{uv} \quad ,$$

$$g(x) = \sum_v c_v f_v(x) \quad , \quad c_v = \langle f_v(x)|g(x)\rangle \quad ,$$

for any other function $g(x)$ which belongs to the same Hilbert space.

Hermitian operators

- An observable is an operator which has a real-valued expectation: $\langle Q\rangle^* = \langle Q\rangle = \int f^*\hat{Q}f\,dx = \langle f|\hat{Q}f\rangle$.
- But as we just showed, $\langle f|\hat{Q}f\rangle = \langle\hat{Q}f|f\rangle^*$; since the LHS is real-valued, so is the RHS, and the complex conjugation comes off:

$$\boxed{\langle f|\hat{Q}f\rangle = \langle\hat{Q}f|f\rangle} \; .$$

Hermitian operator
(same Hermite as the polynomials)

Observables are Hermitian operators, and *vice versa*.

- Few operators are Hermitian. Momentum is, for example:

$$\langle f|\hat{p}f\rangle = -i\hbar\int_{-\infty}^{\infty} f^*\frac{d}{dx}f\,dx = \cancelto{0}{-i\hbar f^* f\Big|_{-\infty}^{\infty}} + i\hbar\int_{-\infty}^{\infty}\frac{d}{dx}f^*f\,dx = \int_{-\infty}^{\infty}\left(-i\hbar\frac{d}{dx}f\right)^* f\,dx = \langle\hat{p}f|f\rangle \quad .$$

The raising and lowering operators are not, quite apart from being complex: as in the lemma we proved in Lecture 6 (pp. 2-3),

$$\langle f|\hat{a}_\pm f\rangle = \int_{-\infty}^{\infty} f^*\left(\hat{a}_\pm f\right)dx = \int_{-\infty}^{\infty}\left(\hat{a}_\mp f\right)^* f\,dx = \langle\hat{a}_\mp f|f\rangle \quad .$$

Hermitian operators (continued)

- But the combinations $\hat{a}_+\hat{a}_-$ and $\hat{a}_-\hat{a}_+$ are Hermitian, as one can show with two applications of the lemma:

$$\langle f\,|\,\hat{a}_\pm\hat{a}_\mp f\rangle = \int_{-\infty}^{\infty} f^*\left(\hat{a}_\pm\hat{a}_\mp f\right)dx = \int_{-\infty}^{\infty}\left(\hat{a}_\mp f\right)^*\left(\hat{a}_\mp f\right)dx = \int_{-\infty}^{\infty}\left(\hat{a}_\pm\hat{a}_\mp f\right)^* f dx = \langle \hat{a}_\pm\hat{a}_\mp f\,|\,f\rangle \quad .$$

  They better be, as they appear in the Hamiltonian for the quantum simple harmonic oscillator.

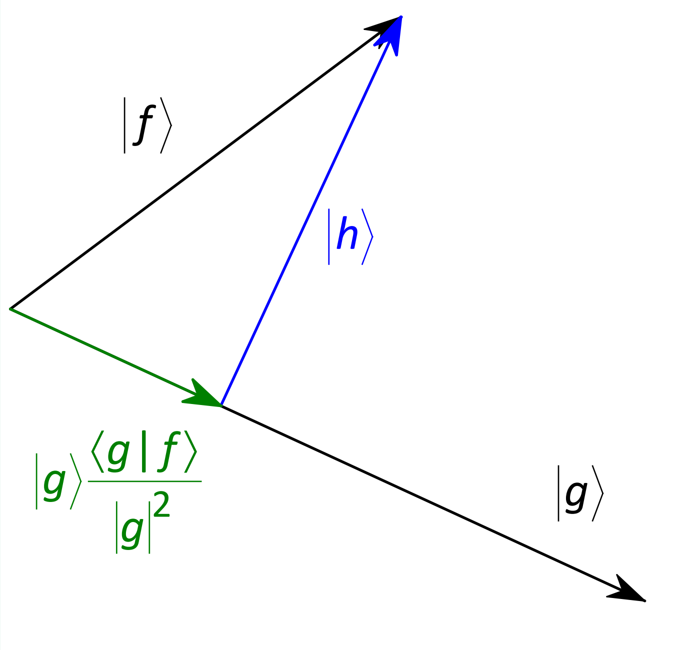
- An operator $\hat{Q}^\dagger$ such that $\langle f\,|\,\hat{Q}g\rangle = \langle \hat{Q}^\dagger f\,|\,g\rangle$, for all f and g, is called the Hermitian conjugate, or **adjoint**, of $\hat{Q}$.
  - For example, the raising and lowering operators are each other's Hermitian conjugate, as we just showed in the last line of page 8.
  - A Hermitian operator is equal to its own Hermitian conjugate; it is **self-adjoint**.
- Related terminology: a state is called **determinate** for observable $\hat{Q}$ if it is an eigenfunction of $\hat{Q}$.
- Also related: two unique states are called **degenerate** if they share the same eigenvalue for an observable $\hat{Q}$.

The Schwartz inequality

Suppose $f(x)$ and $g(x)$ are square-integrable, nonzero, and that inner products involving $|f(x)\rangle$ and $|g(x)\rangle$ exist. Then $|\langle f|g\rangle| \leq |f||g|$, with the equality corresponding to linearly-dependent f and g.

- No matter how many dimensions in their Hilbert space, $|f\rangle$ and $|g\rangle$ define directions in that space, and the two of them define a plane in that space.
- In that plane, we can use the Pythagorean theorem.
- So construct a right triangle with $|f\rangle$, its projection onto $|g\rangle$, and the vector difference of this projection with $|f\rangle$, which we will call $|h\rangle$:

$$|h\rangle = |f\rangle - |g\rangle\frac{\langle g|f\rangle}{\langle g|g\rangle} \quad .$$



The Schwartz inequality (continued)

- Then find the length of $|h\rangle$:

$$|h|^2 = \langle h|h\rangle = \left(\langle f| - \frac{\langle f|g\rangle}{|g|^2}\langle g|\right)\left(|f\rangle - |g\rangle\frac{\langle g|f\rangle}{|g|^2}\right)$$

$$= \langle f|f\rangle - \frac{\langle f|g\rangle}{|g|^2}\langle g|f\rangle - \langle f|g\rangle\frac{\langle g|f\rangle}{|g|^2} + \frac{\langle f|g\rangle}{|g|^2}\langle g|g\rangle\frac{\langle g|f\rangle}{|g|^2} = |f|^2 - \frac{\langle f|g\rangle\langle g|f\rangle}{|g|^2} \quad .$$

- And rearrange: $|f|^2|g|^2 - \langle f|g\rangle\langle g|f\rangle = |g|^2|h|^2 \geq 0$, as the RHS is positive definite. Now recall

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^* g\,dx \quad , \quad \langle g|f\rangle = \int_{-\infty}^{\infty} g^* f\,dx = \langle f|g\rangle^* \quad ; \text{so} \quad \boxed{|\langle f|g\rangle|^2 \leq |f|^2|g|^2} \quad , \quad \text{q.e.d.}$$

- Equality would mean $|h|^2 = 0$; that is, $|f\rangle$ and $|g\rangle$ differ by a multiplicative factor (are linearly dependent).