(8) Matrix Mechanics

1 Thus Far

- Configuration determined by wavefunction $\psi(x)$
- Time evolution related to energy $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- Observables (like energy)
  - correspond to operators ($\hat{E} = i\hbar\frac{\partial}{\partial t}$)
  - which have eigenfunctions ($\phi_E(x) = e^{-i\omega t}$)
  - with eigenvalues ($\hbar\omega$)
  - which correspond to measurable values of the observable
  - for which the probability is $\mathbb{P}_E = |\langle\phi_E(x)|\psi(x)\rangle|^2$
  - and should you make such a measurement on the state $\psi(x)$
  - and get eigenvalue $\hbar\omega$
  - the state will collapse to the eigenfunction $\phi_E(x)$
  - and remain their forever!

Last time I got a good question about how we could be sure that $\langle x\rangle$ is real, given the obviously complex terms in this expression:

Superpositions Move

$$\begin{aligned}\langle x\rangle &= \int_{-\infty}^{\infty}\left(\sum_n c_n\phi_n(x)\,e^{-i\omega_n t}\right)^* x\left(\sum_m c_m\phi_m(x)\,e^{-i\omega_m t}\right)dx \\ &= \sum_{n,m} c_n^* c_m e^{i(\omega_n-\omega_m)t}\underbrace{\int_{-\infty}^{\infty}\phi_n^*(x)\,x\,\phi_m(x)\,dx}_{\neq\delta_{mn}}\end{aligned}$$

The easy answer, which hit me later, is that for every term in the sum in which $n \neq m$, there is a term with n and m reversed. These are complex conjugate pairs (since x is real, or $\hat{x}$ is Hermitian if you like), and thus their sum must be real. For every term with $n = m$, the exponential goes to 1 and $c_n^* c_m = |c_n|^2$.

2 This Time

- Clicker Question Review
- Connection to Matrix Mechanics

3 Connection to Matrix Mechanics

Here I digress briefly to discuss the strong analogy between the mathematics of operators and that of linear algebra. (This will probably only be enlightening for students with a strong understanding of vector and matrix manipulation, and it is not critical in this course.)

If we use superposition to express a state as a linear combination of orthonormal basis functions

$$\psi(x) = \sum_n c_n \psi_n(x) \tag{1}$$

we can write the coefficients that appear in this sum as a vector $\vec{c}$. Orthonormality requires that the basis functions satisfy

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_m(x)\, dx = \delta_{mn} \quad \text{where} \quad \delta_{mn} = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{otherwise} \end{cases}$$

We could also use a continuous set of basis functions, as in the Fourier transform

$$\psi(x) = \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx}\, dx$$

in which case $\tilde{\psi}(k)$ plays the role of $\vec{c}$, but we will stick to the discrete case here.

We start to clarify the linear algebra analogy by looking at the normalization of $\mathbb{P}(x)$, which we can write as

$$
\begin{aligned}
\langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} \mathbb{P}(x)\, dx = \int_{-\infty}^{\infty} \psi^*(x)\, \psi(x)\, dx \\
&= \int_{-\infty}^{\infty} \left(\sum_n c_n \psi_n(x) \right)^* \left(\sum_m c_m \psi_m(x) \right) dx \\
&= \sum_{n,m} c_n^* c_m \int_{-\infty}^{\infty} \psi_n(x)^*\, \psi_m(x)\, dx = \sum_{n,m} c_n^* c_m\, \delta_{mn} \\
&= \sum_n |c_n|^2 = \left[c_1^*, c_2^*, \ldots, c_n^*\right] \cdot \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} \\
&= \vec{c}^{\,\dagger} \cdot \vec{c} \equiv |\vec{c}|^2
\end{aligned}
$$

where the † indicates the conjugate of the transpose, also known as the Hermitian adjoint. Thus, $\langle\psi|\psi\rangle$ is equal to the inner product of $\vec{c}$ with its conjugate, or the norm squared of $\vec{c}$. Not surprisingly, a properly normalized wavefunction corresponds to a vector with a norm of 1.

Similarly, given two states built from different linear combinations of the same basis functions,

$$
\psi_a(x) = \sum_n a_n \psi_n(x) \quad \text{and} \quad \psi_b(x) = \sum_n b_n \psi_n(x)
$$

we find that the overlap integral between two states

$$
\begin{aligned}
\langle\psi_a|\psi_b\rangle &= \int_{-\infty}^{\infty} \psi_a^*(x)\, \psi_b(x)\, dx \\
&= \sum_{n,m} a_n^* b_m\, \delta_{mn} \\
&= \sum_n a_n^*\, b_n = \vec{a}^{\,\dagger} \cdot \vec{b}
\end{aligned}
$$

is the inner product of their coefficient vectors.

In this context, operators play the role of matrices, such that

$$\begin{aligned}\langle\psi_a|\hat{A}|\psi_b\rangle &= \int_{-\infty}^{\infty}\psi_a^*(x)\,\hat{A}\,\psi_b(x)\,dx \\ &= \sum_{n,m} a_n^* b_m\,A_{n,m} \\ &= \vec{a}^{\dagger}\cdot\mathbf{A}\cdot\vec{b}\end{aligned}$$

where $A_{n,m}$ are the elements of matrix $\mathbf{A}$. These matrix elements describe the action of $\hat{A}$ on the set of basis functions used to make $\psi_a(x)$ and $\psi_b(x)$ and are equal to

$$A_{n,m} = \langle\psi_n|\hat{A}|\psi_m\rangle \text{ where } \{n,m\}\in\mathbb{Z} \tag{2}$$

Having identified states like $|\psi_a\rangle$ with vectors, and operators with matrices, some of the statements of the previous section can be seen in a new light.

For instance, the idea that operator order is important is exactly the same as saying that matrix multiplication is non-commutative. We also see that eigenfunctions of a given operator correspond to eigenvectors of the matrix which represents that operator

$$\hat{A}|\psi_{A,n}\rangle = \alpha_n|\psi_{A,n}\rangle \quad\leftrightarrow\quad \mathbf{A}\cdot\vec{a} = \alpha\,\vec{a} \tag{3}$$

such that $\mathbf{A}$ is diagonal in the basis of its own eigenfunctions, in which case $A_{n,m} = \alpha_n\delta_{mn}$.

We can also look at the definition of the Hermitian operator in this context.

Hermitian Operators

$$
\begin{aligned}
\langle \hat{A}\, \psi_a | \psi_b \rangle &= (\mathbf{A} \cdot \vec{a})^{\dagger} \cdot \vec{b} \\
&= (\mathbf{A} \cdot \vec{a})^{T*} \cdot \vec{b} \\
&= \left(\vec{a}^{T} \cdot \mathbf{A}^{T}\right)^{*} \cdot \vec{b} \\
&= \vec{a}^{\dagger} \cdot \mathbf{A}^{\dagger} \cdot \vec{b} \\
&= \langle \psi_a | \hat{A}^{\dagger} | \psi_b \rangle \\
&= \langle \psi_a | \hat{A} | \psi_b \rangle \quad \because \quad \hat{A} = \hat{A}^{\dagger}
\end{aligned}
$$

While we will use concepts like "orthonormal basis functions" in this class, we will not make frequent use of the linear algebra approach to QM, rather we will stick to the language of "wave mechanics". Linear algebra is, however, used extensively in QM and serves as the foundation for "matrix mechanics". Of course, this is all just notational conventions; physics is the same either way!

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4 Next Time

No new pset posted... Exam on Thursday!

- Energy eigenstates.