(9) Qualitative Eigenstates

1   Last Time

- Energy Eigenstates: the states the don't move
- The infinite square well: our first 1D potential

2   This Time

- Qualitative properties of Energy eigenfunctions in any 1D potential
- The general rules of EESs in 1D potentials

3   Inner Products and Overlap Integrals

- Sh. 1.(1-8)

For the most part, in this class I try to keep the math as unintrusive as possible in hopes that this will let us focus on the physical systems we are trying to model. However, sometimes we have to focus on our mathematical tools to avoid getting lost in an array of symbols that we don't understand.

This was brought to the fore in the last lecture with the questions about the physical meaning of the "overlap integral" or "inner product" or "projection" written in Dirac notation as

$$
\begin{aligned}
\langle \psi_a | \psi_b \rangle &= \int_{-\infty}^{\infty} \psi_a^*(x)\, \psi_b(x)\, dx \\
&= \vec{a}^\dagger\, \vec{b}
\end{aligned}
$$

where the vector version is for expansions in a common orthonormal basis (see the part on Matrix Mechanics in the previous lecture).

The meaning of $\langle \psi_a | \psi_b \rangle$ in words, if ψ_a and ψ_a are normalized states, is something like "how similar is state A to state B?"

1

Before we go further, let me make a quick note about Dirac notation

$$|\hat{A}\psi\rangle = \hat{A}\,\psi(x) = \hat{A}|\psi\rangle \qquad \text{Ket means nothing}$$
$$\langle\hat{A}\psi| = (\hat{A}\,\psi(x))^{\dagger} = \langle\psi|\hat{A}^{\dagger} \qquad \text{Bra means adjoint}$$

When they come together, it means "do the overlap integral".

Identical states will have an overlap of 1. States which differ only by an overall phase will give a result with magnitude 1 (e.g., -1 if they are $180°$ out of phase). States which have nothing in common will have zero overlap. (An example is a pair of localized particle at different locations.)
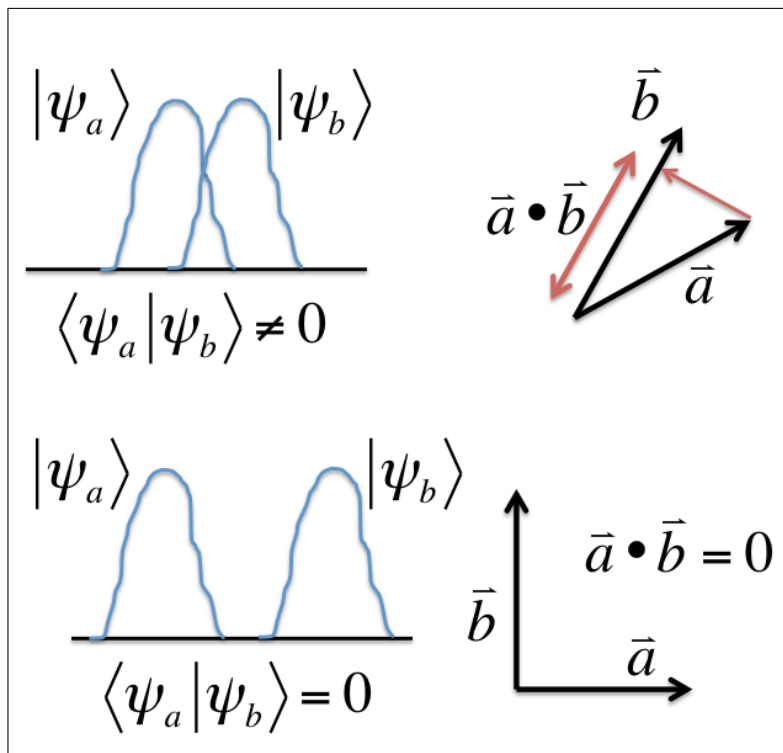
This is essentially identical to the dot-product of 2 vectors. If the vectors are normalized, their dot product will be between 1 and -1, with these two extremes are reached for vectors that are parallel and anti-parallel.

If we expand our state in terms of the eigenfunctions of some operator which corresponds to an observable, then the interpretation becomes "how much of each

eigenfunction do I have in this state". (Recall that you can always do this for Hermitian operators, since they all come with a complete basis of orthogonal eigenfunctions.)

For example, Energy Eigenstates:

$$\langle \phi_5 | \psi \rangle = \int_{-\infty}^{\infty} \phi_5^*(x) \sum_n c_n \phi_n(x) \, dx$$

$$= \sum_n c_n \int_{-\infty}^{\infty} \phi_5^*(x) \phi_n(x) \, dx$$

$$= \sum_n c_n \delta_{5,n} = c_5$$

How much ϕ_5 is in ψ? c_5!

An intuitive feeling for what operators do in this context is somewhat more challenging, but much can be learned by sticking with our expansion in an eigenfunction basis. On operator acting on a state multiplies each component by the associated eigenvalue

$$\hat{A} | \psi \rangle = \sum_n a_n c_n \psi_{A,n}(x)$$

Putting this together with the corresponding ket gives the expectation value

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_m c_m^* \sum_n a_n c_n \delta_{mn}$$

$$= \sum_n a_n c_n^* c_n = \sum_n a_n \mathbb{P}_n$$

In summary, physical interpretations of general expression with Dirac brackets are vague, but if you put them together in meaningful combinations the message

can be quite precise (what is the probability of measuring a_n, what is the expectation value of A for state ψ, what is the matrix element for converting from basis A to basis B, ...). The potentially vague physical interpretation should not be confused with an imprecise mathematical expression; the mapping from Dirac brackets to overlap integrals is unambiguous.

4 Comment on the Schrödinger Equation

When we encountered the Schrödinger equation, I told you that

$$\hat{E} = \left(\frac{-\hbar^2}{2m}\partial_x^2 + V(x) \right) \quad \leftarrow \quad \text{Energy Operator}$$

$$i\hbar\partial_t = \hat{E} \quad \leftarrow \quad \text{Schrödinger}$$

Combining these two expressions and operating on a wavefunction

$$\Rightarrow i\hbar\partial_t\,\psi(x,t) = \left(\frac{-\hbar^2}{2m}\partial_x^2 + V(x) \right)\psi(x,t)$$

As a technical note about nomenclature,

$\psi(x,t)$ is the **state** of the system at time t
We can expand them as $\psi(x,t) = \sum_n c_n(t)\,\phi_n(x)$

Note that the basis states ϕ_n are NOT time dependent

$\psi_2(x) = \hat{O}\,\psi_1(x)$: operators change the **state**
by mapping $\phi_n(x) \rightarrow \sum_m \mathbf{O}_{mn}\phi_m(x)$

This is analogous to, say, a rotation in 2 dimensions in which

Basis Rotation in 2D

$$\hat{i}_2 = \cos\theta\,\hat{i} + \sin\theta\,\hat{j}$$
$$\hat{j}_2 = \cos\theta\,\hat{j} - \sin\theta\,\hat{i}$$
$$\text{for}\quad \hat{R}_2 = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

but there is nothing really special about the basis states; operators act on any state in the same way. This too is analogous to vector rotation:

General Rotation in 2D

$$|v_2\rangle = \hat{R}_2|v_1\rangle$$
$$\vec{v}_2 = x_1\left(\cos\theta\,\hat{i} + \sin\theta\,\hat{j}\right) + y_1\left(\cos\theta\,\hat{j} - \sin\theta\,\hat{i}\right)$$
$$\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}\begin{bmatrix} x_1 \\ y_1 \end{bmatrix}$$

Operators have no sense of TIME
$\Rightarrow \partial_t$ is not really a regular operator

Since we can't say what it does without knowing another operator, $\hat{E}$.

So we need to be careful when considering commutators involving $\hat{E}$.

$$\begin{aligned} \left[\hat{p}, \hat{E}\right] &= \left[\hat{p}, \frac{\hat{p}^2}{2m} + V(x)\right] \\ &= \frac{1}{2m}\left[\hat{p}, \hat{p}^2\right] + [\hat{p}, V(x)] \\ &= \frac{1}{2m}\left(\hat{p}^3 - \hat{p}^3\right) + i\hbar F(x) \\ &= i\hbar F(x)\quad \text{where}\ \ F(x) = -\partial_x V(x) \end{aligned}$$

which is correct, and notably NOT the same as

$$
\begin{aligned}
\left[\hat{p}, \hat{E}\right] &\overset{?}{=} [\hat{p}, i\hbar\,\partial_t] \\
&= \hbar^2\,[\partial_x, \partial_t] \\
&= (\partial_x\,\partial_t - \partial_t\,\partial_x) = 0
\end{aligned}
$$

(since the order or partial derivatives doesn't matter). Fundamentally, we cannot use ∂_t in a commutator because we can't say what it does to a state without knowing $\hat{E}$, thus to compute the value of the commutator we must use the other side of the Schrödinger equation in which $\hat{E}$ is written in terms of operators with well defined actions.

5 Energy Eigenstates in 1D

- E&R 5.(5-8), Li. 7.1, Sc. 3.3

Last time we left off with energy eigenstates of a particular potential; the infinite square well. Our formulation for these eigenstates looked like

> ## Energy ES
>
> $$\hat{E}\ \phi_E(x)\ =\ E\ \phi_E(x)$$
>
> where $\psi_E(x,t) = \phi_E(x)e^{-i\omega t}$ and $E = \hbar\omega$

This formulation is helpful because it gave us a time-independent PDE to solve, rather than the full Schrödinger equation.

> ## Energy ES in SE
>
> $$E\ \phi_E(x)\ =\ \left(\frac{-\hbar^2}{2m}\partial_x^2 + V(x)\right)\ \phi_E(x)$$

Now, suppose that instead of the infinite square well, or some flat potential where plane-waves are good solutions, you want to find the energy eigenstates in an arbitrary potential.

> *Given any 1-D potential, what does the energy eigenstate look like?*

We can rearrange the Schrödinger equation a little to make an important feature more clear.
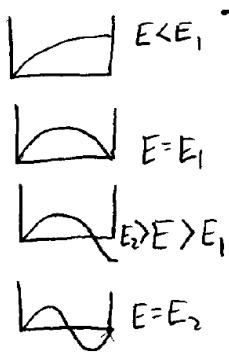
> ## 1D Energy ES
>
> $$\frac{-\hbar^2}{2m}\partial_x^2\ \phi_E(x)\ =\ (E - V(x))\ \phi_E(x)$$
> $$\partial_x^2\ \phi_E(x)\ =\ -k^2(x)\ \phi_E(x)$$
> $$\text{where}\quad k^2(x) = \frac{2m}{\hbar^2}\left(E - V(x)\right)$$

Such that if $V(x)$ changes slowly on a spatial scale of $1/k(x)$, and $E > V(x)$, the solutions are oscillatory (like $e^{\pm ikx}$). If, on the other hand, $E < V(x)$, the solutions are exponential (like $e^{\pm \alpha x}$ with $\alpha^2 = -k^2$).

Let's try this in the infinite square well potential.

Shooting Method in the Infinite Well

• Integrate ODE $\phi_E'' + \frac{2m}{\hbar^2} k^2(x) \phi_E = 0$ E controls _curvature_!

$E < E_1$

$E = E_1$

$E_2 > E > E_1$

$E = E_2$

① _Node Thm_ (1d QM) { - ground state has no nodes
                        - 1st state has one
                        - n^{th} " " n }
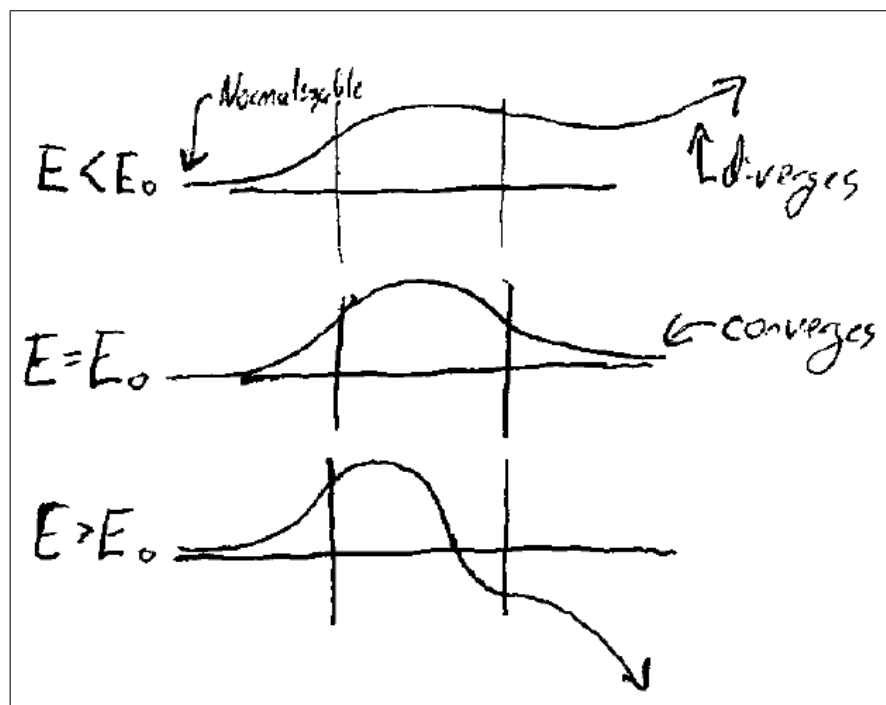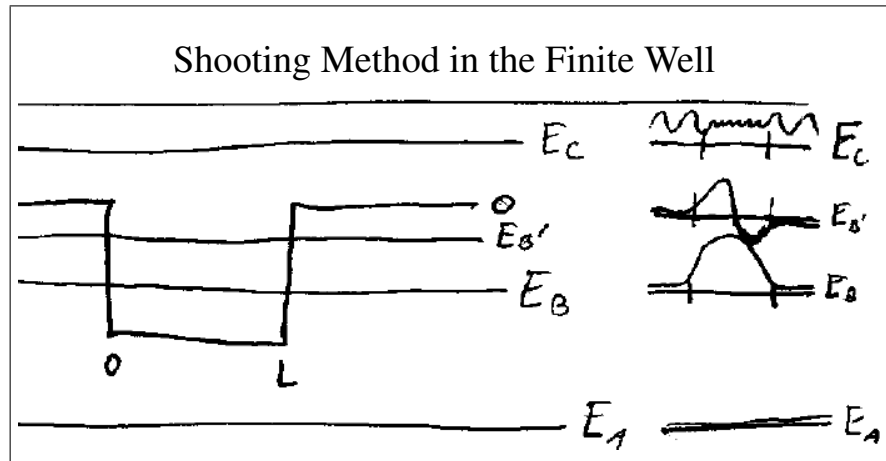
② Bound States $\Leftrightarrow$ _discrete energies_

③ Unbound $\Longrightarrow$ _continuous energies_
   ($\Rightarrow \phi \neq 0$ @ ∞)

Some interesting features of these solutions:

• These functions may always be real (e.g., $\langle p \rangle = 0$).

• The ground state has no nodes.

• The number of nodes increases with each bound state.

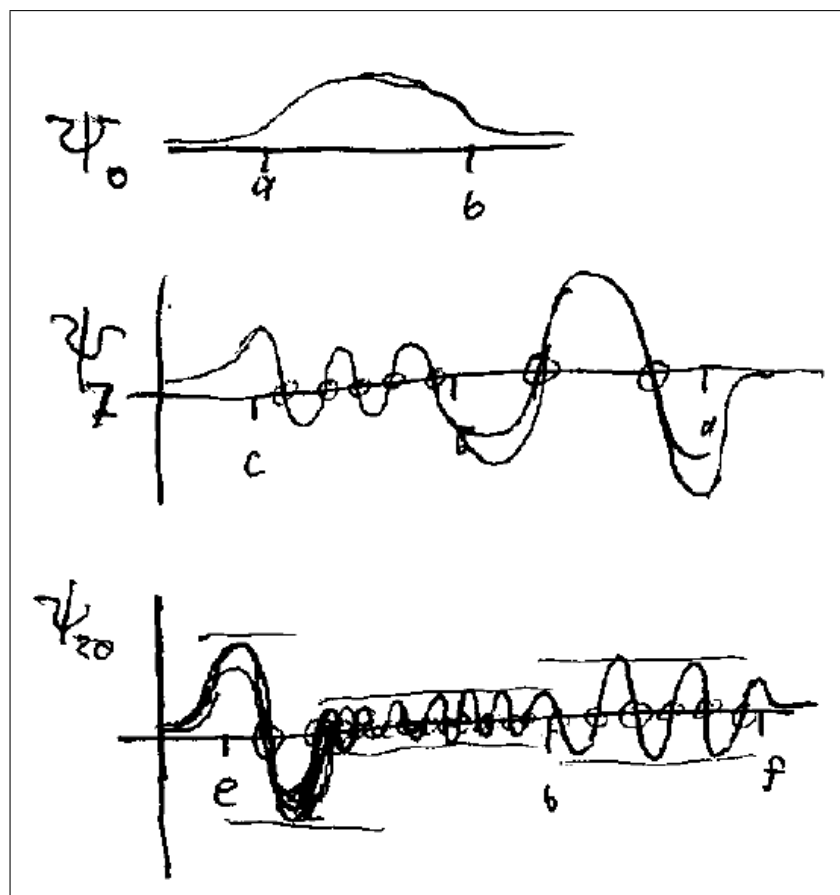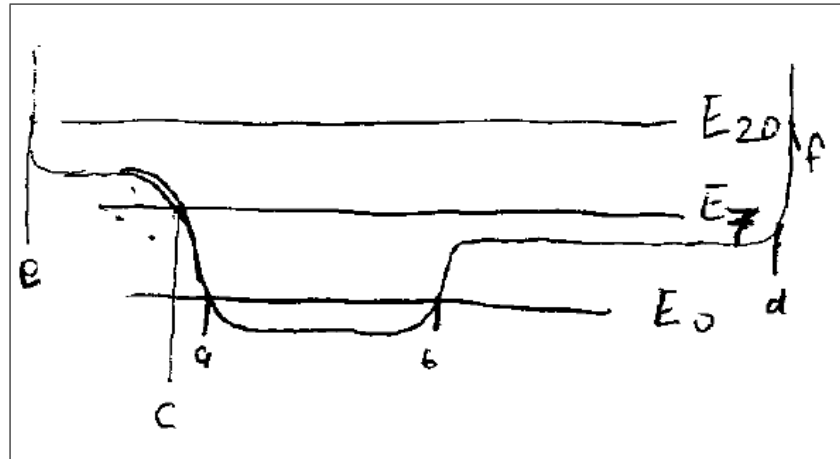We can use this technique to get a first look at the energy eigenstates of the finite square well...

Shooting Method in the Finite Well

Bound vs. Unbound

- Bound states give discrete energies ($E < V(x)$ left and right)
- Unbound states give continuous energies

9

And also for stranger potentials.

6 Next Time

- How to walk through walls and bounce off of cliffs!