Arvind Borde / PHY 19, Week 10: The Wavefunction (continued)

§10.1 Schrödinger's Equation

In 1d, the $\mathcal{S}$ eq. for $\Psi(x,t)$, the wave function for a particle with potential energy, $U(x)$, is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

The equation is dimensionally consistent: Every term has dimension [E][Ψ].

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Knowing $\Psi(x,0)$, the wavefunction at some initial instant of time, $t=0$, the $\mathcal{S}$ eq. allows us to figure out its evolution. That is, it allows us to find $\Psi(x,t)$ at any other time.

Note 1: Ψ is complex, in general.

Note 2: If Ψ_1 and Ψ_2 are solutions of the $\mathcal{S}$ eq., then so is $A_1\Psi_1 + A_2\Psi_2$ (A_i constant).

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$$-\frac{\hbar^2}{2m}\frac{\partial^2(A_1\Psi_1 + A_2\Psi_2)}{\partial x^2} + U(x)(A_1\Psi_1 + A_2\Psi_2)$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2 A_1\Psi_1}{\partial x^2} + U(x)A_1\Psi_1$$

$$+ -\frac{\hbar^2}{2m}\frac{\partial^2 A_2\Psi_2}{\partial x^2} + U(x)A_2\Psi_2$$

$$= A_1 i\hbar\frac{\partial\Psi_1}{\partial t} + A_2 i\hbar\frac{\partial\Psi_2}{\partial t}$$

$$= i\hbar\frac{\partial}{\partial t}(A_1\Psi_1 + A_2\Psi_2)$$

3 In other words, the $\mathcal{S}$ eq. is linear.

§10.2 Interpretation

$|\Psi(x)|^2 dx$ is interpreted as the probability that a particle will be found between x and $x+dx$.

Because of this we require that

$$\int_{-\infty}^{\infty}|\Psi|^2 dx \equiv \int_{-\infty}^{\infty}\Psi^*\Psi\, dx = 1.$$

This forces $\Psi \to 0$ as $|x| \to \infty$.

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The S equation, it turns out, is not the probability police: It allows solutions that are un-normalizable.

But it *does* police evolution: If you *start* normal (ized), it ensures you stay so. In other "words":

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi^*\Psi dx = \int_{-\infty}^{\infty}\left(\frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}\right)dx = 0$$

5 To see this, multiply the $\mathcal{S}$ eq. by $\Psi^*/(i\hbar)$:

$$\Psi^*\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}U(x)\,|\Psi|^2$$

Its complex conjugate is

$$\Psi\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\Psi\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}U(x)\,|\Psi|^2$$

Adding the two,

6 $$\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t} = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \Psi\frac{\partial^2\Psi^*}{\partial x^2}\right)$$

ADDITIONAL NOTES

The left-hand side is the quantity whose integral over x we wish to show is zero.

The right hand side may be rewritten as

$$\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)$$

Integrating this over x from $-\infty$ to ∞, we get

$$\frac{i\hbar}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]_{-\infty}^{\infty} = 0$$

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§10.3 Separable Wavefunctions

For $\Psi(x,t) = \psi(x)\phi(t)$, the $\mathcal{S}$ eq. becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\phi(t) + U(x)\psi(x)\phi(t) = \phi(x)i\hbar\frac{d\phi}{dt}$$

Dividing by $\psi(x)\phi(t)$, we get

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x) = \frac{1}{\phi(t)}i\hbar\frac{d\phi}{dt}$$

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The two will be equal $\forall x$ and $\forall t$ iff each side is a constant, E, with the dimensions of energy. So we get a time-dependent equation,

$$i\hbar\frac{d\phi}{dt} = E\phi(t)$$

and a time-independent one

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi(x)$$

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(1) Solve the time-dependent equation.

$$\int\frac{d\phi}{\phi(t)} = \frac{E}{i\hbar}\int dt$$

$$ln\,\phi(t) = \frac{E}{i\hbar}t + C = -i\omega t + C$$

where we've used $E = \hbar\omega (= hf)$.

This becomes

$$\phi(t) = (e^C)e^{-i\omega t}$$

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We'll drop the e^C term because it will be absorbed by the eventual normalization of $\Psi(x,t)$.

So, $\phi(t) = e^{-i\omega t}$ gives the time dependence of *all* separable wavefunctions.

Unless otherwise stated, we'll assume that all the wavefunctions we consider are separable.

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§10.4 A Free Particle (No Forces)

In the absence of forces, $U(x) = 0$.

§10.4.1 Classical behavior

The particle will obey Newton's first law of motion: it will stay at rest or continue in uniform motion.

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ADDITIONAL NOTES

§10.4.2 Quantum mechanical behavior

We ask what the $\mathcal{S}$ eq. says.

Keep the following in mind, remembering these: $\omega \equiv 2\pi f$, $k \equiv 2\pi/\lambda$, and $\hbar \equiv h/2\pi$:

$$E = hf \qquad p = \frac{h}{\lambda}$$
$$= \hbar\omega \qquad = \hbar k$$

Further $E = p^2/2m$ for a particle of mass m.

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The time-independent $\mathcal{S}$ eq. becomes:

$$\frac{d^2\psi}{dx^2} = -k^2\psi(x), \qquad k^2 = \frac{2mE}{\hbar^2}$$

The general solution is a linear combination of two independent solutions, found by inspection,

$$\psi(x) = A\,sin\,kx + B\,cos\,kx$$

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Another way: Observe that $(\psi'^2 + k^2\psi^2)'$

$$= 2\psi'\psi'' + 2k^2\psi'\psi = 2\psi'(\psi'' + k^2\psi) = 0$$

So $\psi'^2 + k^2\psi^2 = C_1^2$, or $\psi'^2 = k^2\big((C_1/k)^2 - \psi^2\big)$.

$$\int \frac{\psi'}{\sqrt{(C_1/k)^2 - \psi^2}}dx = \int k\,dx$$

$$\psi = (C_1/k)\,sin(kx + C_2)$$
$$= \left[\frac{C_1}{k}\,cos\,C_2\right] sin\,kx + \left[\frac{C_1}{k}\,sin\,C_2\right] cos\,kx$$

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But, we have a problem: the function

$$\psi(x) = A\,sin\,kx + B\,cos\,kx$$

is not normalizable.

We get around this by constructing a wave packet by superposing solutions of this type.

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§10.5 A Particle in a Box

This is a particle confined to move in a fixed space, say $0 \leqslant x \leqslant L$. We model this by

$$U(x) = \begin{cases} 0 & 0 \leqslant x \leqslant L \\ \infty & \text{elsewhere.} \end{cases}$$

§10.5.1 Classical behavior

The particle with either sit at rest in the box, or will bounce at uniform speed between the walls.

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§10.5.2 Quantum mechanical behavior

Inside the box, we have a free particle, so the time-independent equation has the general solution

$$\psi(x) = A\,sin\,kx + B\,cos\,kx$$

Outside the box, the time–independent equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi(x)$$

suggests that $\psi \to 0$, as $U(x) \to \infty$.

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ADDITIONAL NOTES

So, we require that the interior wavefunction obey $\psi = 0$ at the boundaries $x = 0$ and $x = L$:

$$\psi(0) = 0 \Rightarrow A\,sin\,0 + B\,cos\,0 = 0 \Rightarrow B = 0.$$

$$\psi(L) = 0 \Rightarrow A\,sin\,kL = 0 \Rightarrow kL = n\pi,$$

where $n = 0, 1, 2, \ldots$

For each allowed value of n, we get a solution of the $\mathcal{S}$ eq., $\psi_n(x) = A_n\,sin(n\pi x/L)$.

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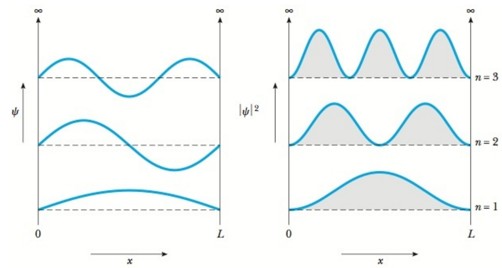
The wavefunctions, ψ_0, ψ_1, and ψ_2, with the associated probability densities $|\psi_n|^2$:



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§10.5.3 Energy levels

Since $kL = n\pi$, we get,

$$E = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

In other words, we have quantized energy levels.

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§10.6 A Particle in a Finite Square Well

This is a particle in a "potential well" of depth U:

$$U(x) = \begin{cases} 0 & 0 \leqslant x \leqslant L \\ U & \text{elsewhere.} \end{cases}$$

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§10.6.1 Classical behavior

This will depend on the total energy E.

If $E \leqslant U$, the particle will be confined to the well, and will bounce between the walls.

If $E > U$, the particle will escape the well.

To explore the CM-QM differences, we'll look at $E \leqslant U$.

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§10.6.2 Quantum mechanical behavior

In the well, we again have a free particle, so the time-independent equation has the same general solution

$$\psi(x) = A\,sin\,kx + B\,cos\,kx$$

We cannot assume here, though, that $\psi(0) = \psi(L) = 0$. We need to first get the wavefunction outside the well.

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ADDITIONAL NOTES

This exterior wave function is obtained from

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi(x)$$

which reduces to

$$\frac{d^2\psi}{dx^2} = \frac{2m(U-E)}{\hbar^2}\psi(x) \equiv \alpha^2\psi(x)$$

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There are two independent solutions, $e^{\alpha x}$ and $e^{-\alpha x}$ of this equation.

The general solution is

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$$

Since we need $\psi(x) \to 0$ as $x \to \pm\infty$, we get

$$\psi(x) = \begin{cases} Ce^{+\alpha x} & x < 0 \\ De^{-\alpha x} & x > L \end{cases}$$

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The previous interior solution, must match these "smoothly" at the boundaries: we must have

$$A\,sin\,0 + B\,cos\,0 = B = Ce^0 = C$$

$$A\,sin\,kL + B\,cos\,kL = De^{-\alpha L}$$

No matter the details of this, there's a nonzero probably that the particle will escape even with $E < U$.

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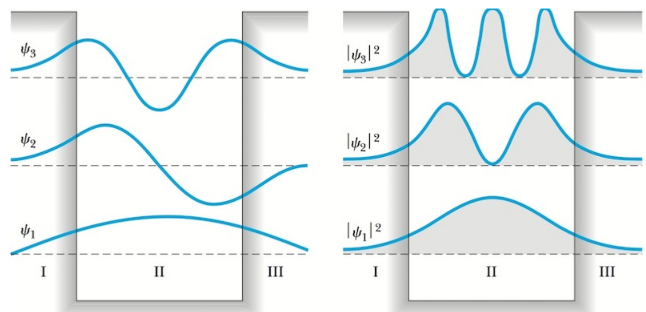
The wavefunctions, ψ_1, ψ_2, and ψ_3, with the associated probability densities $|\psi_n|^2$:



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§10.7 The Simple Harmonic Oscillator

The potential energy is

$$U = \frac{1}{2}Kx^2$$

where $K = m\omega^2$ and m is the mass of the particle.

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§10.7.1 Classical behavior

The total energy is

$$E = \frac{1}{2}Kx^2 + \frac{1}{2}mv^2.$$

At the extreme position $(x = A)$, $v = 0$; we get

$$E = \frac{1}{2}KA^2$$

The particle oscillates between A and $-A$.

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ADDITIONAL NOTES

§10.7.2 Quantum mechanical behavior

The time-ind. $\mathcal{S}$ eq. becomes

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}m\omega^2x^2 - E\right)\psi(x)$$

Not so easy to solve, but try

$$\psi(x) = C_0 e^{-m\omega x^2/2\hbar}$$

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(2) What's $\psi'(x)$?

$$\psi'(x) = \quad \psi(x)\left(\frac{-m\omega x}{\hbar}\right)$$

(3) What's $\psi''(x)$?

$$\psi''(x) = \quad \psi(x)\left(\frac{m\omega x}{\hbar}\right)^2 - \psi(x)\left(\frac{m\omega}{\hbar}\right)$$

Matches right side of the $\mathcal{S}$ eq., if $E = \frac{1}{2}\hbar\omega$.

We have the ground state wave function.

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§10.7.3 Energy levels

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

The quantum oscillator can penetrate the classically forbidden region.

The smallness of the energy level gaps is why we do not see them in day-to-day experience.

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§10.8 Tunneling (Square Barrier Penetration)

This is (in some senses) the opposite of a particle in a well of finite depth: a free particle encounters a square potential of height U.

§10.8.1 Classical behavior

If $E < U$ the particle bounces off the barrier.

If $E > U$ the particle "steps over" the barrier, with a reduction in speed.

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§10.8.2 Quantum mechanical behavior

Say barrier is located between $x = 0$ and $x = L$. Assuming $U = 0$ outside the barrier, we get standard free particle solutions for $x < 0$ and $x > L$.

Choose an *initial* state $\Psi(x, 0) = 0$ for $x > L$.

We get from the $\mathcal{S}$ eq. on the left

$$\Psi(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$$

35 One wave moving right, another moving left.

On the right

$$\Psi(x,t) = Fe^{i(kx-\omega t)}$$

Within the barrier

$$\Psi(x,t) = Ce^{-\alpha x - i\omega t} + De^{+\alpha x - i\omega t}$$

where

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar}$$

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ADDITIONAL NOTES