Arvind Borde / PHY 19, Week 10: The Wavefunction

§10.1 The wave function

Postulate:

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We'll first consider a particle in 1d.

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Interpretation: ____________________________

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We assume that Ψ is single-valued and continuous.

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§10.1.1 Normalization:

Because of the link with probabilities, we require that

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = \_\_\_$$

This allows us to fix C in a wave function represented by $Cf(x)$.

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(1) Find C in the wavefunction $\Psi(x) = Ce^{-|x|/x_0}$, where x_0 is fixed.

$$\int_{-\infty}^{\infty} |\Psi|^2 dx =$$

So,

$$C =$$

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(2) What's the probability that a particle given by the previous wavefunction will be found in $(-x_0, x)$?

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§10.1.2 Evolution

In general we'll have $\Psi(x,t)$ and our job will be to determine the evolution of Ψ from a given initial state.

Ψ evolves according to an equation proposed by Erwin Schrdingier.

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ADDITIONAL NOTES

§10.2 A Free Particle

This is a particle with no forces acting in it. To connect with De Broglie's ideas, we take

$$\Psi(x,t) =$$

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(3) Find $\Psi(x,0)$, if $a(k) = (C\alpha/\sqrt{\pi})e^{-\alpha^2 k^2}$ where C and α are constants.

$$=$$

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§10.3 Forces

In the presence of a force, $F = -dU/dx$, where $U(x)$ is the potential energy, Schrödinger proposed this equation for $\Psi(x,t)$:

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Solving this, in general, is hard. We will confine ourselves to separable wavefunctions of the form $\Psi(x,t) = \psi(x)\phi(t)$. In this case we get

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ADDITIONAL NOTES

§10.3.1 A particle in a box

This a particle confined to move in a fixed space, say $0 \leqslant x \leqslant L$.

The time independent equation becomes:

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§10.3.2 A finite square well

This is particle in "potential well" of depth U. Here the exterior wave function is obtained from

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§10.3.3 The harmonic oscillator

The potential energy for a harmonic oscillator is

where m is the mass of the particle and $\omega = \sqrt{K/m}$.

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ADDITIONAL NOTES

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§10.4 Expectation Values

Many quantities we might wish to measure, such as position, have probabilistic values in quantum mechanics. We define the expectation value of a quantity, $f(x)$ as

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We can use this to find the uncertainty in position for a harmonic oscillator:

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§10.5 Observables and Operators

An observable is any particle property that can be measured.

The position and momentum of a particle are observables, as are KE and PE.

In quantum mechanics, we associate an "operator" that acts on functions with each observable.

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For example, a constant c is an operator, that simply operates on $f(x)$ by $cf(x)$.

Another operator is d/dx.

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ADDITIONAL NOTES

The expectation value $\langle Q \rangle$ of an operator $[Q]$ is

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For example, $\langle KE \rangle$ is

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Here are some common operators:

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§10.6 More on 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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$$\begin{aligned}
&-\frac{\hbar^2}{2m}\frac{\partial^2 (A_1\Psi_1 + A_2\Psi_2)}{\partial x^2} + U(x)(A_1\Psi_1 + A_2\Psi_2) \\
&= -\frac{\hbar^2}{2m}\frac{\partial^2 A_1\Psi_1}{\partial x^2} + U(x)A_1\Psi_1 \\
&\qquad + -\frac{\hbar^2}{2m}\frac{\partial^2 A_2\Psi_2}{\partial x^2} + U(x)A_2\Psi_2 \\
&= A_1 i\hbar\frac{\partial \Psi_1}{\partial t} + A_2 i\hbar\frac{\partial \Psi_2}{\partial t} \\
&= i\hbar\frac{\partial}{\partial t}(A_1\Psi_1 + A_2\Psi_2)
\end{aligned}$$

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

ADDITIONAL NOTES

§10.7 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 $\mathcal{S}$ eq., 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":

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

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

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

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,

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

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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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§10.8 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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ADDITIONAL NOTES

(4) Solve the time-dependent equation.

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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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§10.9 A Free Particle (No Forces)

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

§10.9.1 Classical behavior

The particle will obey Newton's first law of motion:

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§10.9.2 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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ADDITIONAL NOTES

But, we have a problem: the function

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

is not ____________________.

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

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§10.10 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

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

§10.10.1 <u>Classical behavior</u>

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

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§10.10.2 <u>Quantum mechanical behavior</u>

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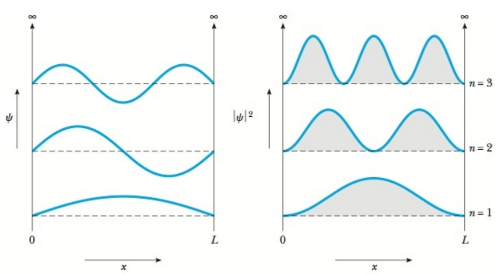
The wavefunctions, ψ_0, ψ_1, and ψ_2, with the associated probability densities $|\psi_n|^2$:



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§10.10.3 <u>Energy levels</u>

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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ADDITIONAL NOTES

§10.11 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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§10.11.1 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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§10.11.2 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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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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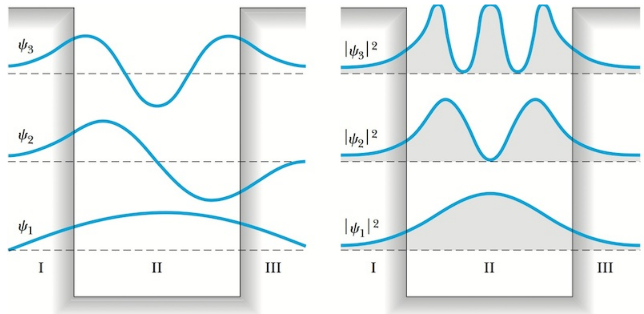
ADDITIONAL NOTES

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



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§10.12 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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§10.12.1 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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§10.12.2 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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(5) What's $\psi'(x)$?

$$\psi'(x) =$$

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

$$\psi''(x) =$$

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§10.12.3 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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ADDITIONAL NOTES

§10.13 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.

§10.13.1 Classical behavior

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

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§10.13.2 Quantum mechanical behavior

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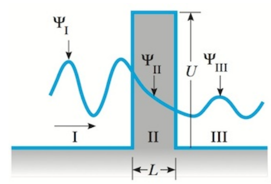
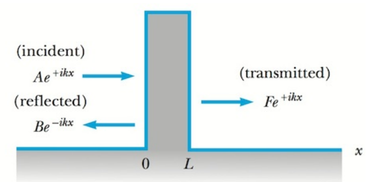
The coefficients are determined from continuity.





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ADDITIONAL NOTES

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