### PHYs-2402

**Lecture 12**

Feb. 26, 2015

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**Announcement**

**Course webpage**


**Textbook**

*Modern Physics, 2/E*

Randy Harris, University of California, Davis

2008 • Addison-Wesley • Cloth, 636 pp
Published 07/26/2007 • Instock

**HW3 (due 3/2)**

13, 15, 20, 31, 36, 41, 48, 53, 63, 66

***** Exam: 3/12

Ch.2, 3, 4, 5

Physics Colloquium: today

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**Chapter 5**

**Bound States: Simple Case**

**Purpose:**

- To make QM useful in real application,
- we must have a way to account for the effects of external forces

Let’s start with the Schrödinger eq. to include these effects.

** interaction of object with its surrounding
Chapter. 5
Bound States: Simple Case

Outline:

• The Schrödinger Equation (for Interacting Particles)
• Stationary States
• Physics Conditions: Well-Behaved Functions
• A Review of Classical Bound States (First)
• Case 1: Particles in a Box – The Infinite Well
• Case 2: The Finite Well
• Case 3: The Simple Harmonic Oscillator
• Expectation Values, Uncertainties, and Operators

The Schrödinger Equation
for Interacting Particles

A Particle Interacting
With What?

F = mg

Simplification:
The Concept of Potential
(replaces all individual
particle-particle interactions
with a single smooth potential)

Why? – see next page

Bound Systems

A bound system is any system of interacting particles where the
nature of the interactions between the particles keeps their
relative separation limited. Classical example: the solar system.

In general, the problem is very difficult. Simplification: motion of a single particle that moves
in a fixed potential energy field \( U(x) \) created by the other particles in the system. A good
approximation when the mass of the particle is small compared to the total mass of the
system (think heavy nucleus ↔ light electron).

Classically allowed region:
\[ E(x) > U(x) \]

Classically forbidden region:
\[ E(x) < U(x) \]
The Infinite Square Well

- a particle in the potential is completely free, except at the two ends where an infinite force prevents it from escaping

Outside the well: \( \psi(x) = 0 \) - the probability of finding the particle = 0

Inside the well:

\[
-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)
\]

- the harmonic oscillator equation

General solution: \( \psi(x) = A\sin kx + B\cos kx \) - constants A and B are fixed by boundary conditions

Continuity of the wave function: \( \psi(0) = \psi(L) = 0 \)

Thus, \( \psi(x) = A\sin kx \)

Thus, \( \psi(x) = A\sin kL = 0 \)

\( kL = 0, \pm \pi, \pm 2\pi, \ldots \)

\( k_n = \frac{n\pi}{L}, \ n = 1, 2, \ldots \)

\( n = \text{quantum number} \) (1D motion is characterized by a single q.n., for 2D motion we need two quantum numbers, etc.)

See next time for details

The Schrodinger Equation

for Interacting Particles

\[
\frac{-\hbar^2}{2m} \frac{d^2\Psi(x, t)}{dx^2} + U(x)\Psi(x, t) = \frac{i\hbar}{\Delta t} \frac{\partial \Psi(x, t)}{\partial t}
\]

Try to add potential energy \( U(x) \)

Adding P.E.

\( (KE + U(x))\Psi(x, t) = E\Psi(x, t) \)

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

\( \rightarrow \text{Time-dependent Schrödinger Eq.} \)

\( \rightarrow \text{To determine the behavior of particle} \)

in (1) CM: solve \( F = \frac{m(d^2r/dt^2)}{\Delta t} \) for \( r \), given knowledge of Net external \( F \) on particle

in (2) QM: solve the Schrödinger eq. for \( \psi(x, t) \), given knowledge of P.E., \( U(x) \)

The Schrödinger Equation

for Interacting Particles

and for Stationary Potentials

\( U = U(x) \)

\( U \neq U(t) \)
**Key Assumption:**

*Factorization of the wave function*

\[ \Psi(x, t) = \psi(x)\phi(t) \]

Wave function may be express as a product of …

**Spatial Part**

**Temporal Part**

Q: Why?, A: allows us to break a differential eq. with 2 independent variables \((x,t)\) into simpler eqs. For position & time, separately!!

What happens with the Schrodinger equation?

\[ -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x) \]

... and factoring out terms constant w.r.t. the partial derivatives …

\[ -\frac{\hbar^2}{2m} \frac{1}{\phi(t)} \frac{\partial^2 \phi(t)}{\partial x^2} + U(x)\psi(x)\phi(t) = i\hbar \frac{\psi(x)}{\phi(t)} \frac{\partial \phi(t)}{\partial t} \]

Divide both sides by \(\psi(x)\phi(t)\)

Variables are separate now!!

\[ \phi(t) = e^{-i(E\hbar)t} \]

**Temporal part**

\[ \Psi(x, t) = \psi(x)\phi(t) \]

\[ \Psi(x, t) = \psi(x)e^{-i(E\hbar)t} \]

**Total wave function**
The probability density is time-independent; i.e., the whereabouts of the particle don't change with time in any observable way.

Quantum Mechanically, electron is not an accelerating charged particles, but rather a stationary "cloud".

The spatial part of $\psi(x,t)$

Replace $C$ by $E$, multiply both sides by $\psi(x)$;

The time-independent Schrodinger equation:

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

NOTE: $\psi(x)$ is Real, but $\psi(x,t)$ is Complex, because $\phi(t) = e^{-i\alpha t}$.

Well-behaved wave functions

Total Probability of finding the particle = 1

The procedure by which we ensure that the wave function gives a unit probability is called Normalization of $\psi(x,t)$

Smoothness of $\psi(x,t)$

Another requirement is that a wave function be...
Normalization of $\psi(x,t)$

$$\int_{\text{all space}} |\Psi(x, t)|^2 \, dx = 1$$

The particle must be somewhere in the universe at any time (the total probability should be $= 1$)

Smoothness of $\psi(x,t)$

1. Continuity of $\psi(x,t)$
2. Continuity of $(d\psi(x)/dx)$

Discontinuity in $\psi(x)$

Short wave length become zero wave length.
i.e. infinite momentum & K.E. (physically unacceptable...)

Smoothness of $\psi(x,t)$

$$\tilde{\psi}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} \, dx$$

Discontinuity in $\psi(x)$

Extremely large $k$ (or short $\lambda$) $\rightarrow$ $\rightarrow$ **Infinite Momentum** impossible
Gaussian Wave Packet

\[ \psi(x) = Ae^{-(x/2\epsilon)^2} e^{ik_0x} \]
\[ \mathcal{F}(k) = ? \]
\[ \mathcal{F}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \]

Find the “Spectral Content”:

The Schrödinger Equation for Interacting Particles

A Particle Interacting With What?

Simplification:
The Concept of Potential
(replaces all individual particle-particle interactions with a single smooth potential)

\[ \text{Energy vs. Position for a mass connected to a spring} \]

Summary

\[ \phi(i) = e^{-i(E/\hbar)t} \]
\[ \frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \]
\[ \Psi(x, t) = \psi(x)e^{-i(E/\hbar)t} \]

Normalization of \( \psi(x,t) \)

Smoothness of \( \psi(x,t) \)

Temporal part
Spatial part
Total wave function

Smooth & Stationary Function
Smooth & Stationary Function
Independent of the motion of “our” Particle

Energy vs. Position for a mass connected to a spring

Classically forbidden region

\[ U(x) = \frac{1}{2} k x^2 \]

Turning points

Classically forbidden region

3rd Newton’s Law?

In Quantum Mechanics – Bound States are Standing Waves

Bound states is one in which a particle's motion is restricted by an external force to finite region of space

Not forbidden

In Quantum Mechanics – Bound States are Standing Waves
In Quantum Mechanics –
Bound States are Standing Waves

The “Ground state”
the lowest energy state
is not at \( E=0 \)

Not forbidden

Consistent with the Uncertainty Relations:
\[
\Delta x \Delta p_x \geq \frac{\hbar}{2}
\]

Today’s Lecture – Chapter. 5
Bound States: Simple Case

Outline:

• Case 1: Particles in a Box – The Infinite Well
• Case 2: The Finite Well
• Case 3: The Simple Harmonic Oscillator
• Expectation Values, Uncertainties, and Operators

5.5 Case. I
Particle in a Box: The Infinite Well

The situation in which the particle-confining \( U(x) \)
allows the simplest solution of the time-independent
Schrödinger equation is called “particle in a box”, or
“infinite well”

CM: simply bounce back & forth

QM: standing waves \( \leftrightarrow \) Schrödinger Eq.
Case I: Particle in a box –
Infinite Potential well

E-field in each capacitor exerts a force, \( F = (-e)E \), inward on the electron. With total \( E < eV_0 \), the electron is bound: Its KE drops to “0” before it can reach a capacitor’s outer plate, and it returns in the opposite direction. So its PE is higher outside: \( U = qV = (-e)(-V_0) \)

\[ U(x) = \begin{cases} 
0 & 0 < x < L \\
U_0 & x < 0, x > L 
\end{cases} \]

1. Continuity of \( \psi(x,t) \)
2. Continuity of \( (d\psi(x)/dx) \)

Region I (0 < x < L)

Since \( U(x) = 0 \) here, the time-independent Schrödinger equation (4-8) is:

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad \text{or} \quad \frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2} \psi(x) \]

For convenience, let us make the following definition (which we very soon see is a wave number, thus the symbol):

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \]  \( \text{(4-11)} \)

Thus,

\[ \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \]
\[ \psi(x) = A \sin kx \quad \text{and} \quad \psi(x) = B \cos kx \]

\[ \psi(x) = A \sin kx + B \cos kx \]

**General solution for region I**

See Appendix K for more detail.

A crucial difference in this region is that the constant \( \alpha^2 \) is positive, where it was negative before (i.e., \(-k^2\)). A pair of independent solutions is

\[ \psi(x) = Ce^{+\alpha x} \quad \text{and} \quad \psi(x) = De^{-\alpha x} \]

and the general solution is the sum:

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

e\( ^{\alpha x} \) diverges as \( x \rightarrow \) negative infinite, i.e. mathematically OK, but physically unacceptable.

so, \( D \) must be zero!!

**Region II** \((x < 0)\)

Here, \( U(x) = U_0 \), so the time-independent Schrödinger equation is

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U_0\psi(x) = E\psi(x) \quad \text{or} \quad \frac{d^2\psi(x)}{dx^2} = \frac{2m(U_0 - E)}{\hbar^2} \psi(x) \]

Again we make a simplifying definition:

\[ \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \quad \text{(4-12)} \]

Thus,

\[ \frac{d^2\psi(x)}{dx^2} = \alpha^2\psi(x) \]

**Region III** \((x > L)\)

Since \( U(x) \) is the same, the mathematical solution of the Schrödinger equation in this region is the same as in region II. Thus,

\[ \psi(x) = Fe^{+\alpha x} + Ge^{-\alpha x} \]

\[ x \rightarrow \pm \infty \]

\[ \psi \rightarrow \infty \]

\[ F = D = 0 \]
However, the physically unacceptable term in this case is $e^{\pm \alpha x}$, which diverges as $x \to +\infty$ for any value of $U_0$; $F$ must be zero.

Altogether, we have

$$\psi(x) = \begin{cases} 
Ce^{\alpha x} & x < 0 \\
A \sin kx + B \cos kx & 0 < x < L \\
Ge^{-\alpha x} & x > L 
\end{cases} \tag{4-13}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $\alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$.