7 Finite well and harmonic oscillator

Slides: Lecture 7a Particles in potential wells – introduction

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.9
Particles in potential wells

Quantum mechanics for scientists and engineers

David Miller
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Slides: Lecture 7b The finite potential well

Text reference: Quantum Mechanics for Scientists and Engineers
Section 2.9
Particles in potential wells

The finite potential well

Quantum mechanics for scientists and engineers

David Miller
Finite potential well

Lesson 7
Particles in potential wells

Insert video here (split screen)

Insert number 2
Particle in a finite potential well

We will choose the height of the potential barriers as $V_0$ with 0 potential energy at the bottom of the well.

The thickness of the well is $L_z$

Now we will choose the position origin in the center of the well.
Particle in a finite potential well

If there is an eigenenergy $E$ for which there is a solution then we already know what form the solution has to take sinusoidal in the middle exponentially decaying on either side.
Particle in a finite potential well

For some eigenenergy $E$

with $k = \sqrt{2mE / \hbar^2}$

and $\kappa = \sqrt{2m(V_o - E) / \hbar^2}$

for $z < -L_z / 2$

$$\psi(z) = G \exp(\kappa z)$$

for $-L_z / 2 < z < L_z / 2$

$$\psi(z) = A \sin(kz) + B \cos(kz)$$

for $z > L_z / 2$

$$\psi(z) = F \exp(-\kappa z)$$

with constants $A$, $B$, $F$, and $G$
Particle in a finite potential well

Now we need to apply the boundary conditions to solve for the unknown coefficients constants $A$, $B$, $F$, and $G$

\[ \psi(z) = G \exp(\kappa z) \quad z < -L_z / 2 \]

\[ \psi(z) = A \sin k z + B \cos k z \quad -L_z / 2 < z < L_z / 2 \]

\[ \psi(z) = F \exp(-\kappa z) \quad z > L_z / 2 \]

or at least three of them

the fourth could be found by normalization
Particle in a finite potential well

From continuity of the wavefunction at $z = L_z / 2$

$$\psi \left( \frac{L_z}{2} \right) = F \exp \left( -\kappa L_z / 2 \right)$$

$$= A \sin \left( kL_z / 2 \right) + B \cos \left( kL_z / 2 \right)$$

Writing $X_L = \exp \left( -\kappa L_z / 2 \right)$

$$S_L = \sin \left( kL_z / 2 \right)$$

$$C_L = \cos \left( kL_z / 2 \right)$$

gives

$$FX_L = AS_L + BC_L$$
Particle in a finite potential well

Similarly at \( z = -L_z / 2 \)

\[ GX_L = -AS_L + BC_L \]

Continuity of the derivative gives

at \( z = -L_z / 2 \)

\[ \frac{k}{\kappa} GX_L = AC_L + BS_L \]

at \( z = L_z / 2 \)

\[ \frac{-k}{\kappa} FX_L = AC_L - BS_L \]
Particle in a finite potential well

So we have four relations

\[ GX_L = -AS_L + BC_L \]
\[ FX_L = AS_L + BC_L \]
\[ \frac{\kappa}{k} GX_L = AC_L + BS_L \]
\[ -\frac{\kappa}{k} FX_L = AC_L - BS_L \]

Now we need to find what solutions are compatible with these
Particle in a finite potential well

Adding $GX_L = -AS_L + BC_L$

$FX_L = AS_L + BC_L$

gives

$2BC_L = (F + G)X_L$

Subtracting

$-\frac{\kappa}{k}FX_L = AC_L - BS_L$

from

$\frac{\kappa}{k}GX_L = AC_L + BS_L$

gives

$2BS_L = \frac{\kappa}{k}(F + G)X_L$
As long as \( F \neq -G \), we can divide

\[
2BS_L = \frac{\kappa}{k} (F + G) X_L
\]

by

\[
2BC_L = (F + G) X_L
\]

to obtain

\[
\tan\left(\frac{kL_z}{2}\right) = \frac{\kappa}{k}
\]

This relation is effectively a condition for eigenvalues.
Particle in a finite potential well

Subtracting \( GX_L = -AS_L + BC_L \) from \( FX_L = AS_L + BC_L \) gives
\[
2AS_L = (F - G)X_L
\]

Adding \( -\frac{\kappa}{k}FX_L = AC_L - BS_L \) and
\[
\frac{\kappa}{k}GX_L = AC_L + BS_L
\]
gives
\[
2AC_L = -\frac{\kappa}{k}(F - G)X_L
\]
Particle in a finite potential well

Similarly, as long as \( F \neq G \), we can divide by to obtain

\[
2 AC_L = -\frac{\kappa}{k} (F - G) X_L
\]

by

\[
2 AS_L = (F - G) X_L
\]

to obtain

\[-\cot\left(\frac{kL_z}{2}\right) = \frac{\kappa}{k}\]

This relation is also effectively a condition for eigenvalues.
Particle in a finite potential well

For any case other than \( F = G \)

which leaves \( \tan \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

but not \( -\cot \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

or \( F = -G \)

which leaves \( -\cot \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

but not \( \tan \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

then the solutions \( \tan \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

and \( -\cot \left( \frac{kL_z}{2} \right) = \frac{\kappa}{k} \)

are contradictory
So the only possibilities are

1 - \( F = G \)
   and \( \tan \left( \frac{kL_z}{2} \right) = \kappa / k \)

2 - \( F = -G \)
   and \( -\cot \left( \frac{kL_z}{2} \right) = \kappa / k \)
1. $F = G$

and \( \tan\left(\frac{kL_z}{2}\right) = \kappa / k \)

Note from \( 2AS_L = (F - G)X_L \)

and \( 2AC_L = -\frac{\kappa}{k}(F - G)X_L \)

$S_L$ and $C_L$ cannot both be 0

so $A = 0$

Hence in the well we have

$\psi(z) \propto \cos kz$

which is an even function
1 - \( F = -G \)

and \(-\cot\left(\frac{kL_z}{2}\right) = \kappa / k\)

Note from \(2BC_L = \left(F + G\right)X_L\)

and \(2BS_L = \frac{\kappa}{k}\left(F + G\right)X_L\)

\(S_L\) and \(C_L\) cannot both be 0

so \(B = 0\)

Hence in the well we have

\(\psi(z) \propto \sin kz\)

which is an odd function
Particle in a finite potential well

Though we have found the nature of the solutions we have not yet formally solved for the eigenenergies $E$ and hence for $k$ and $\kappa$.

We do this by solving

$$\tan\left(\frac{kL_z}{2}\right) = \kappa / k$$

and

$$-\cot\left(\frac{kL_z}{2}\right) = \kappa / k$$
Solving for the eigenenergies

Change to “dimensionless” units

Use the energy of the first level in the “infinite” potential well width $L_z$

leading to a dimensionless eigenenergy

and a dimensionless barrier height

Also

$$E_1^\infty = \frac{\hbar^2}{2m} \left( \frac{\pi}{L_z} \right)^2$$

$$\varepsilon \equiv \frac{E}{E_1^\infty}$$

$$\nu_o \equiv \frac{V_o}{E_1^\infty}$$

$$k = \sqrt{2mE / \hbar^2} = \left( \frac{\pi}{L_z} \right) \sqrt{E / E_1^\infty} = \left( \frac{\pi}{L_z} \right) \sqrt{\varepsilon}$$

$$\kappa = \sqrt{2m(V_o - E) / \hbar^2} = \left( \frac{\pi}{L_z} \right) \sqrt{(V_o - E) / E_1^\infty} = \left( \frac{\pi}{L_z} \right) \sqrt{\nu_o - \varepsilon}$$
Solving for the eigenenergies

Consequently

\[
\frac{\kappa}{k} = \sqrt{\frac{V_o - E}{E}} = \sqrt{\frac{v_o - \varepsilon}{\varepsilon}}
\]

\[
\frac{kL_z}{2} = \frac{\pi}{2} \sqrt{\frac{E}{E_1^\infty}} = \frac{\pi}{2} \sqrt{\varepsilon} \quad \text{and} \quad \frac{\kappa L_z}{2} = \frac{\pi}{2} \sqrt{\frac{V_o - E}{E_1^\infty}} = \frac{\pi}{2} \sqrt{v_o - \varepsilon}
\]

So
\[
\tan\left(\frac{kL_z}{2}\right) = \frac{\kappa}{k} \quad \text{becomes} \quad \tan\left[\left(\frac{\pi}{2}\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right) / \varepsilon}
\]

or
\[
\sqrt{\varepsilon} \tan\left[\left(\frac{\pi}{2}\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right)}
\]

and
\[
\cot\left(\frac{kL_z}{2}\right) = \frac{\kappa}{k} \quad \text{becomes} \quad -\cot\left[\left(\frac{\pi}{2}\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right) / \varepsilon}
\]

or
\[
-\sqrt{\varepsilon} \cot\left[\left(\frac{\pi}{2}\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right)}
\]
Graphical solution

Choose a specific well depth \( v_o \)
and plot the curve
\[
\sqrt{\left(v_o - \varepsilon\right)}
\]
Graphical solution

Choose a specific well depth $\nu_o$ and plot the curve $\sqrt{(\nu_o - \varepsilon)}$.
Graphical solution

Choose a specific well depth $\nu_o$ and plot the curve $\sqrt{\left(\nu_o - \varepsilon\right)}$
Graphical solution

Choose a specific well depth $v_o$
and plot the curve

$$\sqrt{(v_o - \varepsilon)}$$

Now add the curves
Graphical solution

Choose a specific well depth \( \nu_o \)

and plot the curve

\[
\sqrt{(\nu_o - \varepsilon)}
\]

Now add the curves

\[
\sqrt{\varepsilon} \tan\left(\frac{\pi}{2}\sqrt{\varepsilon}\right)
\]

\( \nu_o = 8 \)
Graphical solution

Choose a specific well depth $v_o$
and plot the curve

$$\sqrt{(v_o - \varepsilon)}$$

Now add the curves

$$\sqrt{\varepsilon} \tan \left( \frac{\pi}{2} \sqrt{\varepsilon} \right)$$

$$-\sqrt{\varepsilon} \cot \left( \frac{\pi}{2} \sqrt{\varepsilon} \right)$$
Graphical solution

For a specific $\nu_o$
the solutions are the values of $\varepsilon$ at the intersections of

$$\sqrt{(\nu_o - \varepsilon)}$$

and

$$\sqrt{\varepsilon} \tan \left(\frac{\pi}{2} \sqrt{\varepsilon}\right)$$

or

$$-\sqrt{\varepsilon} \cot \left(\frac{\pi}{2} \sqrt{\varepsilon}\right)$$
Solutions

These are the solutions for a well depth \( V_0 \) of \( 8E_1^\infty \)

Note that

they are all

lower energies

than the corresponding solutions for the infinitely deep well of the same width

\[
\begin{align*}
V_0 &= 8E_1^\infty \\
\epsilon &= 5.609 \\
\epsilon &= 2.603 \\
\epsilon &= 0.663 \\
n &= 1 \\
n &= 2 \\
n &= 3
\end{align*}
\]
7 Finite well and harmonic oscillator

Slides: Lecture 7c The harmonic oscillator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.10
Particles in potential wells

The harmonic oscillator

Quantum mechanics for scientists and engineers

David Miller
A simple spring will have a restoring force $F$ acting on the mass $M$
Mass on a spring

A simple spring will have a restoring force $F$ acting on the mass $M$ proportional to the amount $y$ by which it is stretched

For some “spring constant” $K$

$$F = -Ky$$

The minus sign is because this is “restoring” it is trying to pull $y$ back towards zero

This gives a “simple harmonic oscillator”
Mass on a spring

From Newton’s second law

\[ F = Ma = M \frac{d^2 y}{dt^2} = -Ky \]

i.e., \[ \frac{d^2 y}{dt^2} = -\frac{K}{M} y = -\omega^2 y \]

where we define \[ \omega^2 = \frac{K}{M} \]

we have oscillatory solutions of angular frequency \[ \omega = \sqrt{\frac{K}{M}} \]

e.g., \[ y \propto \sin \omega t \]
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\[ y \propto \sin \omega t \]
Potential energy

The potential from the restoring force $F$ is

$$V(z) = \int_0^z -F \, dz = \int_0^z Kz_o \, dz_o = \frac{1}{2} Kz^2 = \frac{1}{2} m\omega^2 z^2$$
Harmonic oscillator Schrödinger equation

With this potential energy \( V(z) = \frac{1}{2} m\omega^2 z^2 \)
the Schrödinger equation is

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dz^2} + \frac{1}{2} m\omega^2 z^2 \psi = E\psi
\]

For convenience, we define a dimensionless distance unit
\( \xi = \sqrt{\frac{m\omega}{\hbar}} z \)
so the Schrödinger equation becomes

\[
\frac{1}{2} \frac{d^2 \psi}{d\xi^2} - \frac{\xi^2}{2} \psi = -\frac{E}{\hbar\omega} \psi
\]
Harmonic oscillator Schrödinger equation

One specific solution to this equation

\[ \frac{1}{2} \frac{d^2\psi}{d\xi^2} - \frac{\xi^2}{2}\psi = -\frac{E}{\hbar \omega} \psi \]

is

\[ \psi \propto \exp(-\xi^2 / 2) \]

with a corresponding energy \( E = \hbar \omega / 2 \)

This suggests we look for solutions of the form

\[ \psi_n(\xi) = A_n \exp\left(-\frac{\xi^2}{2}\right) H_n(\xi) \]

where \( H_n(\xi) \) is some set of functions still to be determined.
Harmonic oscillator Schrödinger equation

Substituting \( \psi_n(\xi) = A_n \exp(-\xi^2/2) H_n(\xi) \)

into the Schrödinger equation

\[
\frac{1}{2} \frac{d^2 \psi}{d\xi^2} - \frac{\xi^2}{2} \psi = -\frac{E}{\hbar \omega} \psi
\]

gives

\[
\frac{d^2 H_n(\xi)}{d\xi^2} - 2\xi \frac{dH_n(\xi)}{d\xi} + \left( \frac{2E}{\hbar \omega} - 1 \right) H_n(\xi) = 0
\]

This is the defining differential equation for the Hermite polynomials
Harmonic oscillator Schrödinger equation

Solutions to

\[
\frac{d^2 H_n(\xi)}{d\xi^2} - 2\xi \frac{dH_n(\xi)}{d\xi} + \left(\frac{2E}{\hbar \omega} - 1\right) H_n(\xi) = 0
\]

exist provided

\[
\frac{2E}{\hbar \omega} - 1 = 2n \quad n = 0, 1, 2, \ldots
\]

that is,

\[
E_n = \left( n + \frac{1}{2} \right) \hbar \omega \quad n = 0, 1, 2, \ldots
\]
Harmonic oscillator Schrödinger equation

The allowed energy levels are equally spaced separated by an amount $\hbar \omega$

where $\omega$ is the classical oscillation frequency

Like the potential well there is a “zero point energy” here $\hbar \omega / 2$

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

$n = 0, 1, 2, \ldots$
Hermite polynomials

The first Hermite polynomials are odd or even, i.e., they have a definite parity. They satisfy a “recurrence relation”

\[ H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(n-1)H_{n-2}(\xi) \]

successive Hermite polynomials can be calculated from the previous two.

- \( H_0(\xi) = 1 \)
- \( H_1(\xi) = 2\xi \)
- \( H_2(\xi) = 4\xi^2 - 2 \)
- \( H_3(\xi) = 8\xi^3 - 12\xi \)
- \( H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \)
Harmonic oscillator solutions

Normalizing gives

\[ \psi_n(\xi) = A_n \exp\left(-\frac{\xi^2}{2}\right)H_n(\xi) \]

\[ A_n = \sqrt{\frac{1}{\sqrt{\pi} 2^n n!}} \]

\[ \xi = \sqrt{\frac{m\omega}{\hbar}} z \]

\[ E_n = \left(n + \frac{1}{2}\right) \hbar \omega \quad n = 0, 1, 2, \ldots \]
Harmonic oscillator solutions

Normalizing

\[ \psi_n(\xi) = A_n \exp\left(-\frac{\xi^2}{2}\right) H_n(\xi) \]

gives

\[ A_n = \sqrt{\frac{1}{\sqrt{\pi} 2^n n!}} \]

\[ \xi = \sqrt{\frac{m\omega}{\hbar}} z \]

or

\[ E_n = \left(n + \frac{1}{2}\right) \hbar \omega \quad n = 0, 1, 2, \ldots \]

\[ \psi_n(z) = \sqrt{\frac{1}{2^n n! \sqrt{\pi \hbar}}} \sqrt{\frac{m\omega}{\hbar}} \exp\left(-\frac{m\omega}{2\hbar} z^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} z\right) \]
Harmonic oscillator eigensolutions

\[ A_4 \exp\left(-\frac{\xi^2}{2}\right)\left(16\xi^4 - 48\xi^2 + 12\right) \]

\[ A_3 \exp\left(-\frac{\xi^2}{2}\right)\left(8\xi^3 - 12\xi\right) \]

\[ A_2 \exp\left(-\frac{\xi^2}{2}\right)\left(4\xi^2 - 2\right) \]

\[ A_1 \exp\left(-\frac{\xi^2}{2}\right)\left(2\xi\right) \]

\[ A_0 \exp\left(-\frac{\xi^2}{2}\right) \]
Classical turning points

The intersections of the parabola and the dashed lines give the “classical turning points” where a classical mass of that energy turns round and goes back downhill.