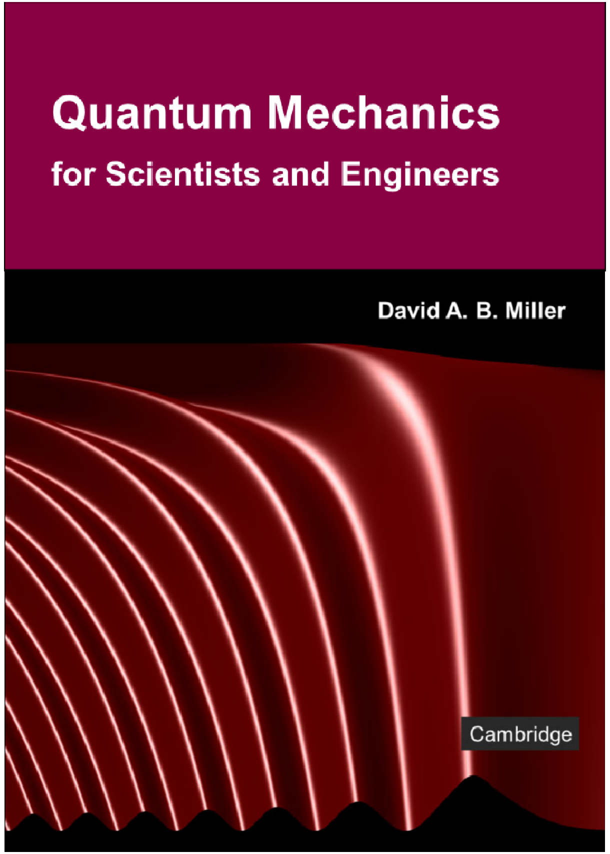
7 Finite well and harmonic oscillator

Slides: Lecture 7a Particles in potential wells – introduction

Text reference: Quantum Mechanics for Scientists and Engineers

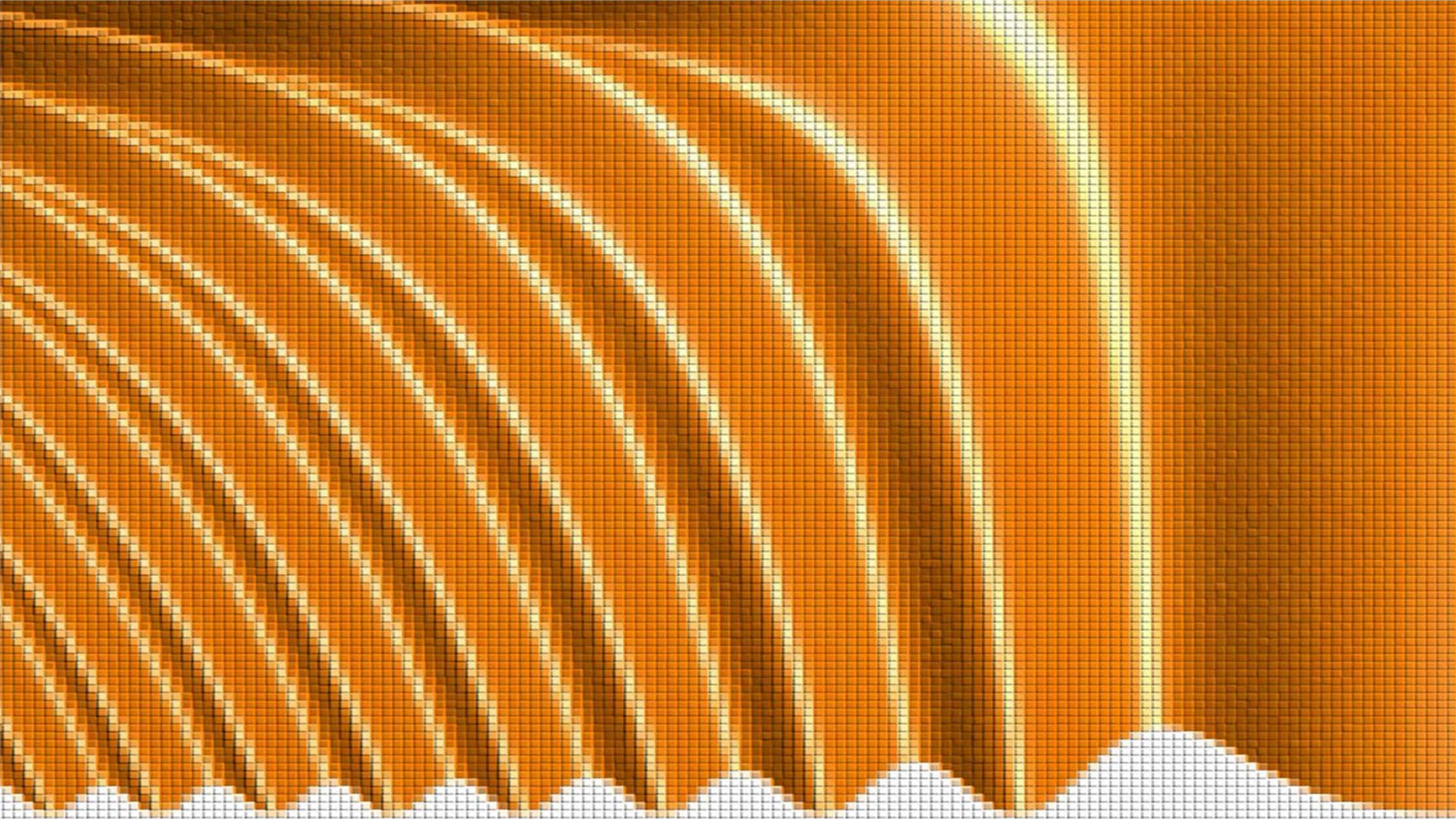
Section 2.9



Particles in potential wells

Quantum mechanics for scientists and engineers

David Miller

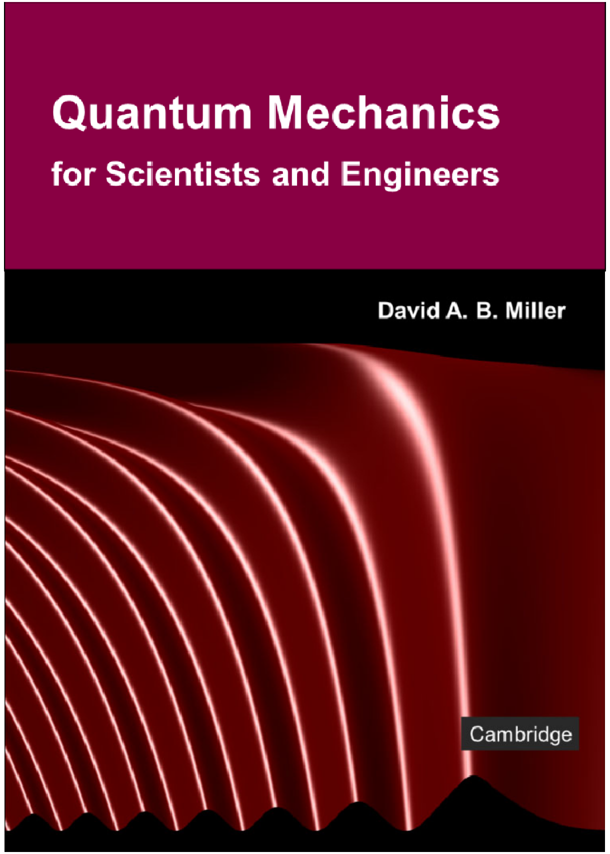


7 Finite well and harmonic oscillator

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

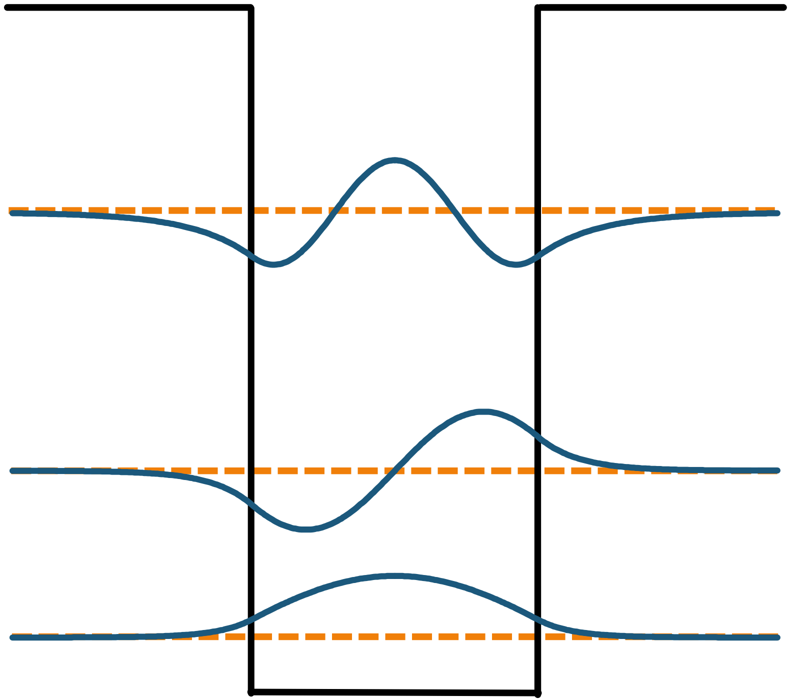
Finite potential well

Insert video here (split screen)

Lesson 7

Particles in potential wells

Insert number 2



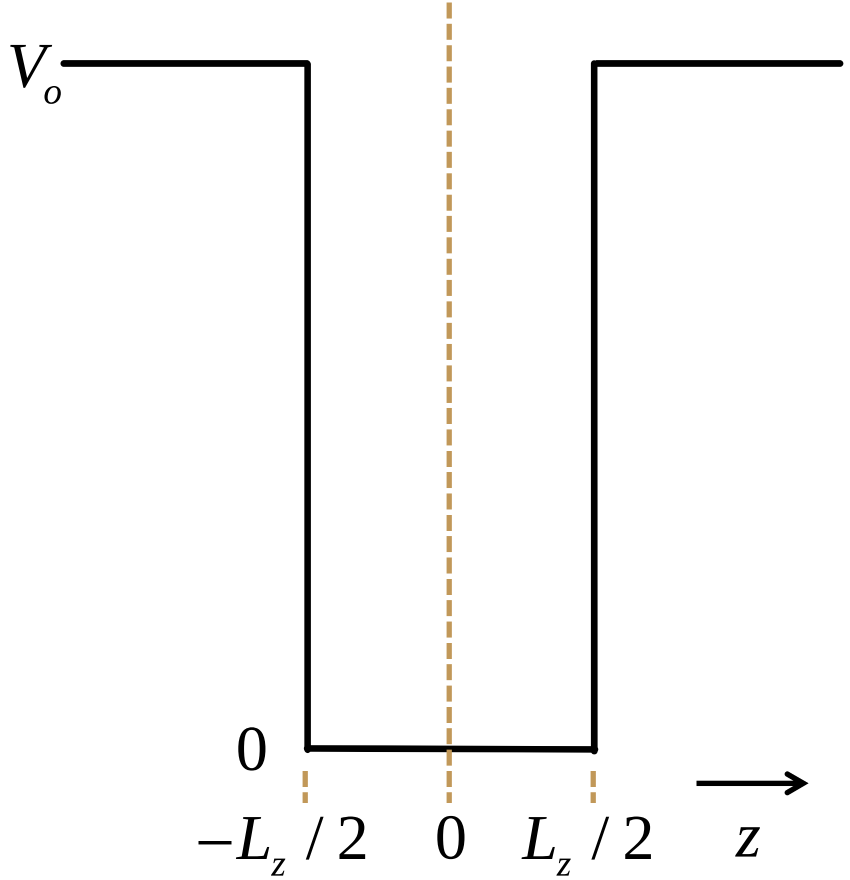
Particle in a finite potential well

We will choose the height of the potential barriers as V_o

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



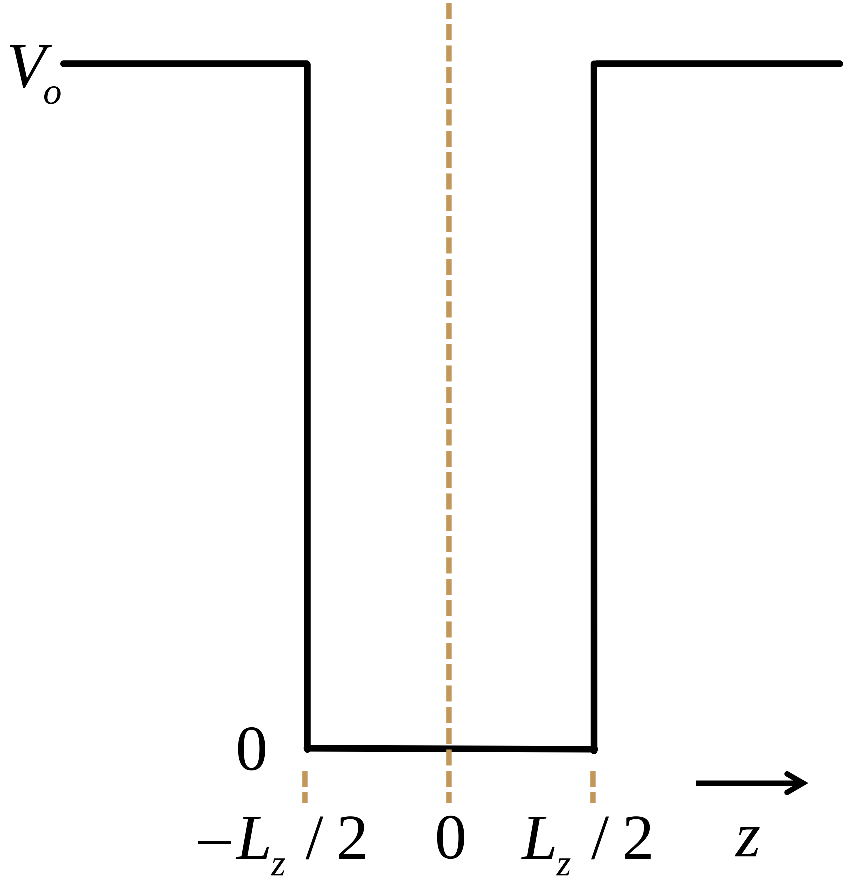
Particle in a finite potential well

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 $z < -L_z/2$

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

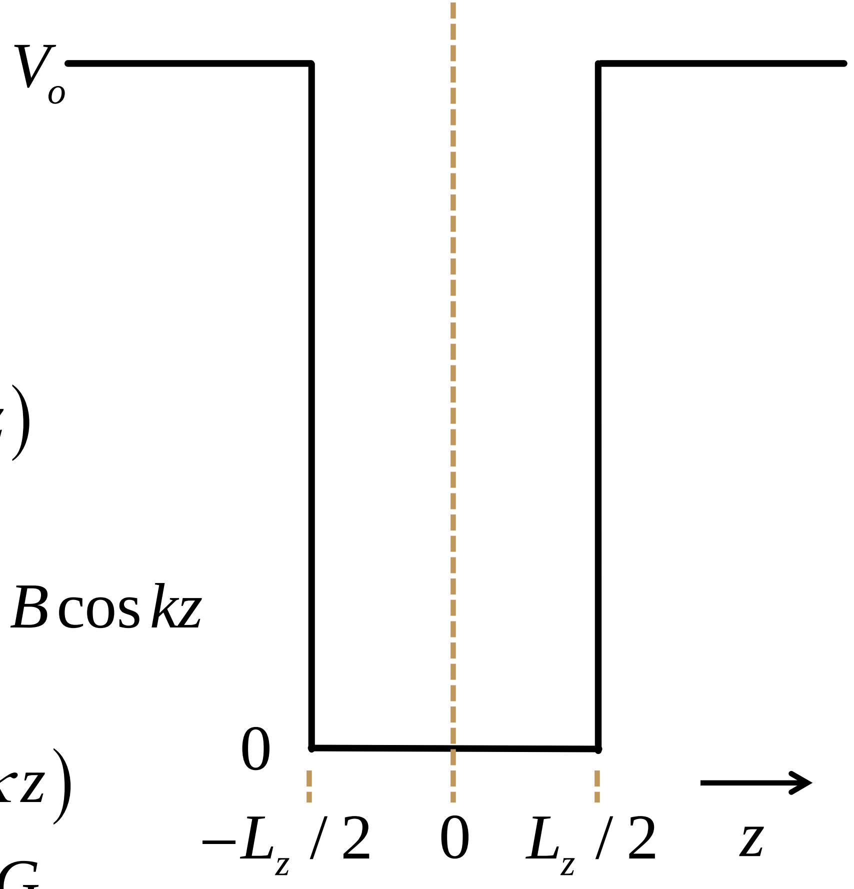
for $-L_z/2 < z < L_z/2$

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

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

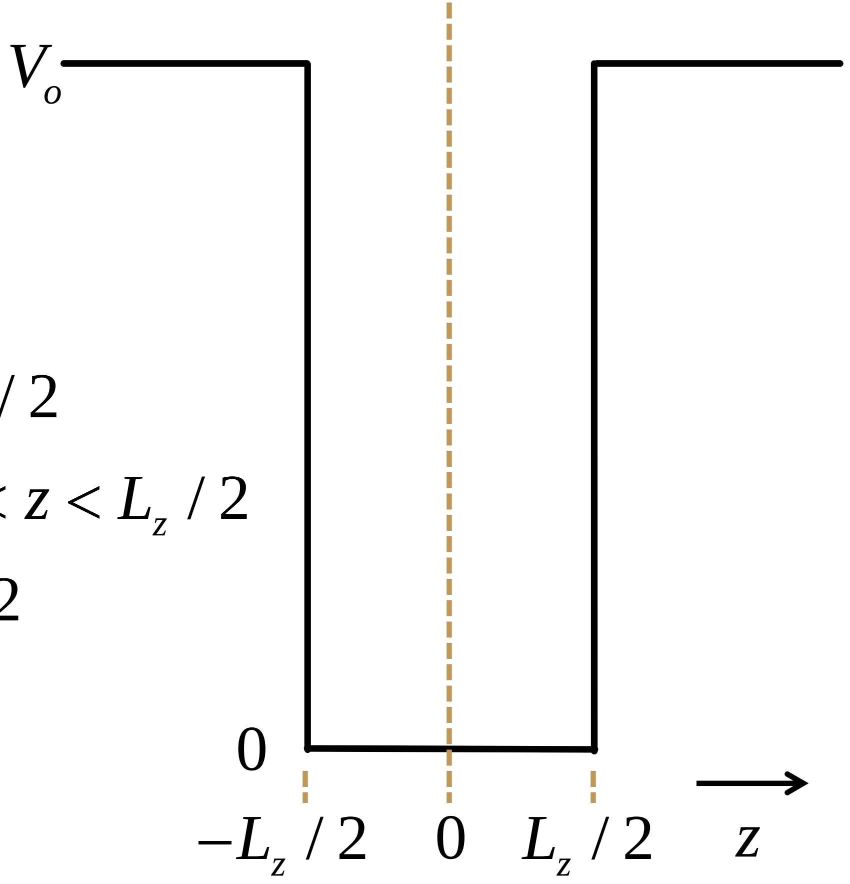
$$\psi(z) = G\exp(\kappa z) \qquad z < -L_z/2$$

$$\psi(z) = A\sin kz + B\cos kz \qquad -L_z/2 < z < L_z/2$$

$$\psi(z) = F\exp(-\kappa z) \qquad z > L_z/2$$

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 $z = L_z / 2$

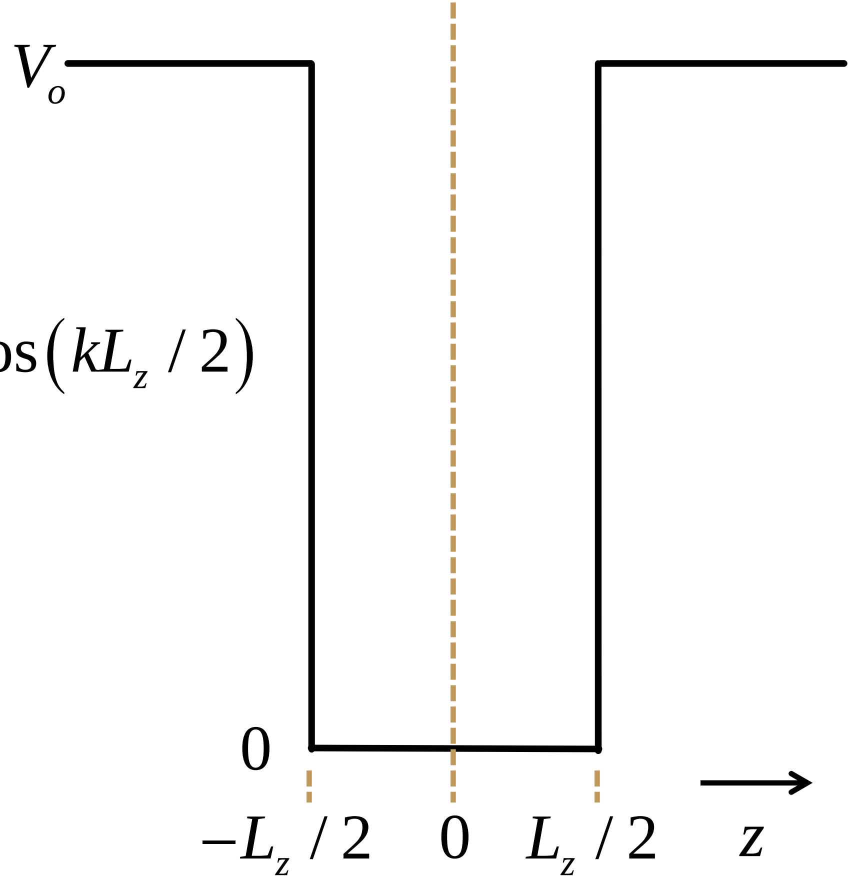
$$\psi\left(L_z / 2\right) = F \exp\left(-\kappa L_z / 2\right)$$
$$= A \sin\left(k L_z / 2\right) + B \cos\left(k L_z / 2\right)$$

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

$$S_L = \sin\left(k L_z / 2\right)$$
$$C_L = \cos\left(k L_z / 2\right)$$

gives

$$F X_L = A S_L + B C_L$$



Particle in a finite potential well

Similarly at $z = -L_z / 2$

$$GX_L = -AS_L + BC_L$$

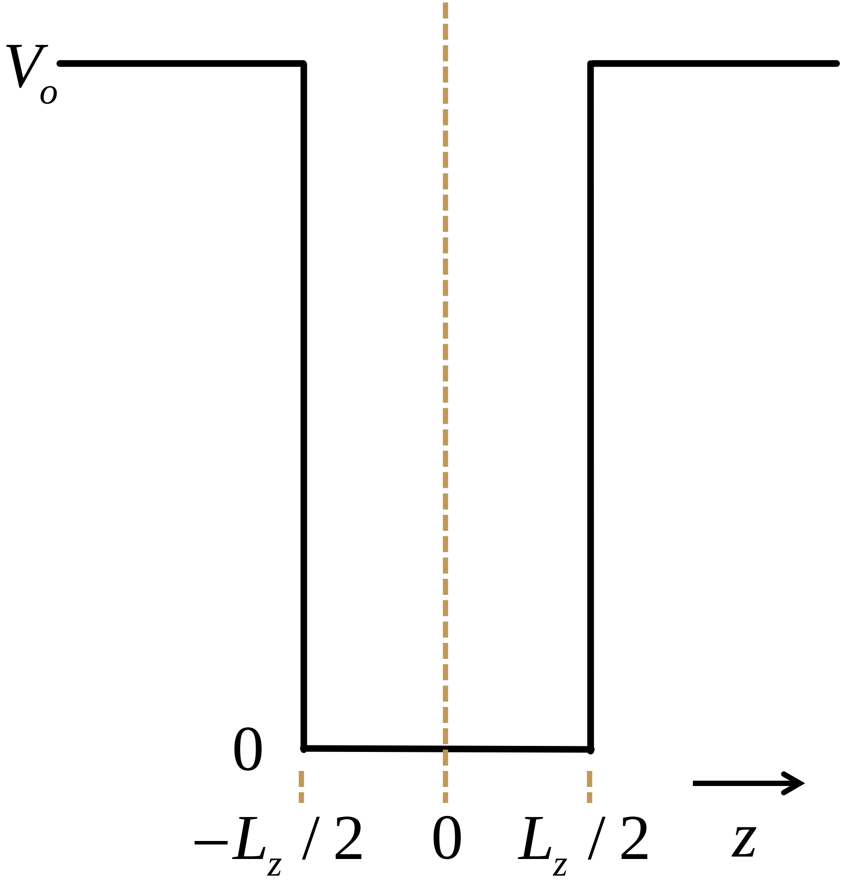
Continuity of the derivative gives

at $z = -L_z / 2$

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

at $z = L_z / 2$

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



Particle in a finite potential well

So we have four relations

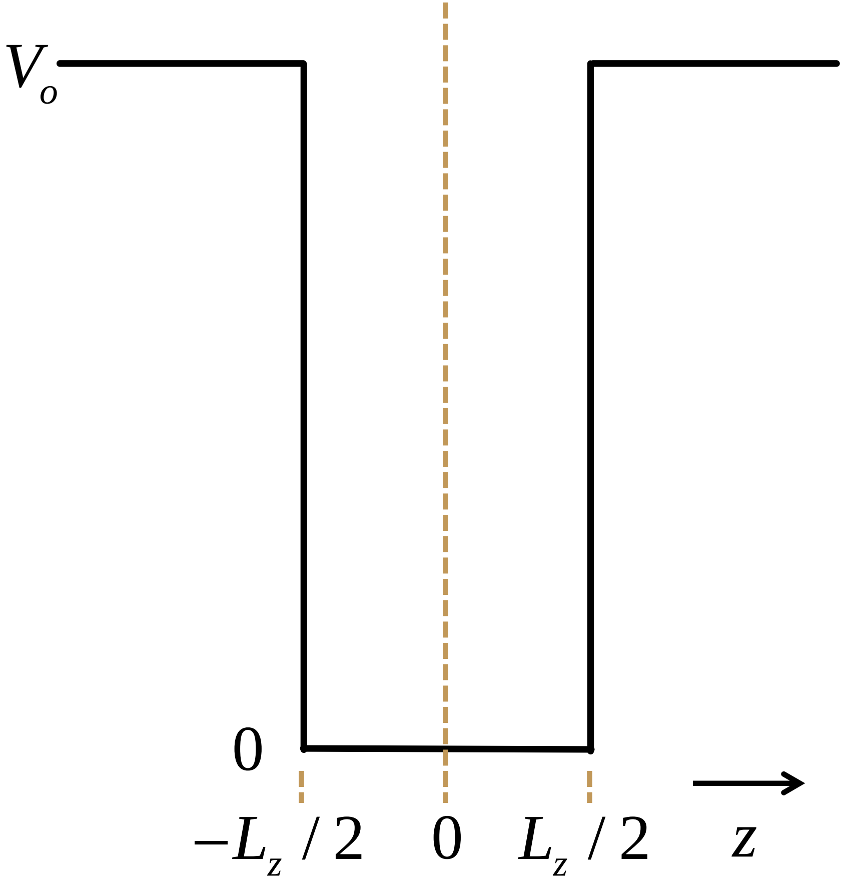
$$GX_L = -AS_L + BC_L$$

$$FX_L = AS_L + BC_L$$

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

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

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

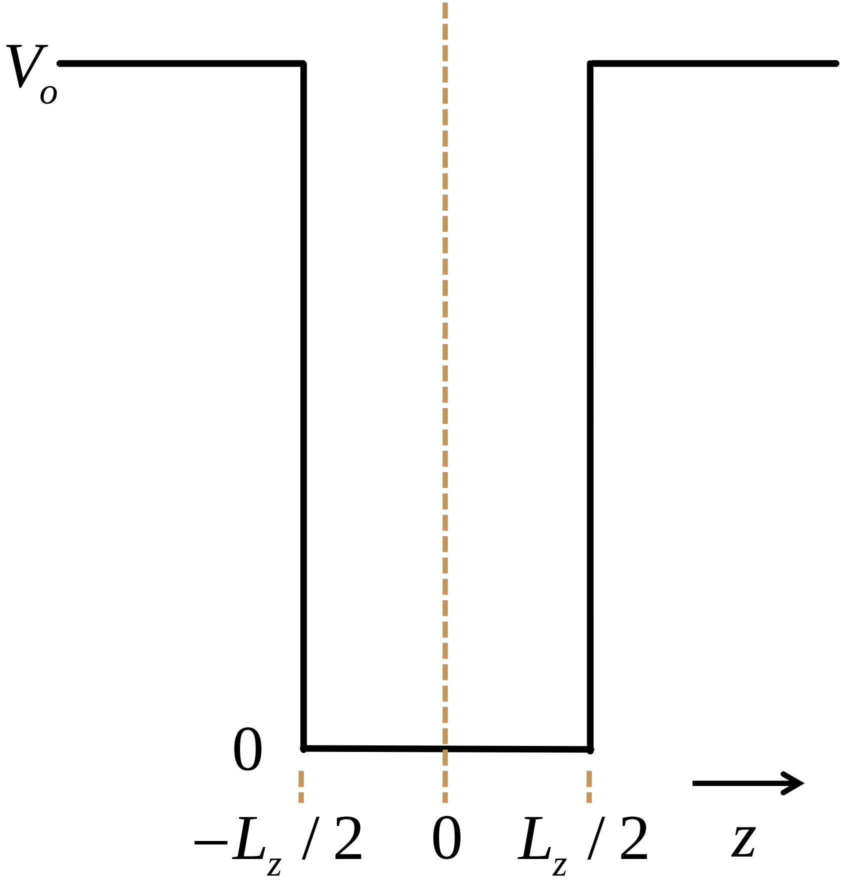
$$2BC_L = (F+G)X_L$$

Subtracting

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

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

gives $2BS_L = \frac{\kappa}{k}(F+G)X_L$



Particle in a finite potential well

As long as $F \neq -G$

we can divide

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

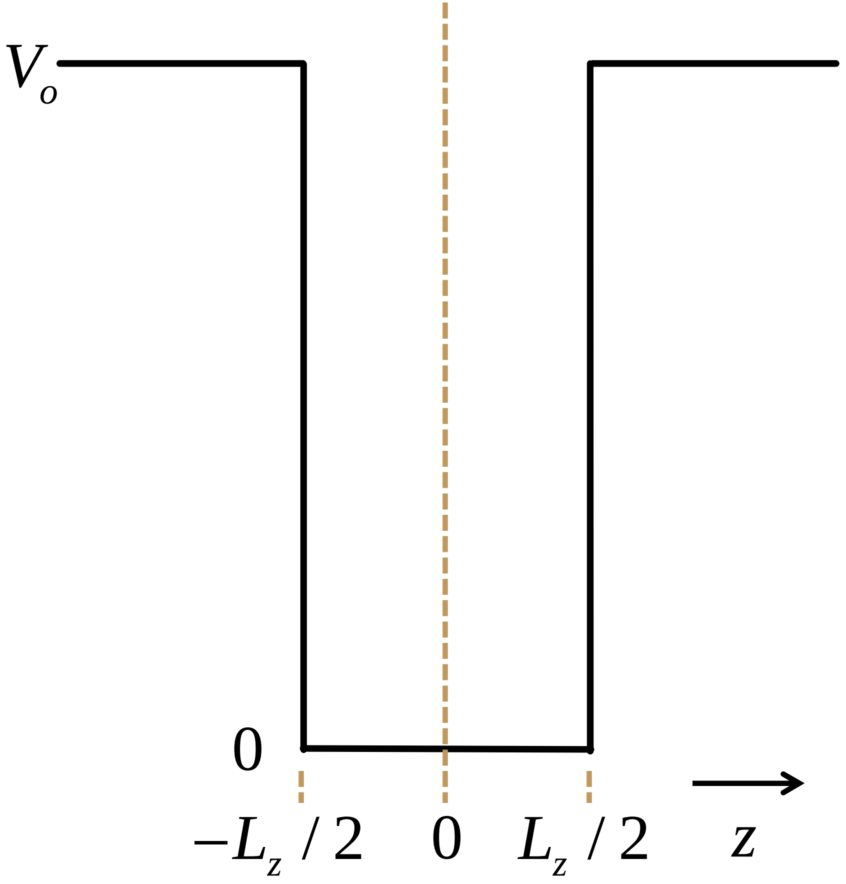
by

$$2BC_L = (F+G)X_L$$

to obtain

$$\tan(kL_z/2) = \kappa/k$$

This relation is effectively a condition for eigenvalues



Particle in a finite potential well

Subtracting $$GX_L = -AS_L + BC_L$$

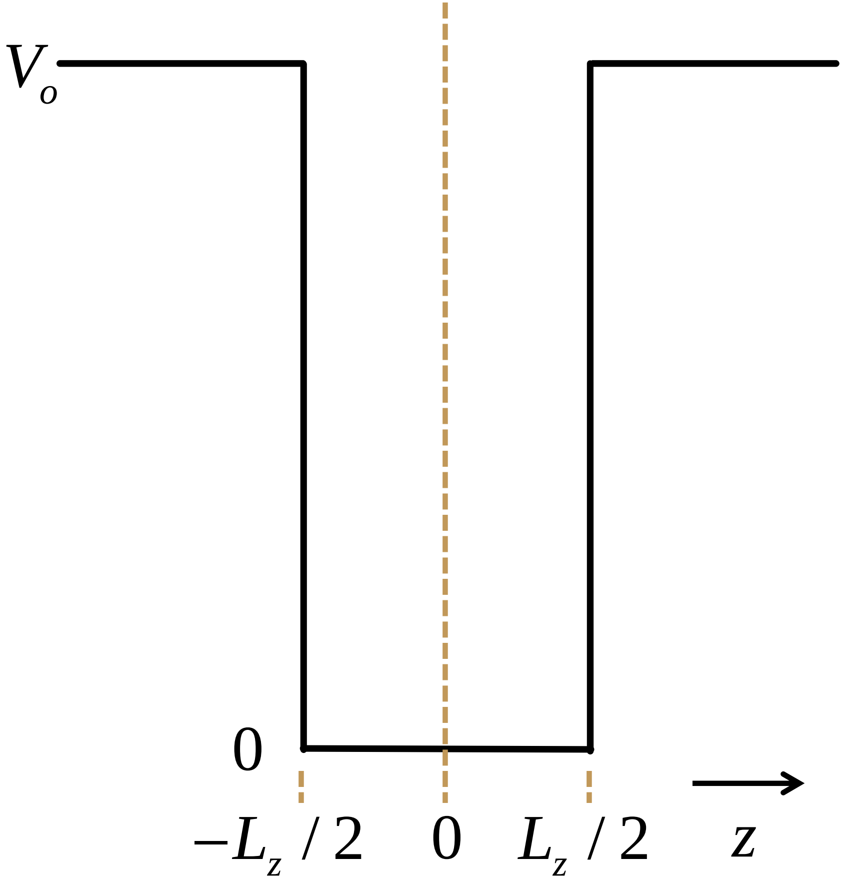
from $$FX_L = AS_L + BC_L$$

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

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

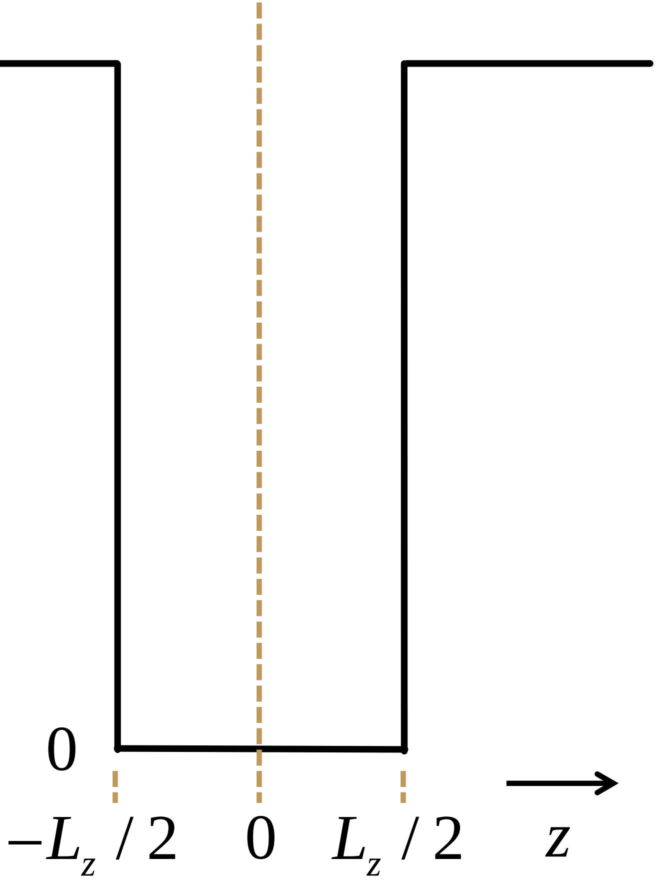
by

$$2AS_L = (F-G)X_L$$

to obtain

$$-\cot(kL_z/2) = \kappa/k$$

This relation is also effectively a condition for eigenvalues



Particle in a finite potential well

For any case other than $F = G$

which leaves $\tan(kL_z/2) = \kappa/k$

but not $-\cot(kL_z/2) = \kappa/k$

or $F = -G$

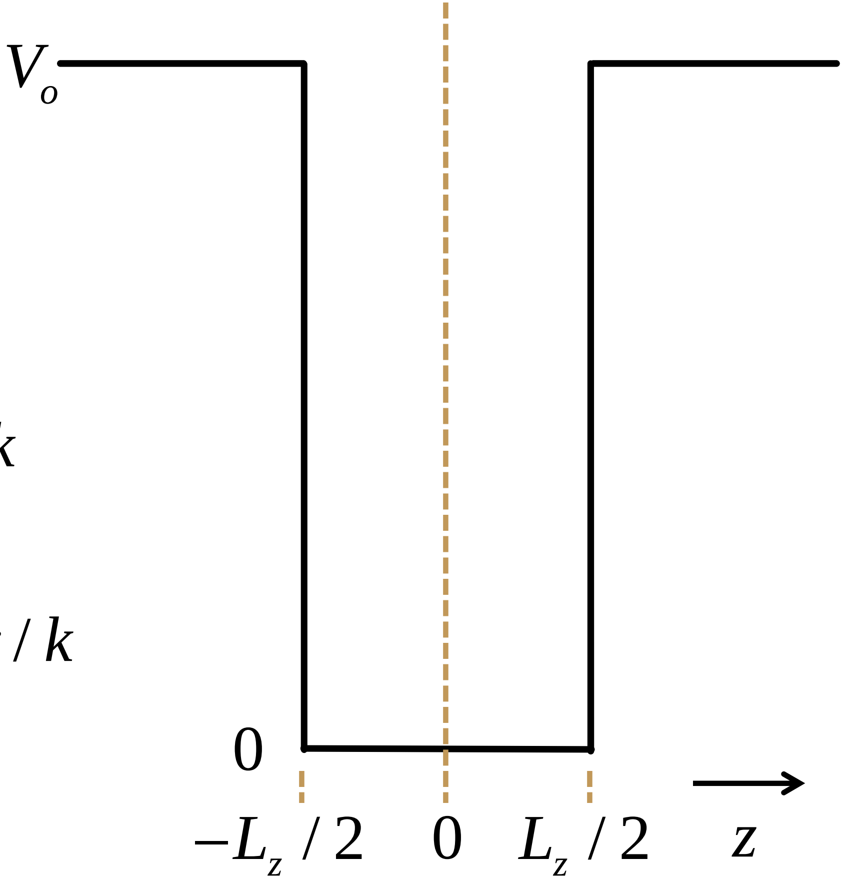
which leaves $-\cot(kL_z/2) = \kappa/k$

but not $\tan(kL_z/2) = \kappa/k$

then the solutions $\tan(kL_z/2) = \kappa/k$

and $-\cot(kL_z/2) = \kappa/k$

are contradictory



Particle in a finite potential well

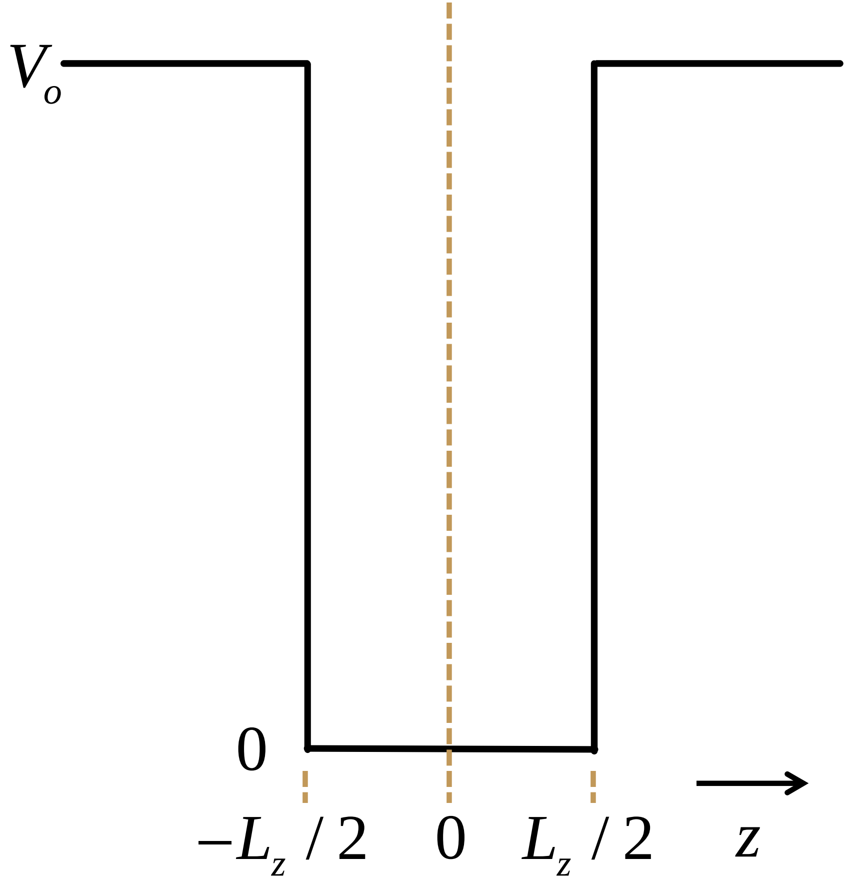
So the only possibilities are

1 - $F = G$

and $\tan\left(kL_z/2\right) = \kappa/k$

2 – $F = -G$

and $-\cot\left(kL_z/2\right) = \kappa/k$



Particle in a finite potential well

1 - $F = G$

and $\tan\left(kL_z / 2\right) = \kappa / k$

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

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

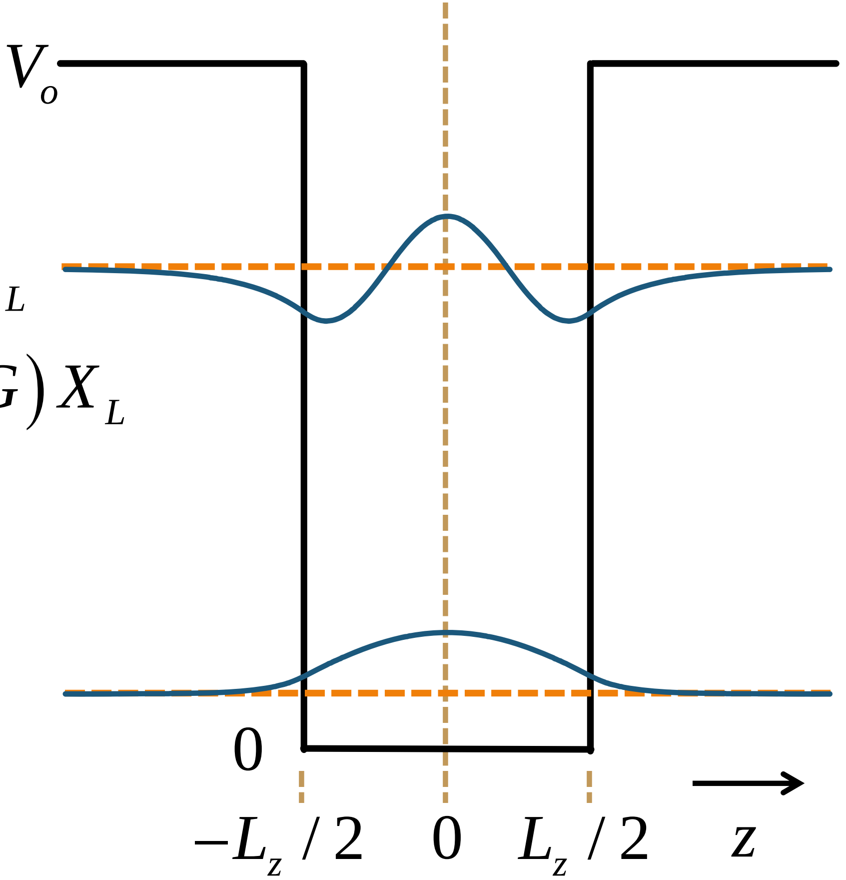
S_L and C_L cannot both be 0

so $A = 0$

Hence in the well we have

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

which is an even function



Particle in a finite potential well

1 - $F = -G$

and $-\cot\left(kL_z / 2\right) = \kappa / k$

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

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

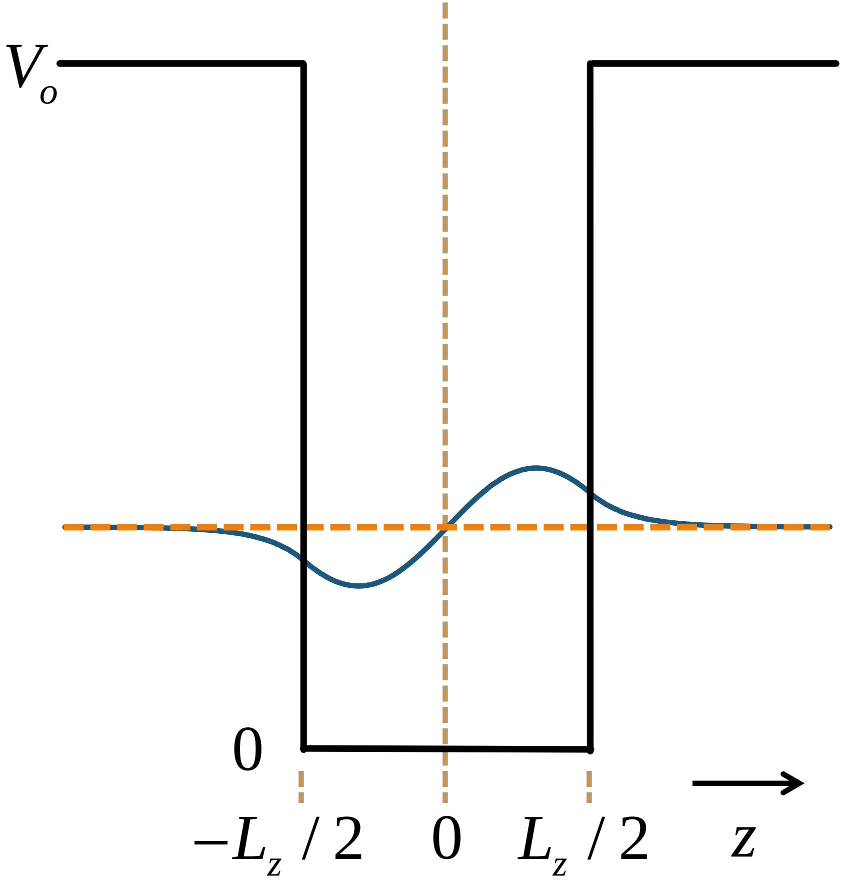
S_L and C_L cannot both be 0

so $B = 0$

Hence in the well we have

$$\psi\left(z\right) \propto \sin kz$$

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

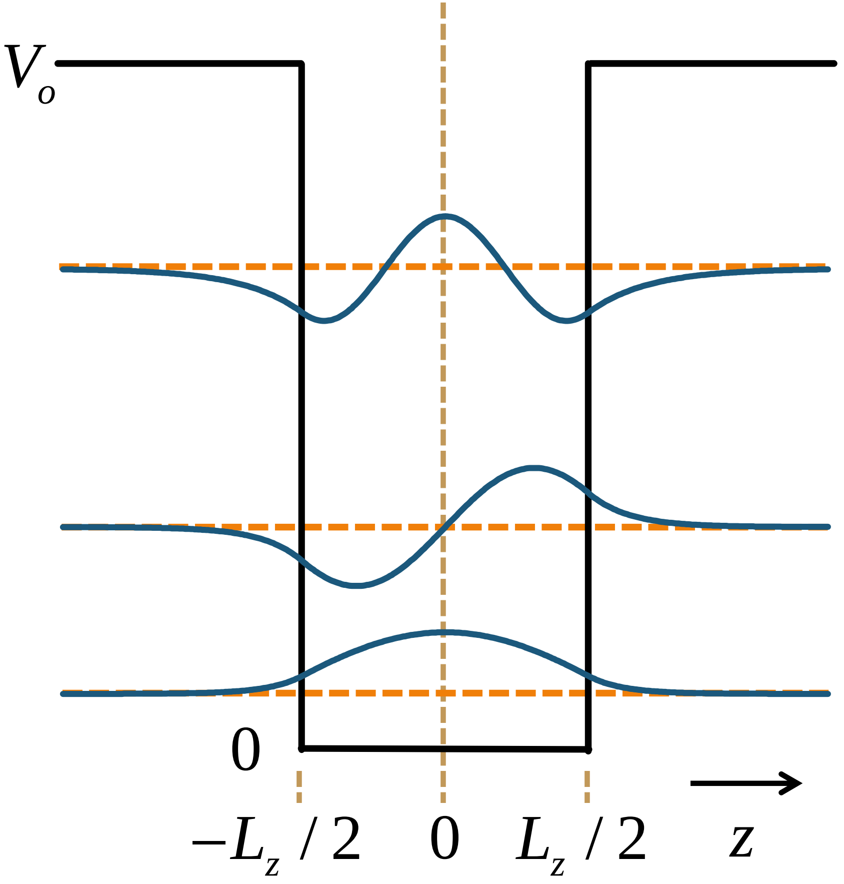
and hence for k and κ

We do this by solving

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

and

$$-\cot\left(kL_z/2\right)=\kappa/k$$



Solving for the eigenenergies

Change to "dimensionless" units

Use the energy of the first level in the "infinite" potential well width L_z

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

leading to a dimensionless eigenenergy

$$\varepsilon \equiv E / E_1^\infty$$

and a dimensionless barrier height

$$v_o \equiv V_o / E_1^\infty$$

Also

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

$$\kappa = \sqrt{2m(V_o - E) / \hbar^2} = (\pi / L_z)\sqrt{(V_o - E) / E_1^\infty} = (\pi / L_z)\sqrt{v_o - \varepsilon}$$

Solving for the eigenenergies

Consequently $\frac{\kappa}{k} = \sqrt{\frac{V_o - E}{E}} = \sqrt{\frac{v_o - \varepsilon}{\varepsilon}}$

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

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

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

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

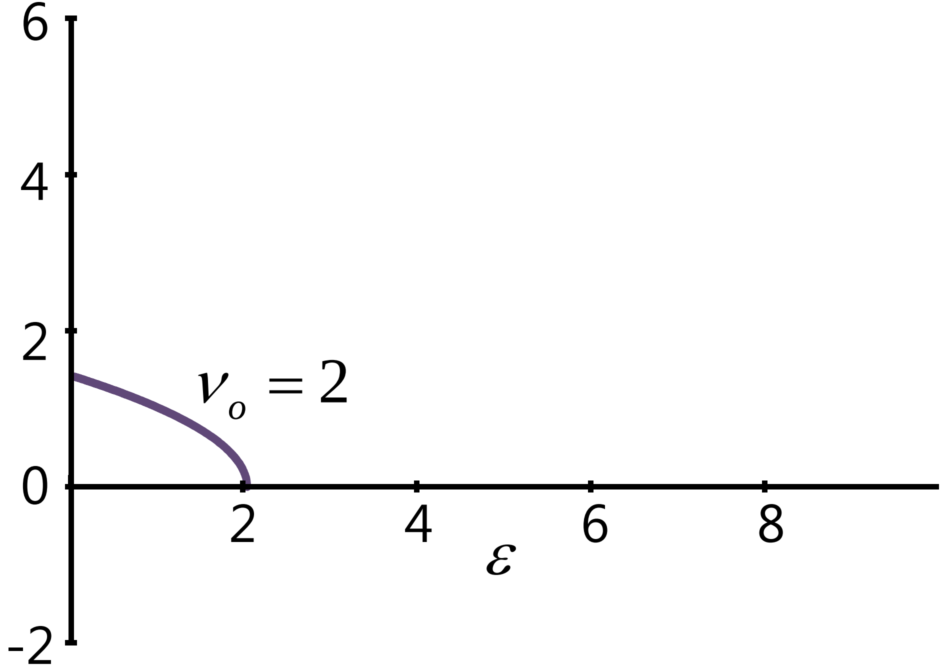
or $-\sqrt{\varepsilon}\cot\left[\left(\pi / 2\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right)}$

Graphical solution

Choose a specific well depth v_o

and plot the curve

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



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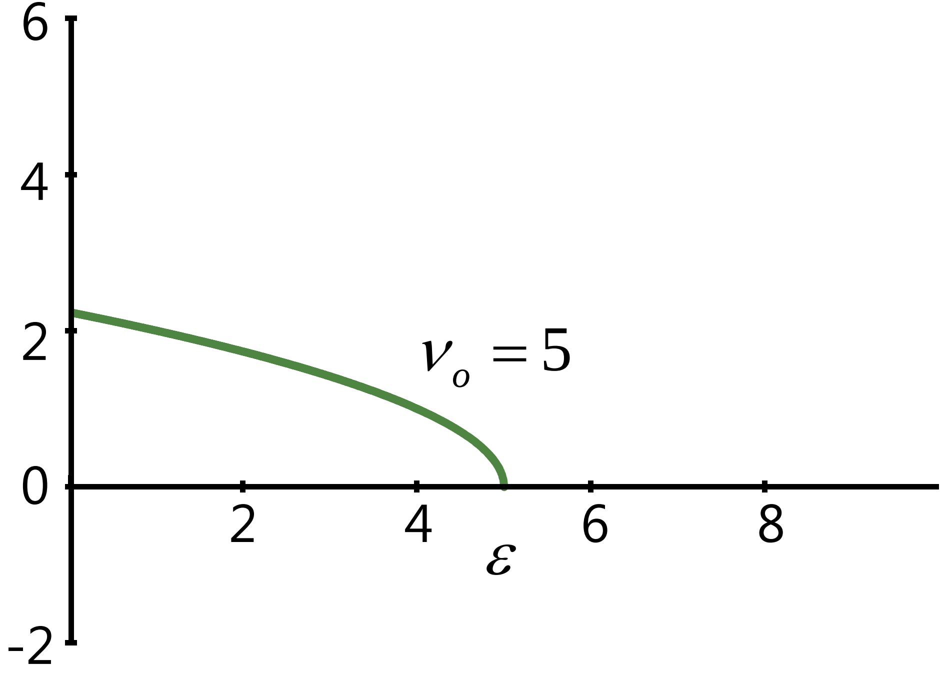

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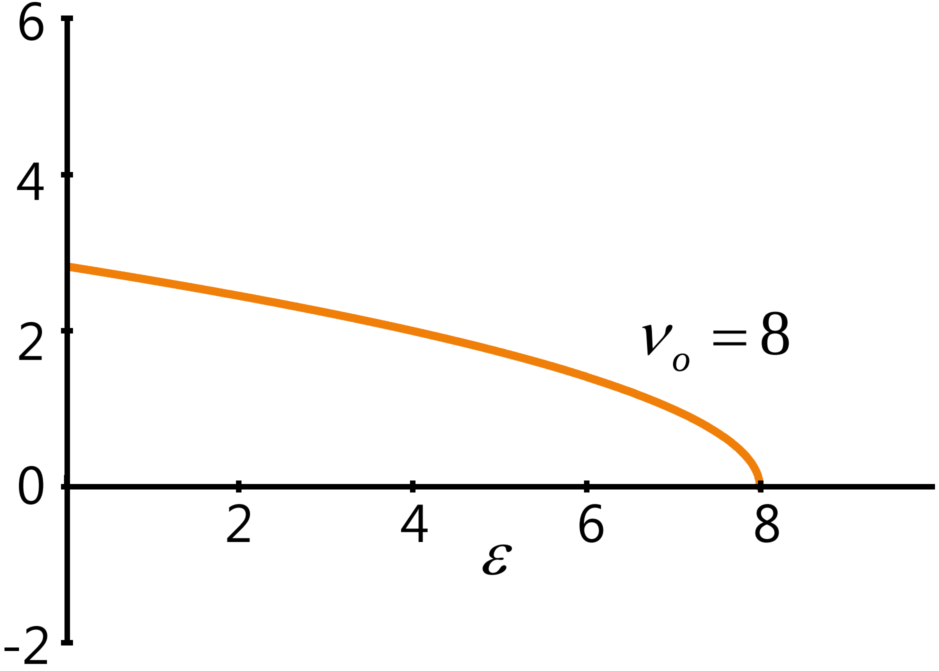


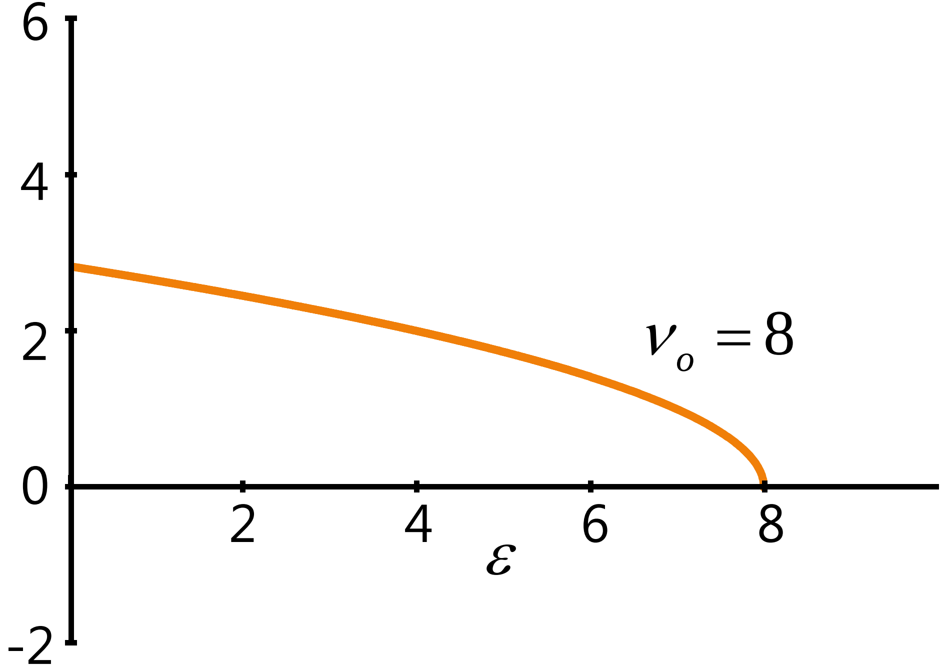
Graphical solution

Choose a specific well depth v_o

and plot the curve

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

Now add the curves



Graphical solution

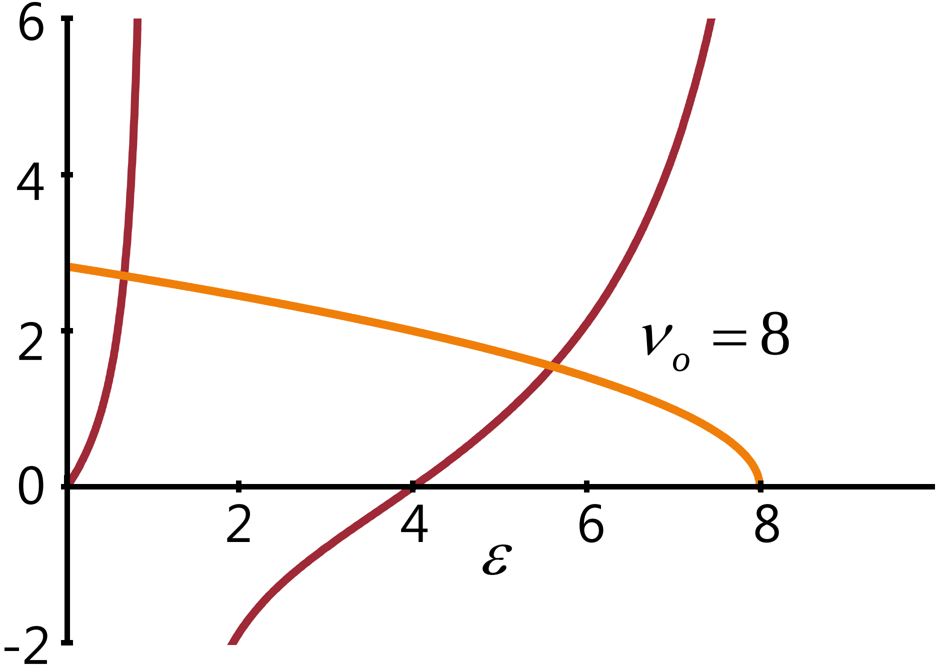
Choose a specific well depth v_o

and plot the curve

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

Now add the curves

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



Graphical solution

Choose a specific well depth v_o

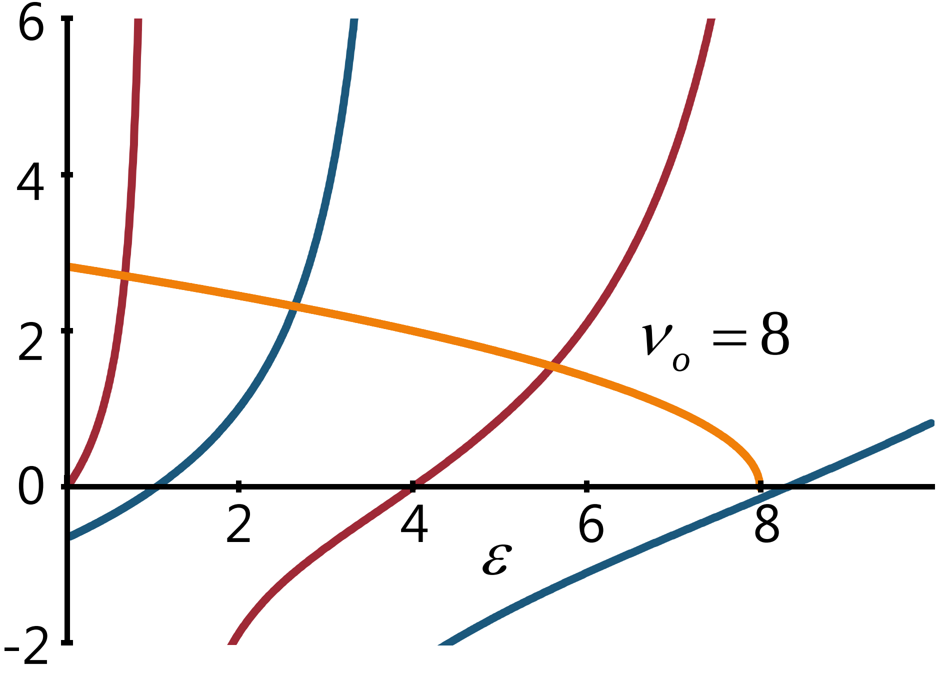
and plot the curve

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

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 v_o

the solutions are the values of ε at the intersections of

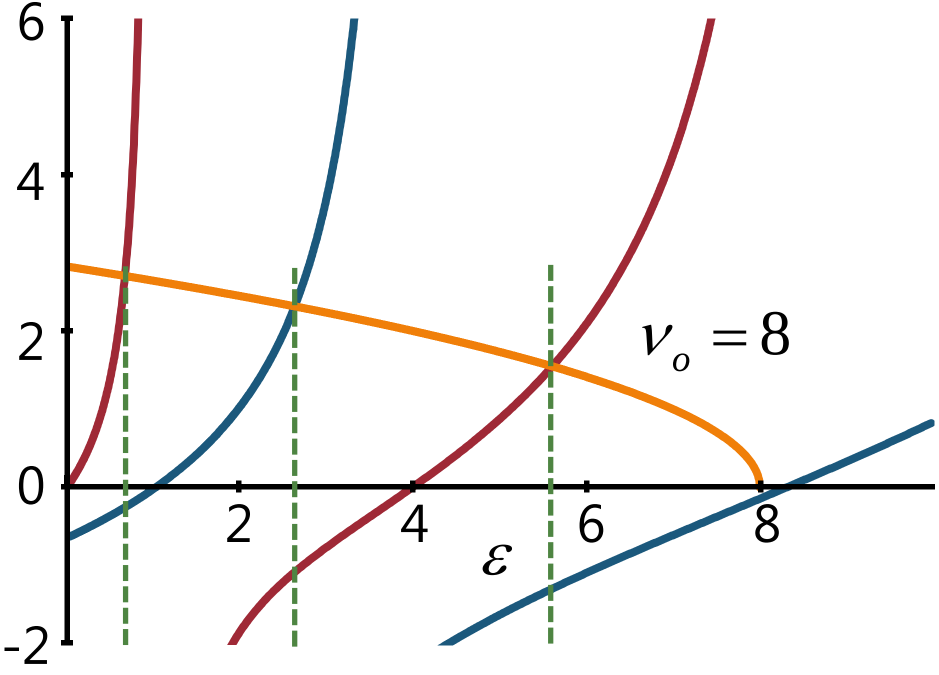
$$\sqrt{(v_o - \varepsilon)}$$

and

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

or

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

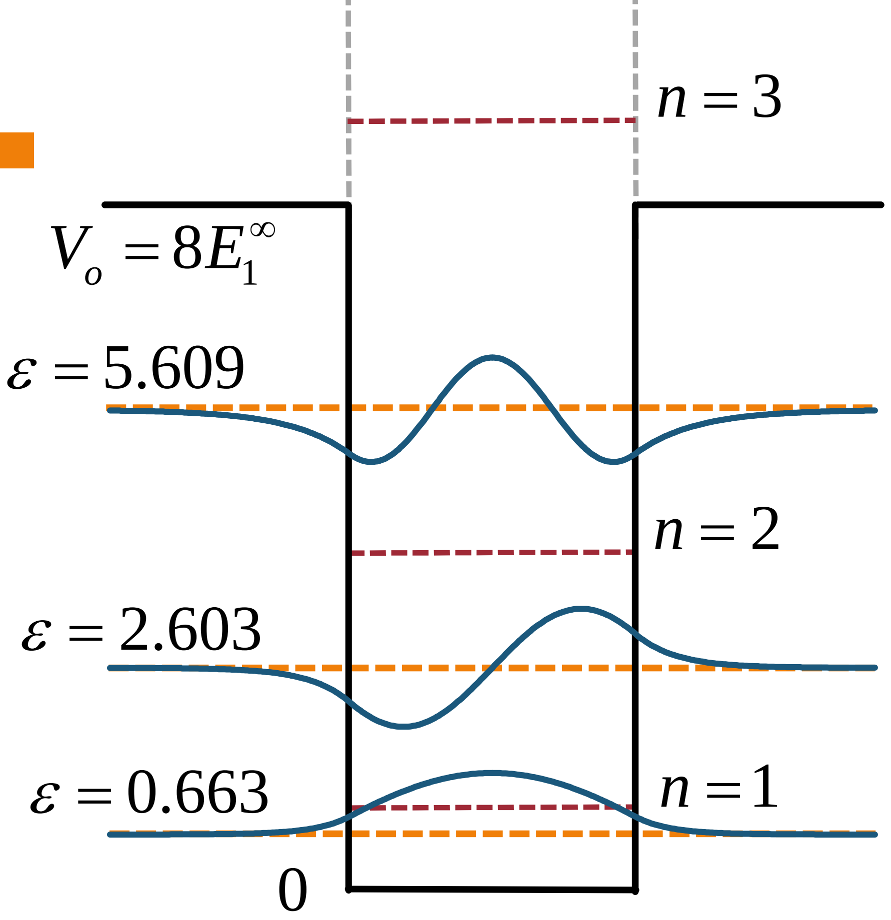


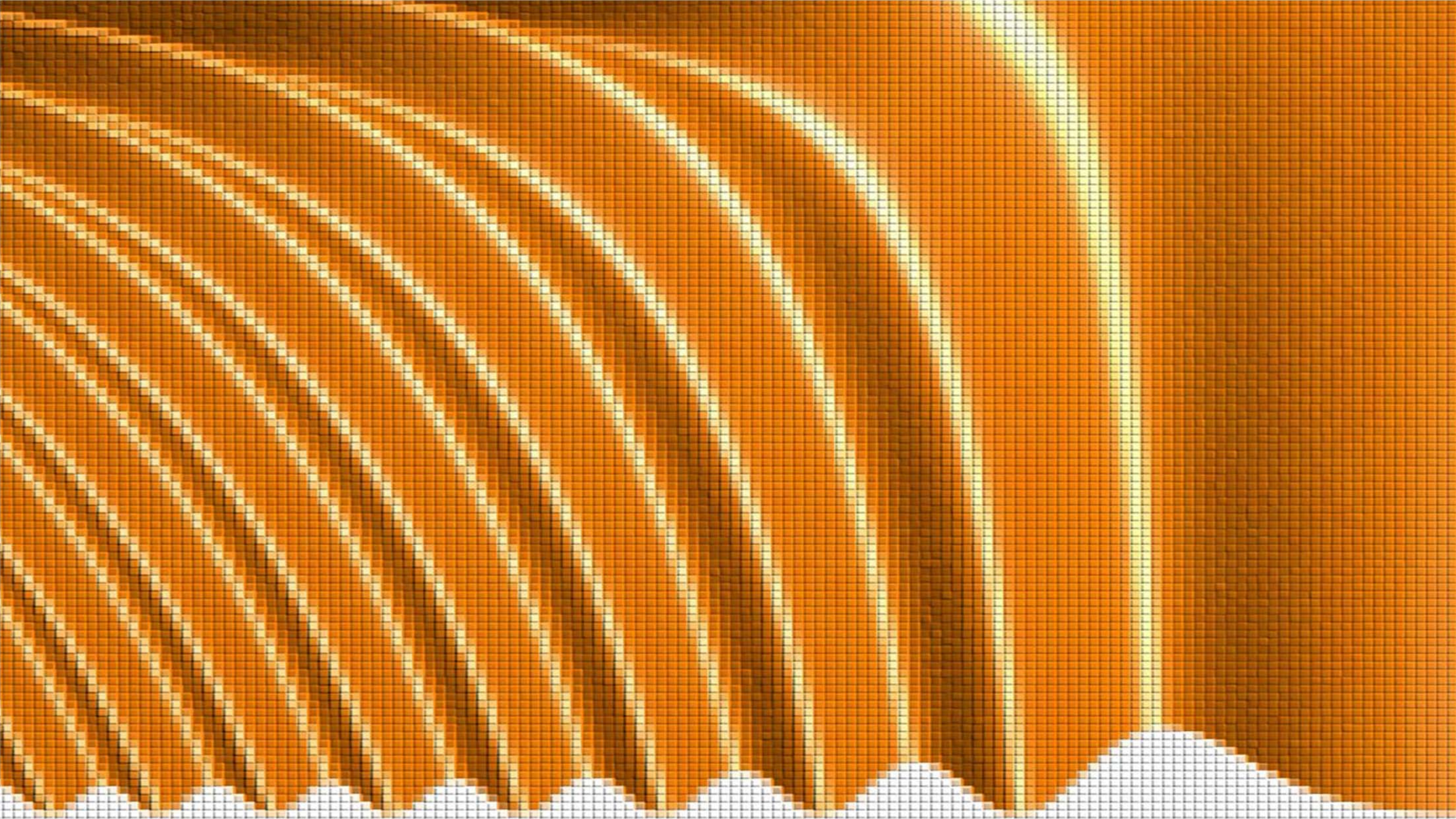
$\varepsilon = 0.663 \quad 2.603 \quad 5.609$

Solutions

These are the solutions for a well depth V_o of $8E_1^{\infty}$

- Note that
  - they are all
    - lower energies
  - than the corresponding solutions for the infinitely deep well of the same width



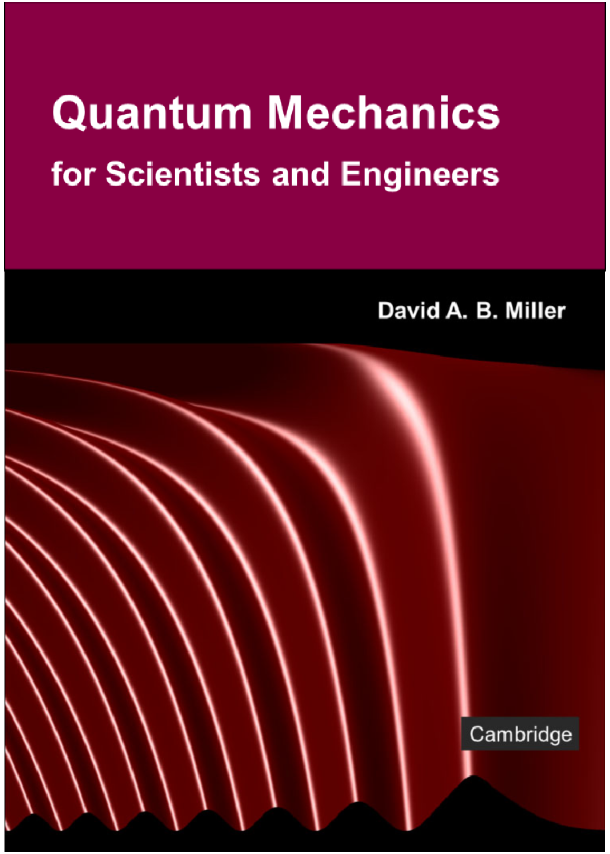


7 Finite well and harmonic oscillator

Slides: Lecture 7c The harmonic oscillator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.10



Particles in potential wells

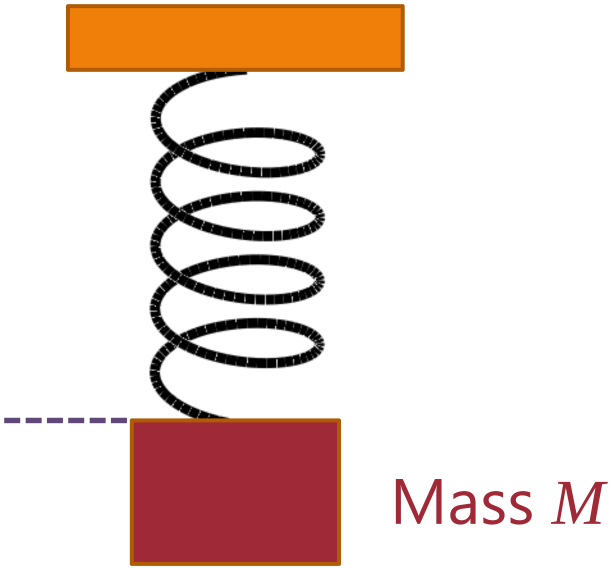
The harmonic oscillator

Quantum mechanics for scientists and engineers

David Miller

Mass on a spring

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

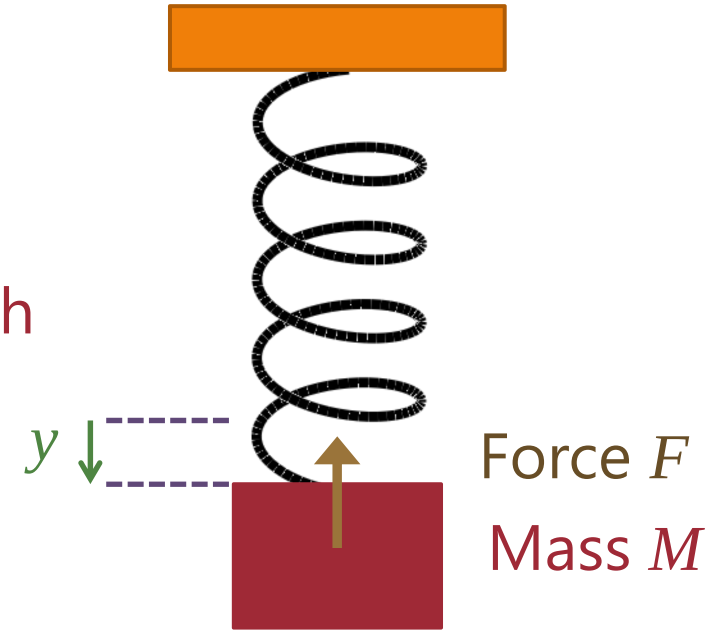
For some "spring constant" K

$$F = -Ky$$

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

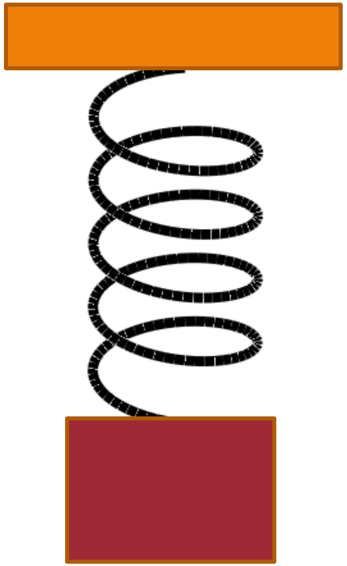
$$F = Ma = M\frac{d^2y}{dt^2} = -Ky$$

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

where we define $\omega^2 = K/M$

we have oscillatory solutions of angular frequency $\omega = \sqrt{K/M}$

e.g., $$y \propto \sin \omega t$$



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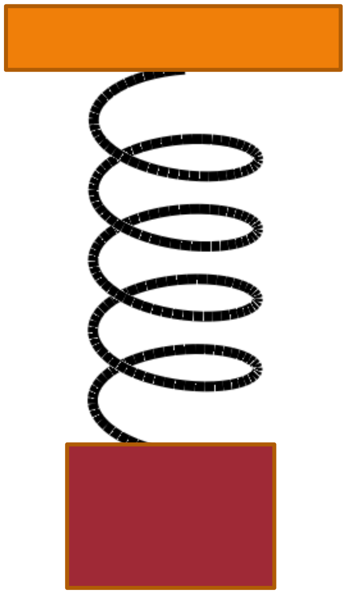
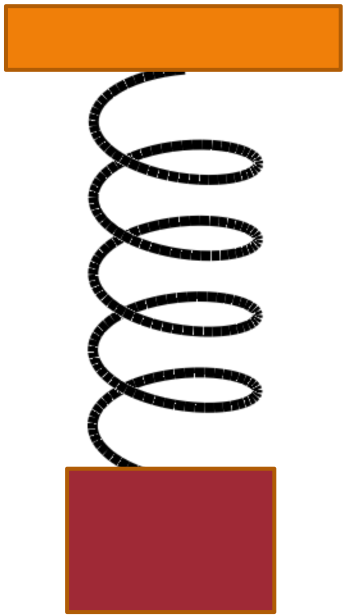


Mass on a spring



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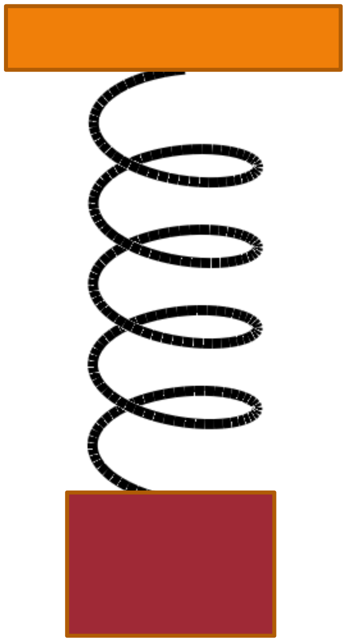

Mass on a spring

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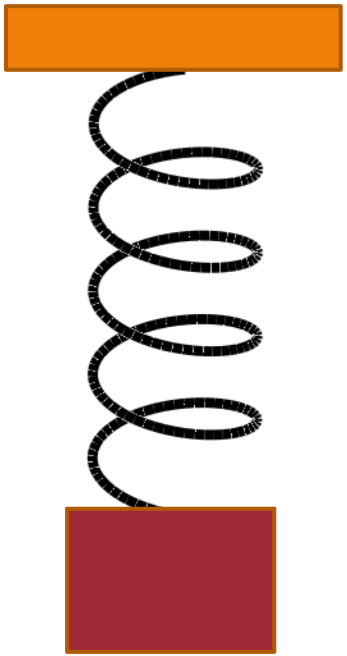

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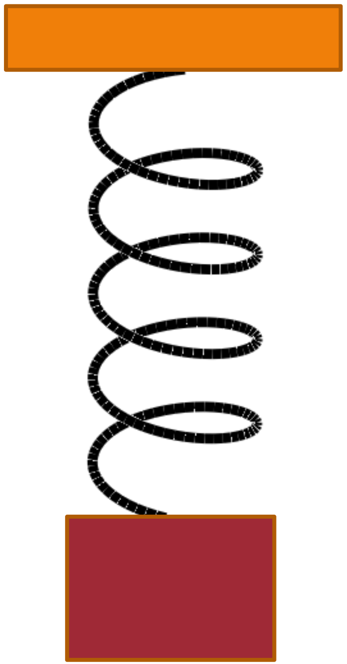
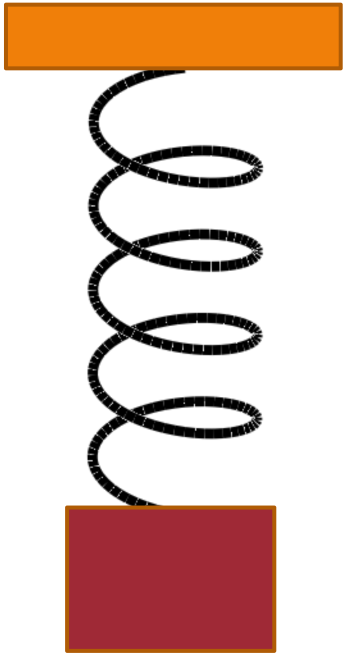


Mass on a spring



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

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

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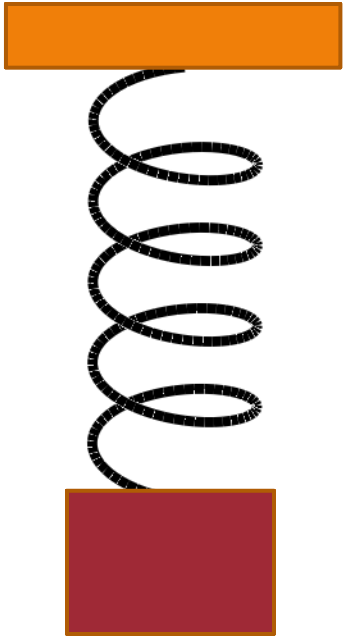
we have oscillatory solutions of angular frequency $\omega = \sqrt{K/M}$

e.g., $$y \propto \sin \omega t$$



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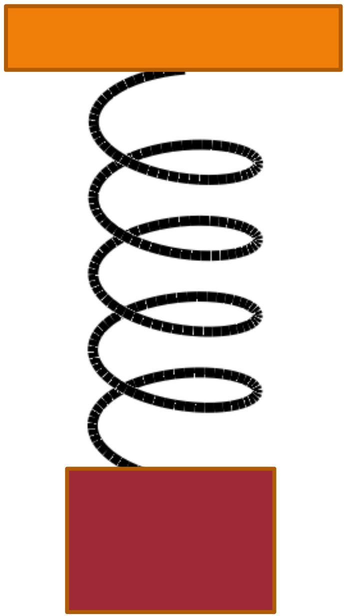

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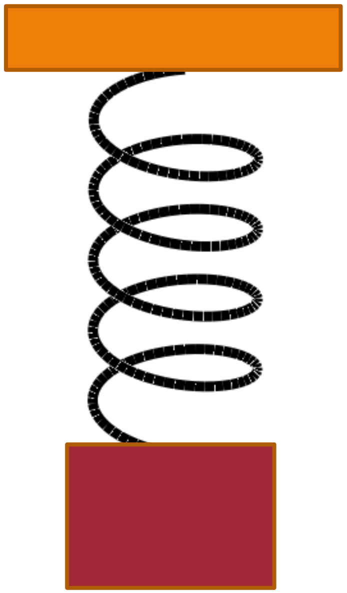

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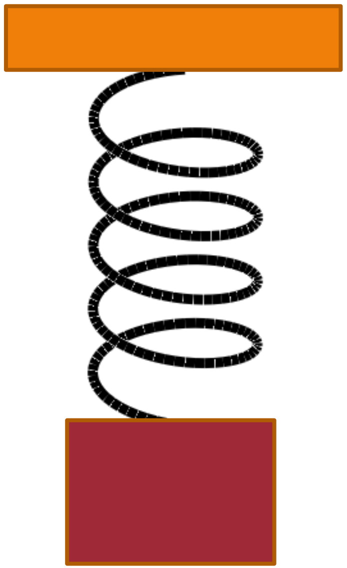

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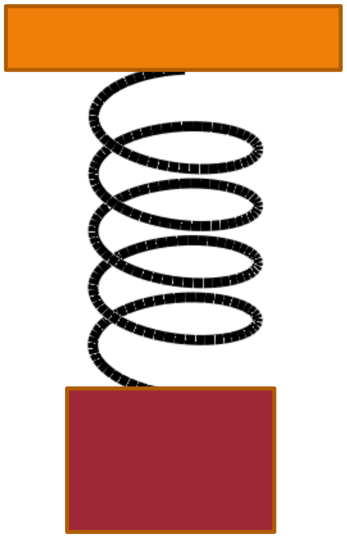

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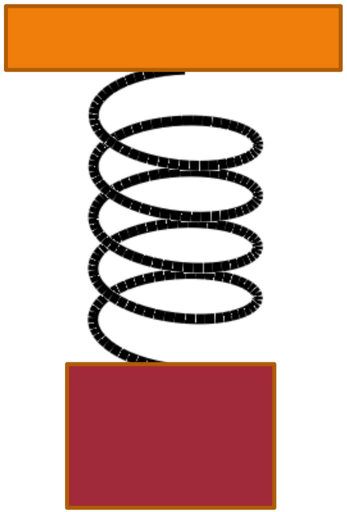

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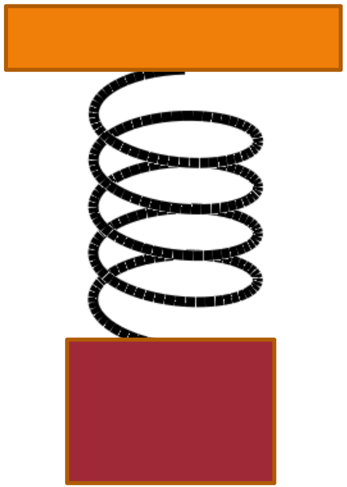

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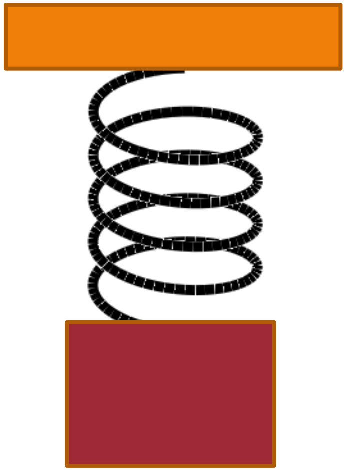

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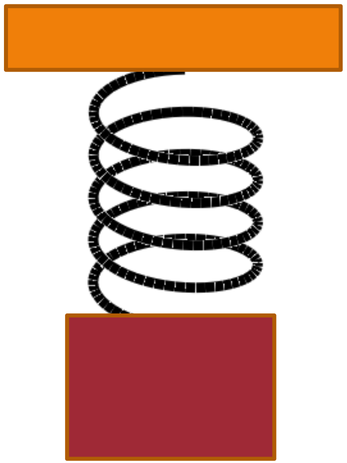

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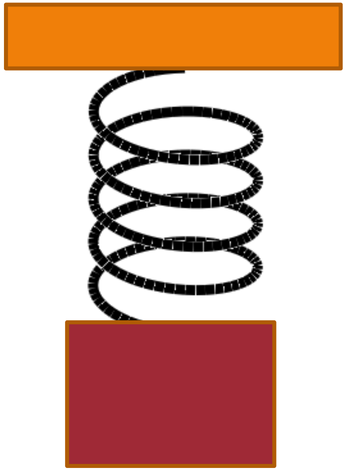

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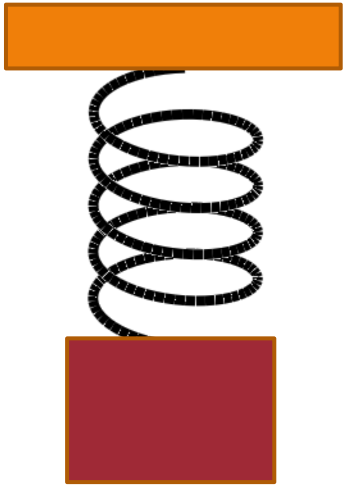

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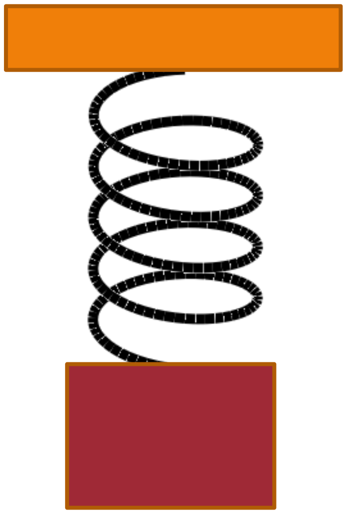

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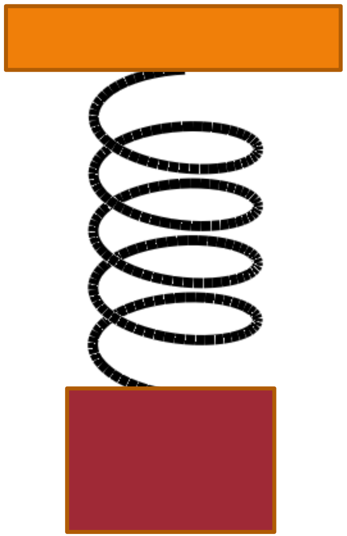

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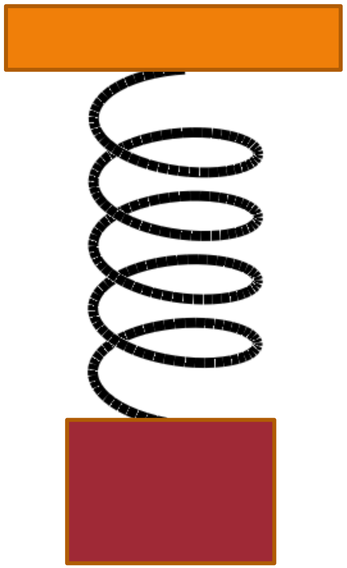
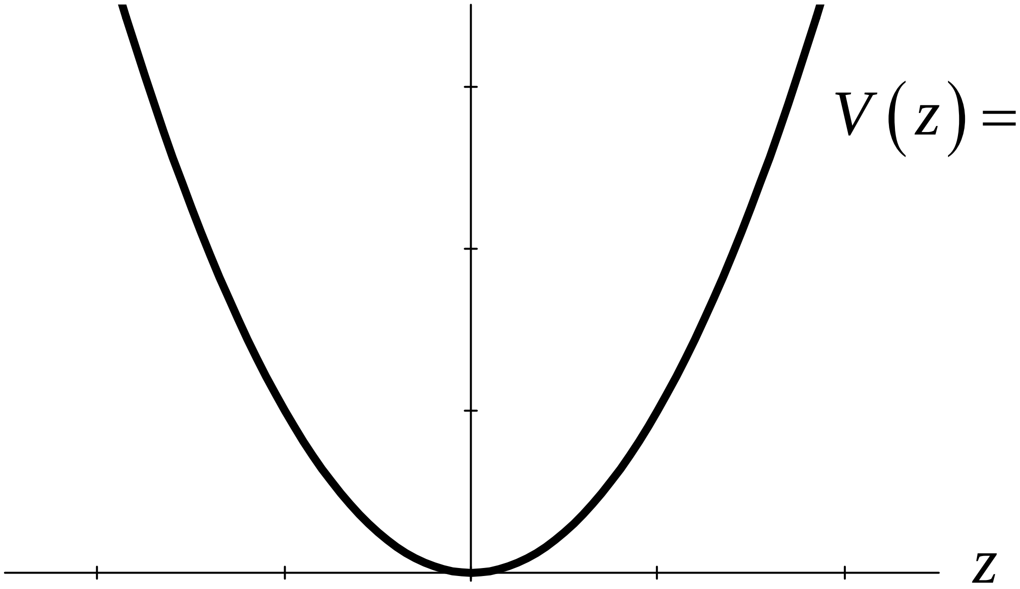
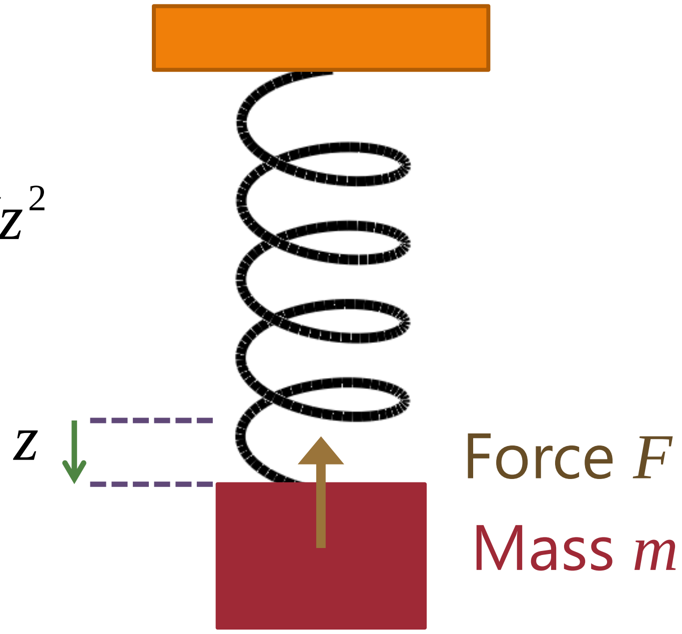


Potential energy



$$V(z) = \frac{1}{2}Kz^2$$



The potential from the restoring force F is

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

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

$$\psi_n(\xi) = A_n \exp\left(-\xi^2/2\right) H_n(\xi)$$

where $H_n(\xi)$ is some set of functions still to be determined

Harmonic oscillator Schrödinger equation

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

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

$$\frac{2E}{\hbar\omega} - 1 = 2n \qquad n = 0, 1, 2, \ldots$$

that is,

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

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

Harmonic oscillator Schrödinger equation

The allowed energy levels are equally spaced

separated by an amount $\hbar\omega$

where ω 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

Note they are either

- 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

$$H_0 = 1$$

$$H_1(\xi) = 2\xi$$

$$H_2(\xi) = 4\xi^2 - 2$$

$$H_3(\xi) = 8\xi^3 - 12\xi$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

Harmonic oscillator solutions

Normalizing

$$\psi_n(\xi) = A_n \exp\left(-\xi^2/2\right) H_n(\xi)$$

gives

$$A_n = \sqrt{\frac{1}{\sqrt{\pi}\, 2^n n!}} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}} z$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

Harmonic oscillator solutions

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$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

or

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

Harmonic oscillator eigensolutions

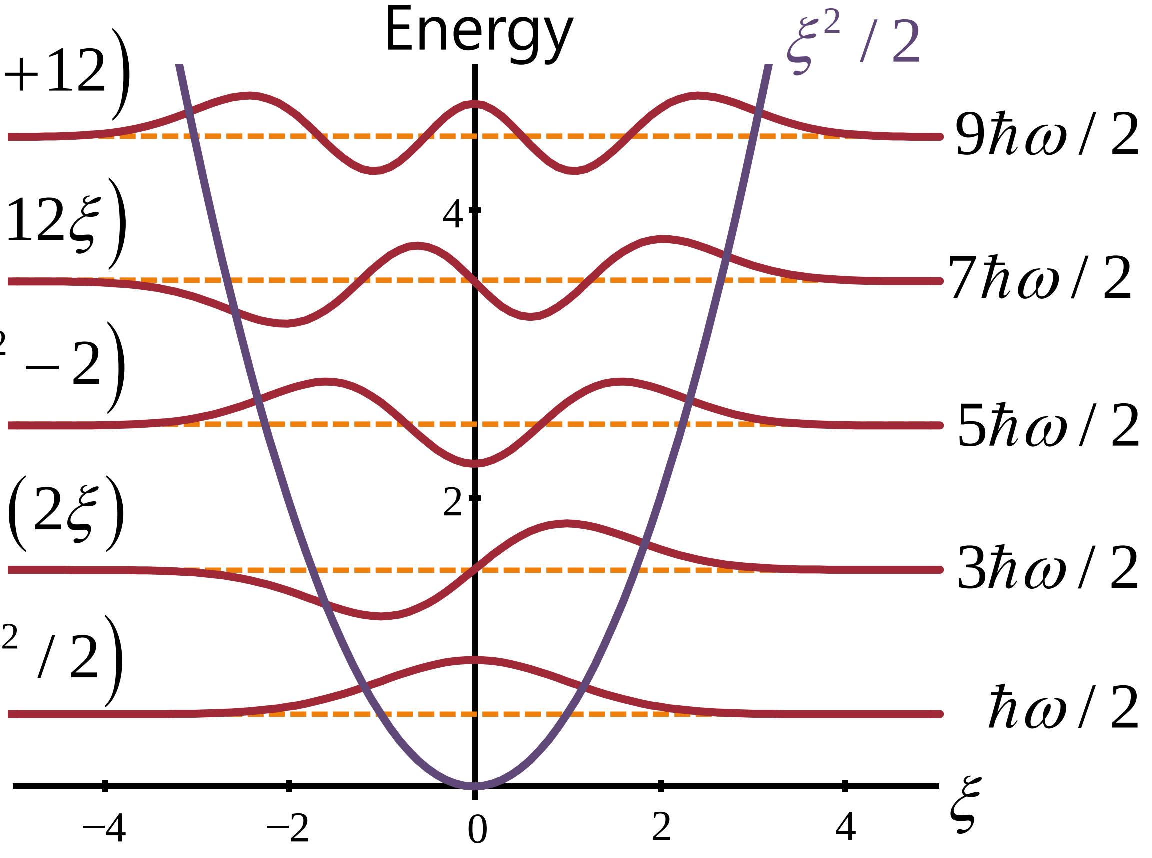
$$A_4 \exp\left(-\xi^2/2\right)\left(16\xi^4 - 48\xi^2 + 12\right)$$

$$A_3 \exp\left(-\xi^2/2\right)\left(8\xi^3 - 12\xi\right)$$

$$A_2 \exp\left(-\xi^2/2\right)\left(4\xi^2 - 2\right)$$

$$A_1 \exp\left(-\xi^2/2\right)\left(2\xi\right)$$

$$A_0 \exp\left(-\xi^2/2\right)$$



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