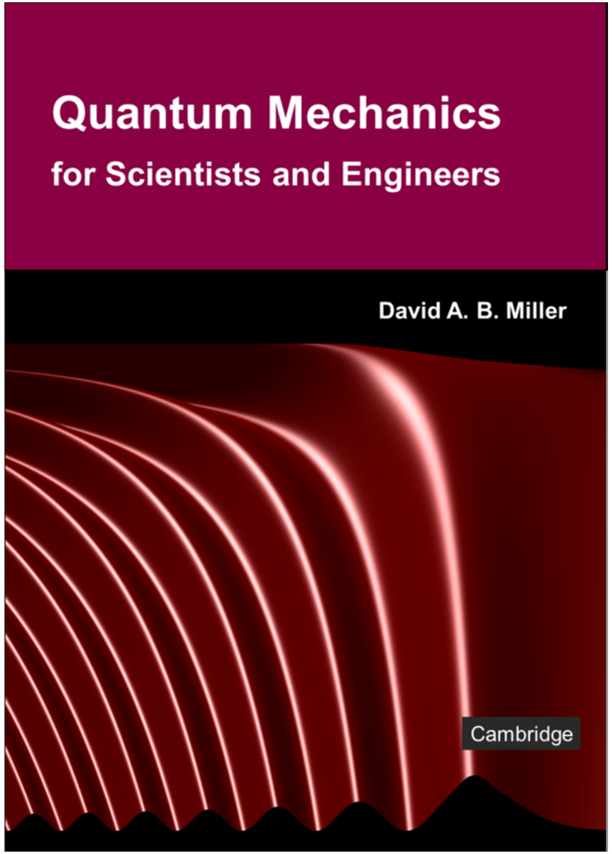
3.2 Finite well and harmonic oscillator

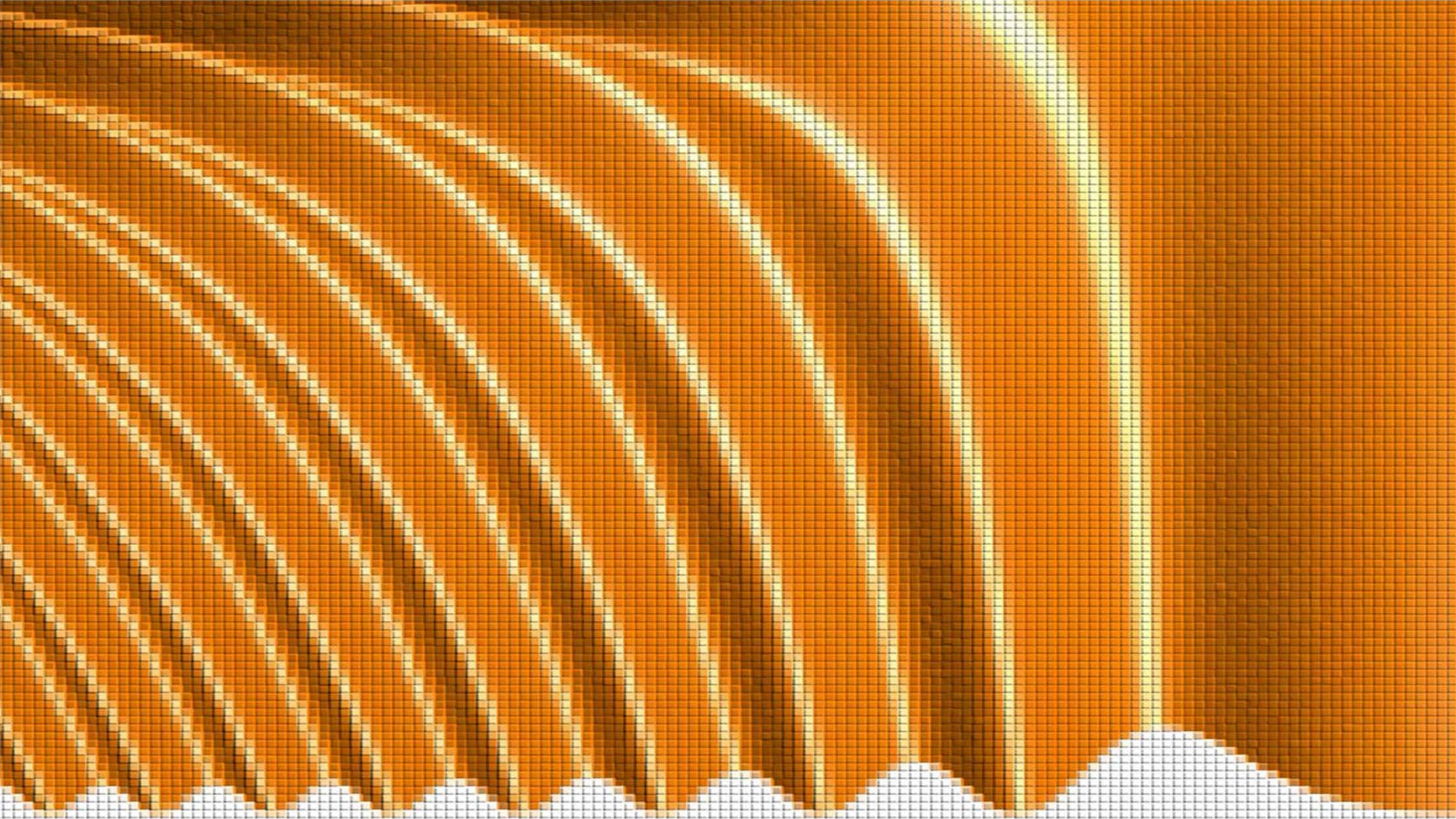
Slides: Video 3.2.1 Particles in potential wells – introduction



Particles in potential wells

Quantum mechanics for scientists and engineers

David Miller

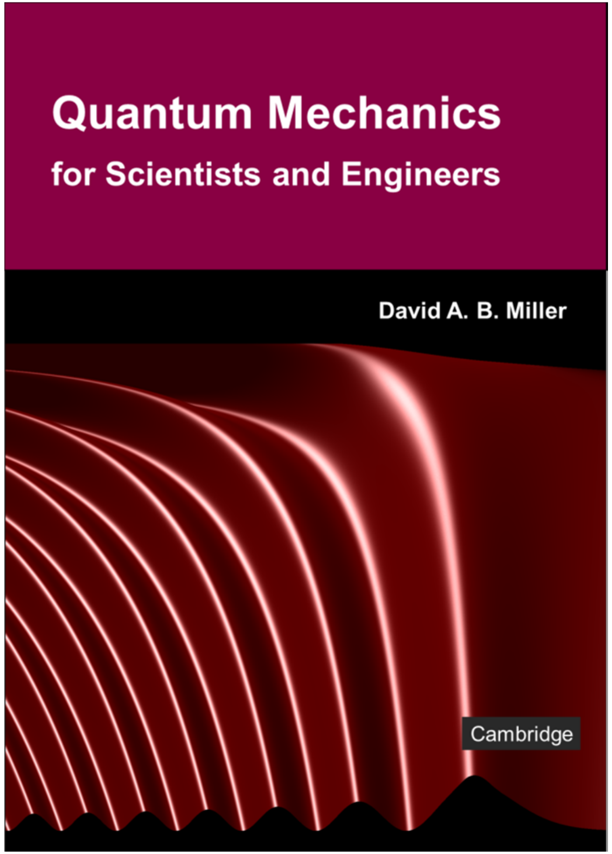


3.2 Finite well and harmonic oscillator

Slides: Video 3.2.2 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

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Finite potential well

Insert video here (split screen)

Lesson 7
Particles in potential wells

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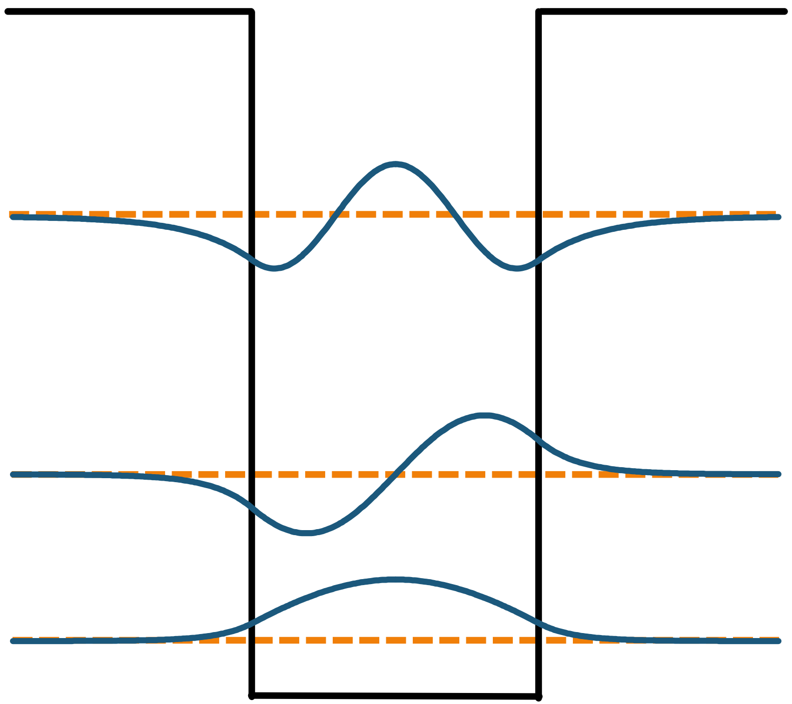


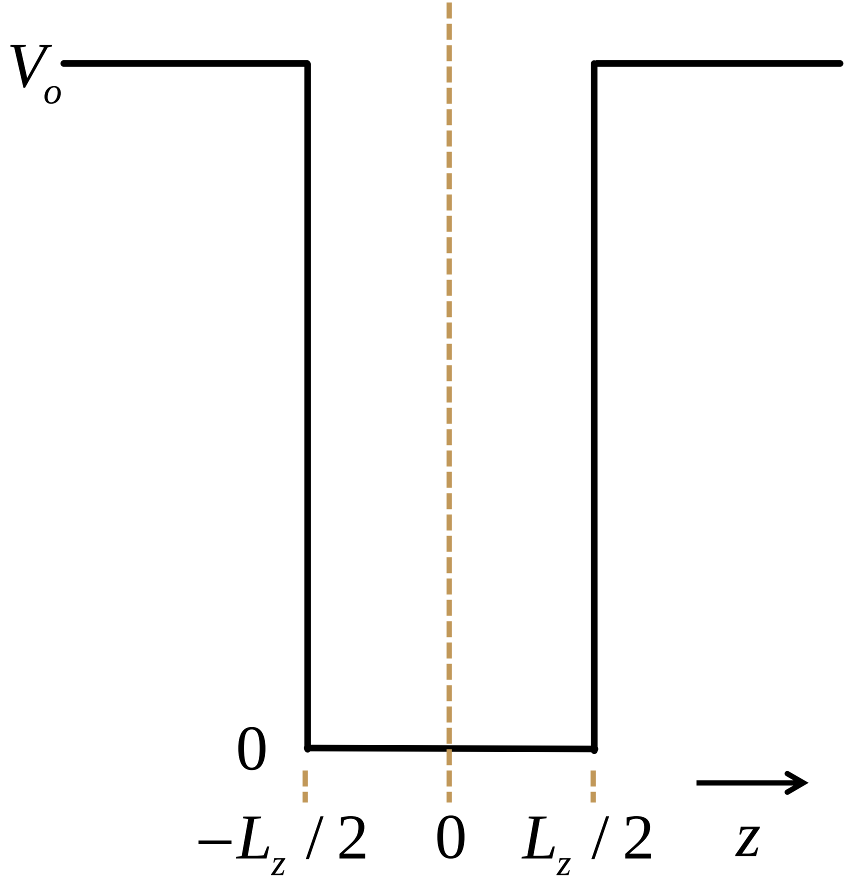
Particle in a finite potential well

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



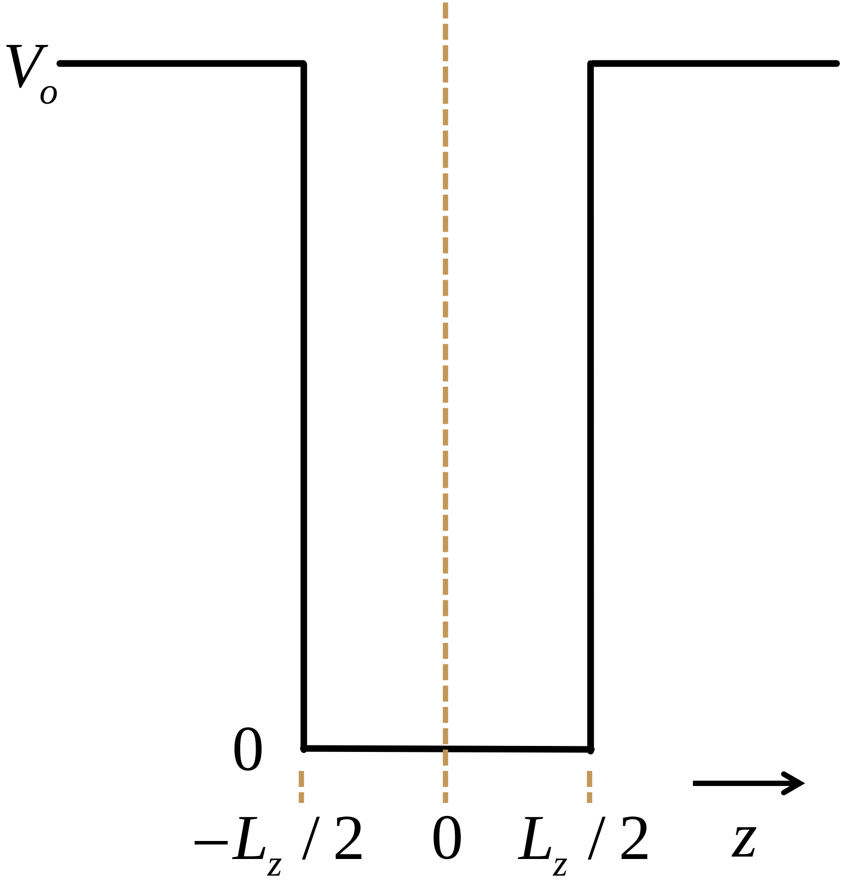
Particle in a finite potential well

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 $z < -L_z/2$

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

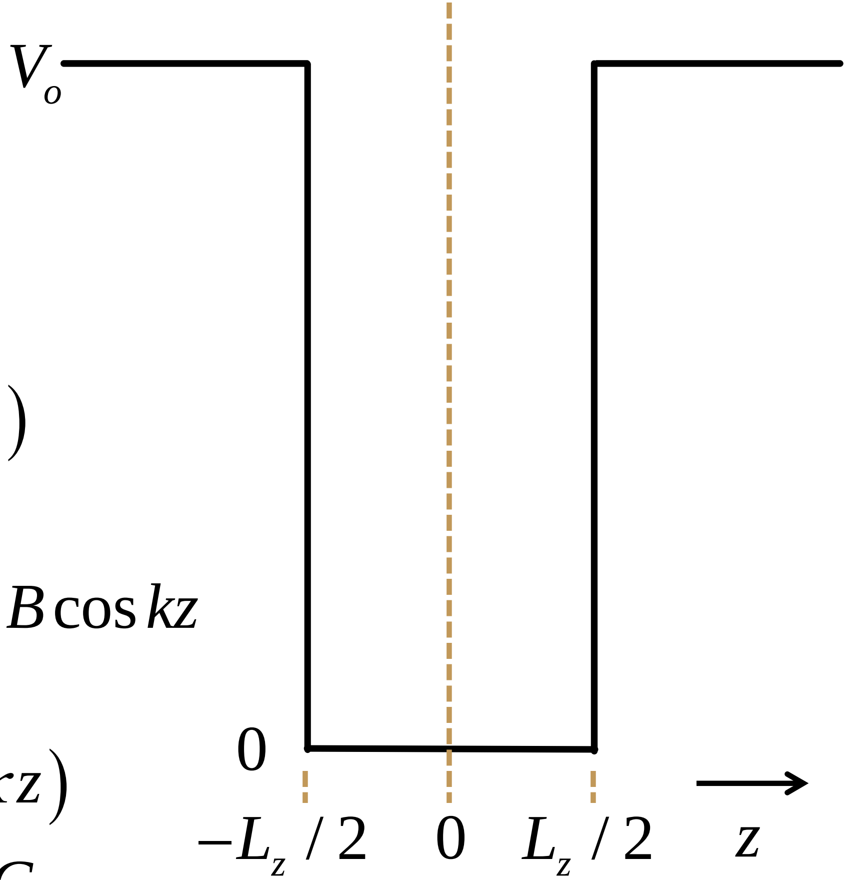
for $-L_z/2 < z < L_z/2$

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

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

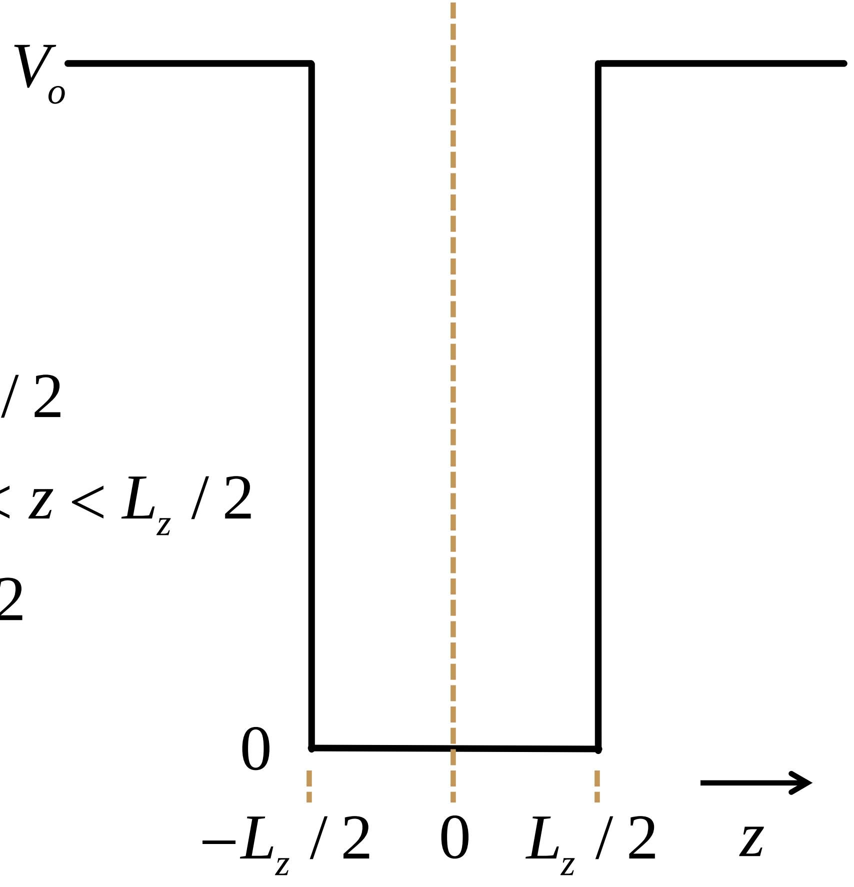
$$\psi(z) = G\exp(\kappa z) \qquad z < -L_z/2$$

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

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

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 $z = L_z / 2$

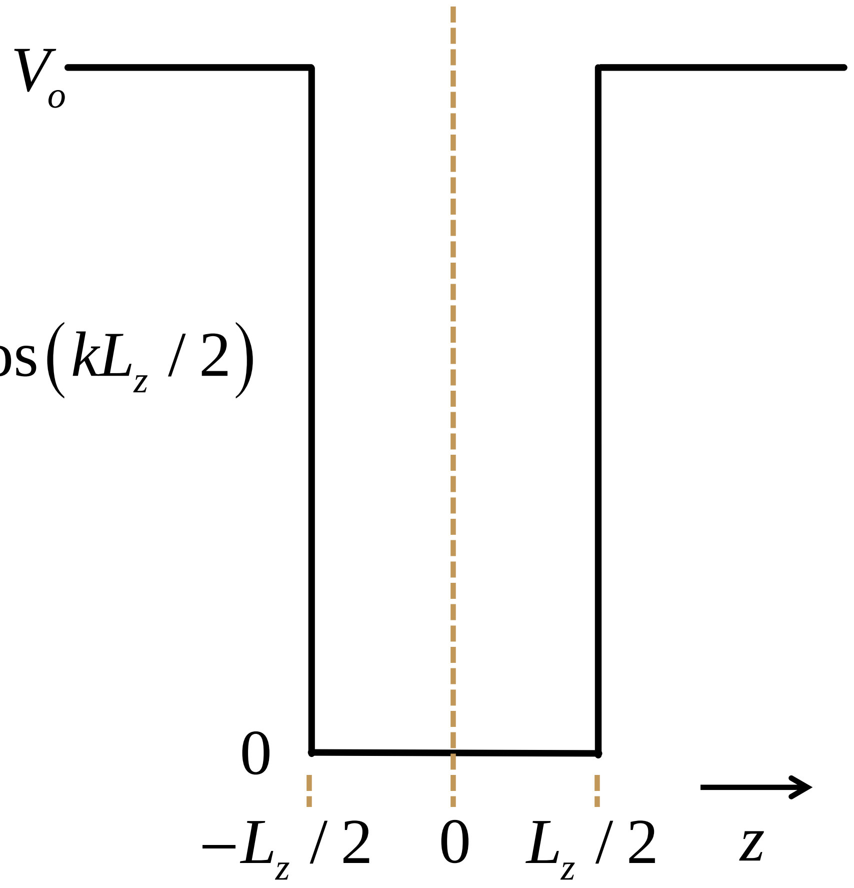
$$\psi\left(L_z / 2\right) = F \exp\left(-\kappa L_z / 2\right)$$
$$= A \sin\left(k L_z / 2\right) + B \cos\left(k L_z / 2\right)$$

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 $z = -L_z / 2$

$$GX_L = -AS_L + BC_L$$

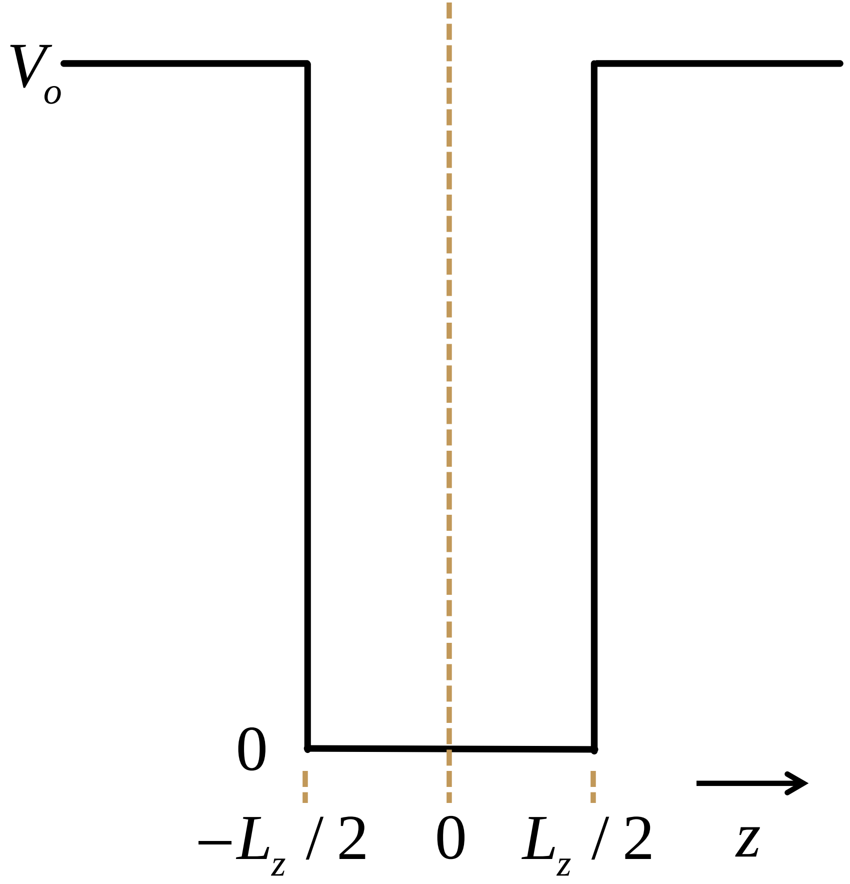
Continuity of the derivative gives

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

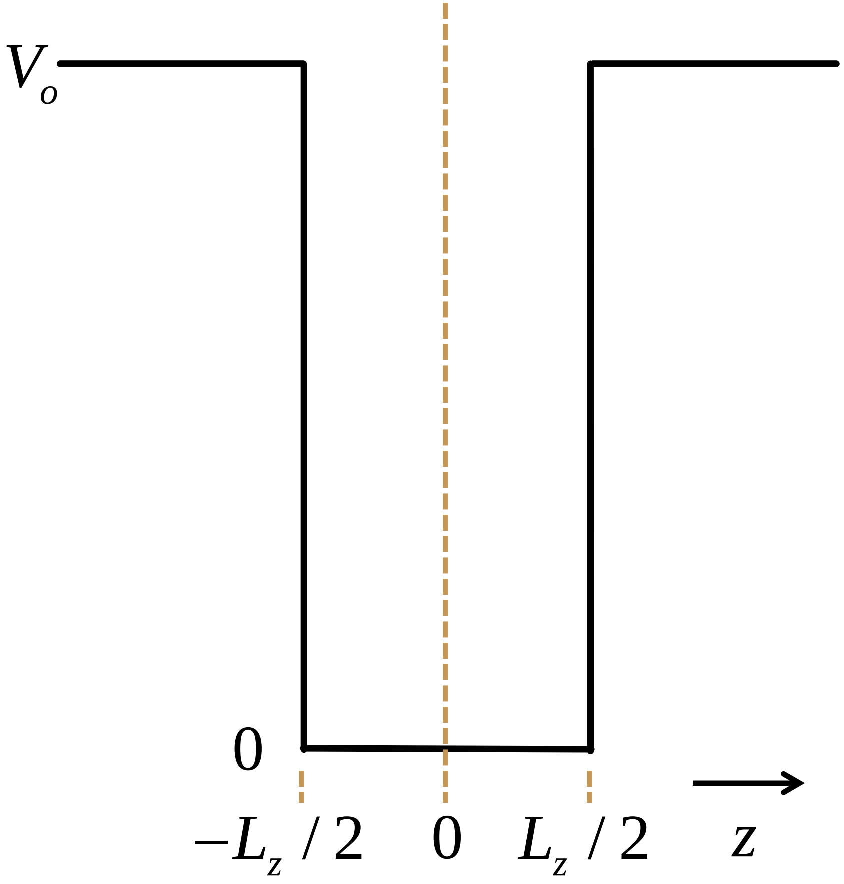
$$GX_L = -AS_L + BC_L$$

$$FX_L = AS_L + BC_L$$

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

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

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

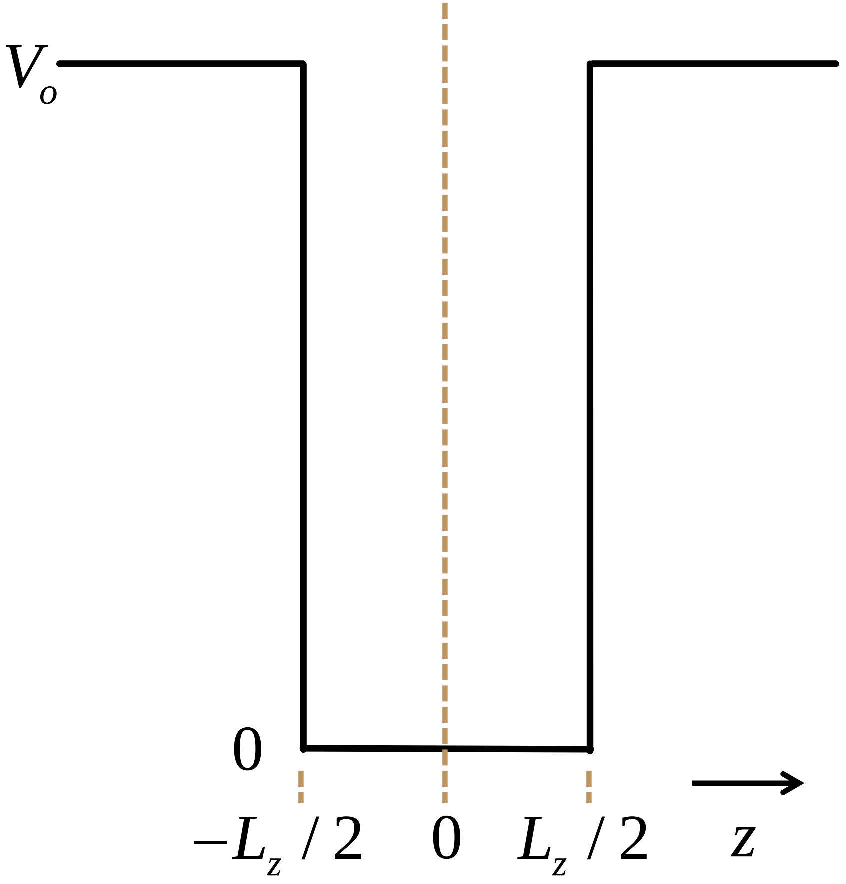
$$2BC_L = \left(F + G\right) X_L$$

Subtracting

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

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

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



Particle in a finite potential well

As long as $F \neq -G$

we can divide

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

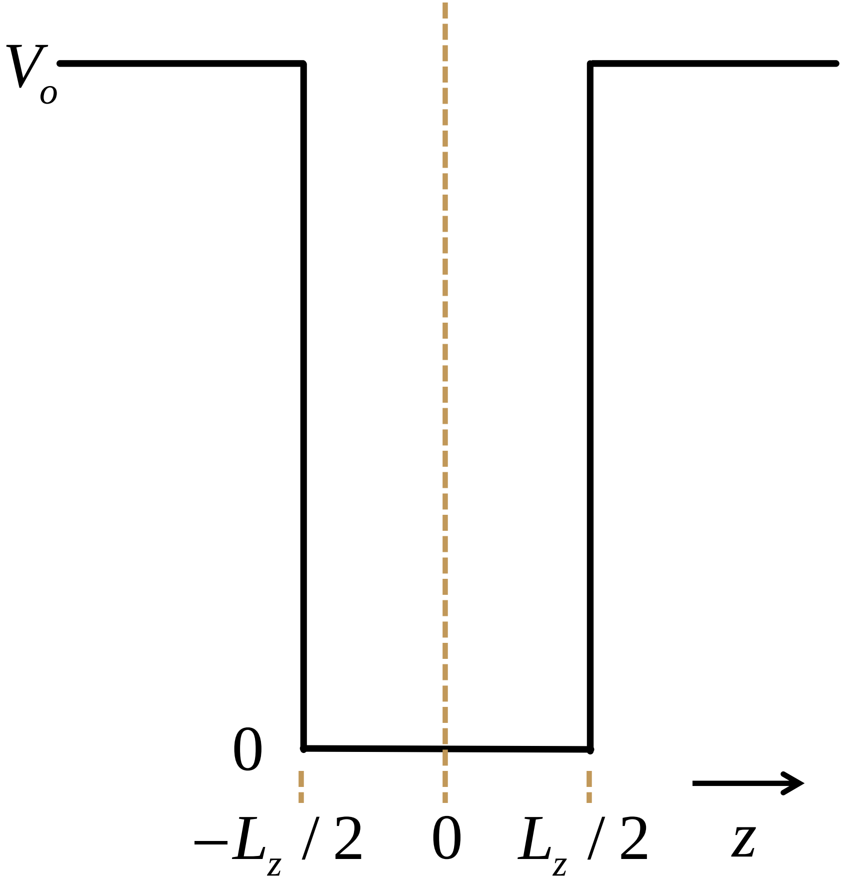
by

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

to obtain

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

This relation is effectively a condition for eigenvalues



Particle in a finite potential well

Subtracting $GX_L = -AS_L + BC_L$

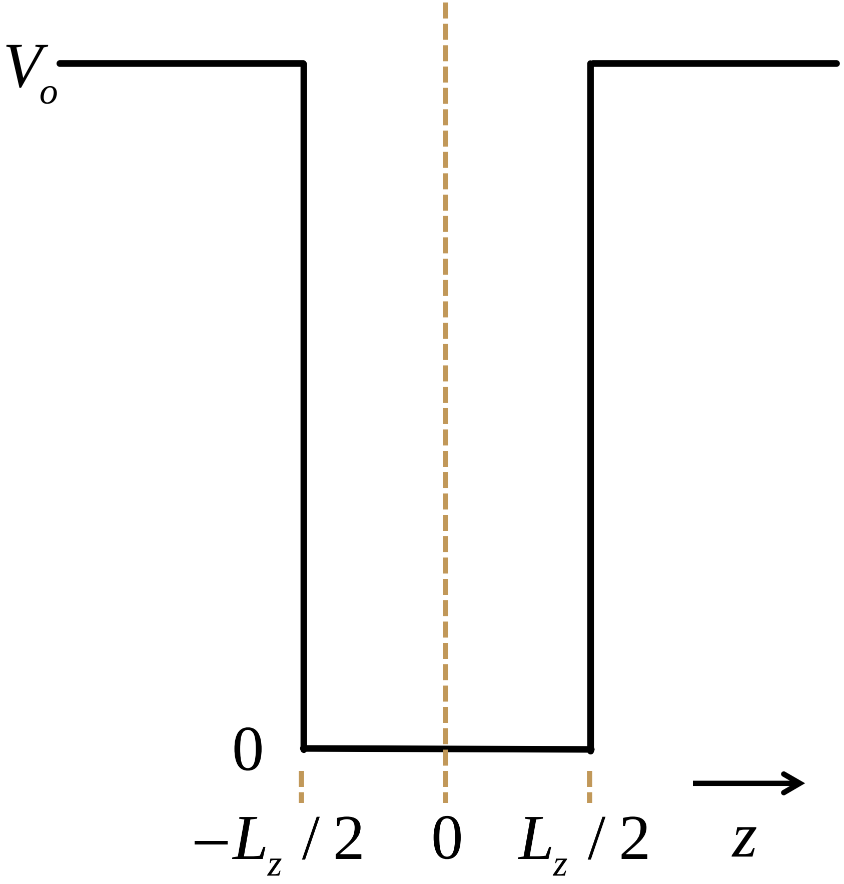
from $FX_L = AS_L + BC_L$

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

Adding $-\dfrac{\kappa}{k}FX_L = AC_L - BS_L$

and $\dfrac{\kappa}{k}GX_L = AC_L + BS_L$

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



Particle in a finite potential well

Similarly, as long as $F \neq G$

we can divide

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

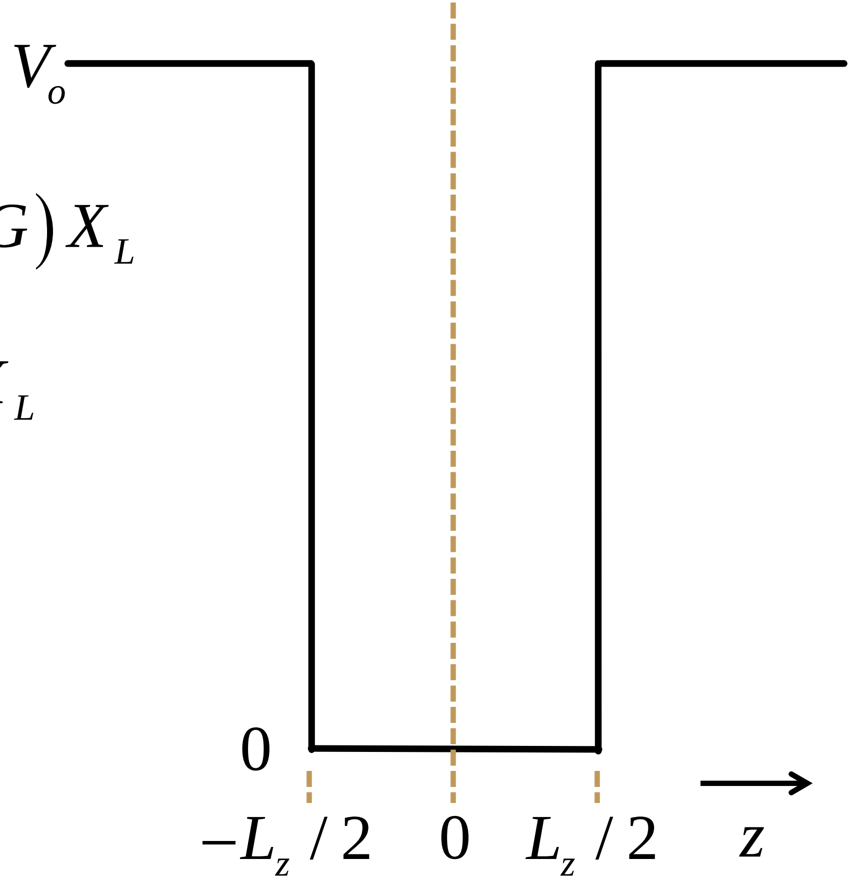
by

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

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 $F = -G$

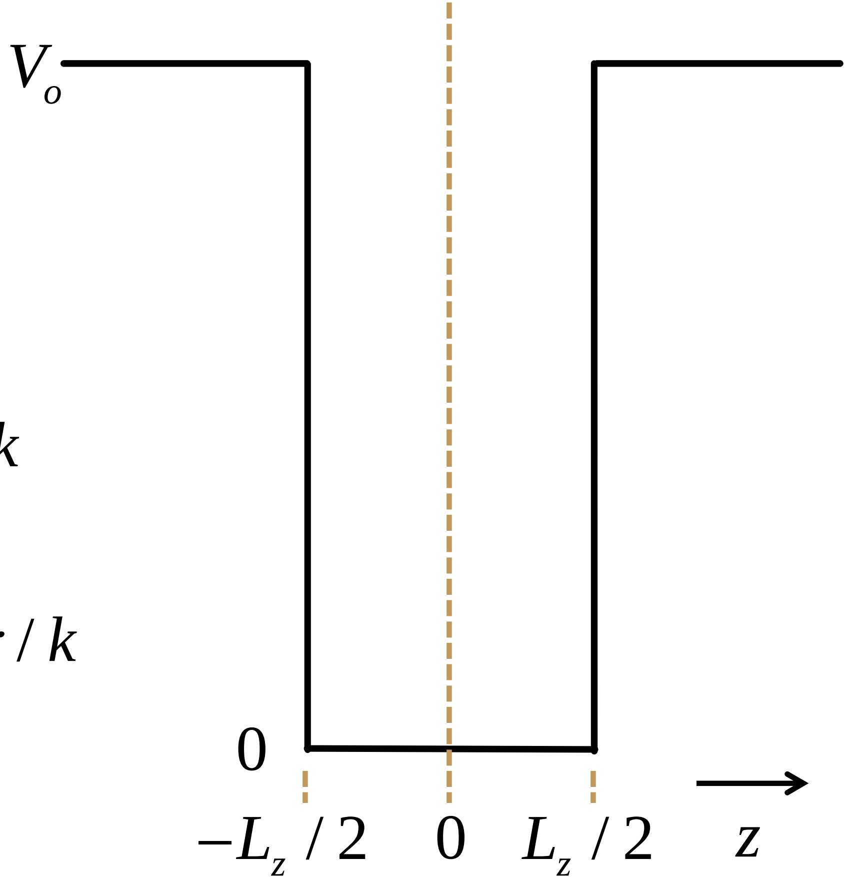
which leaves $-\cot(kL_z/2) = \kappa/k$

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

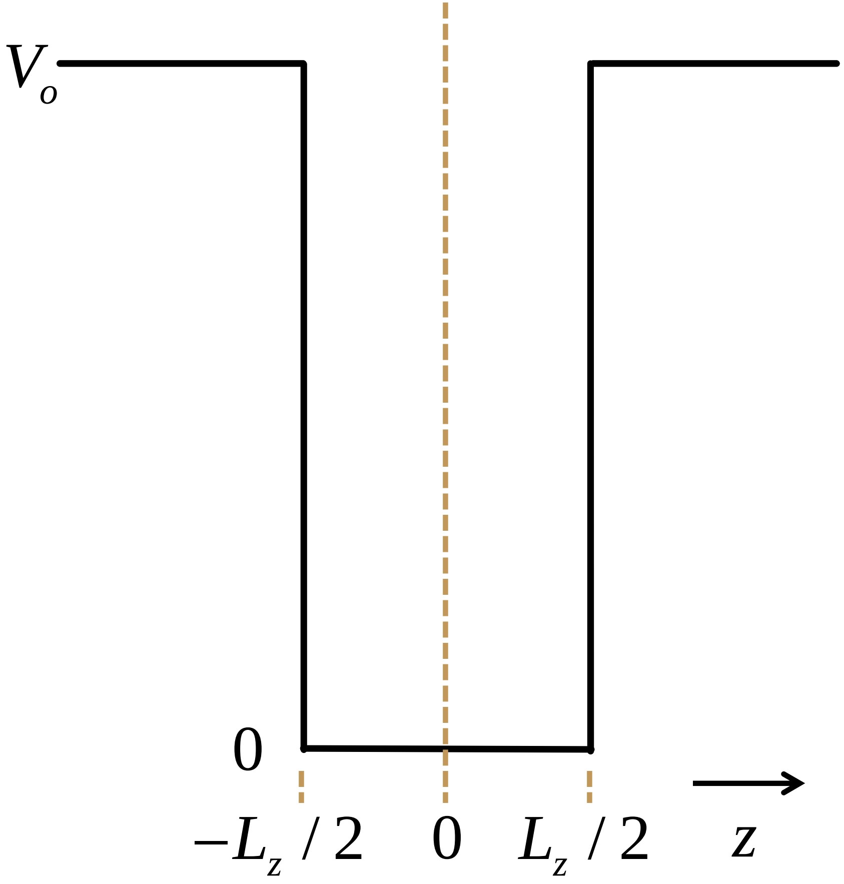
So the only possibilities are

1 - $F = G$

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

2 – $F = -G$

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



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

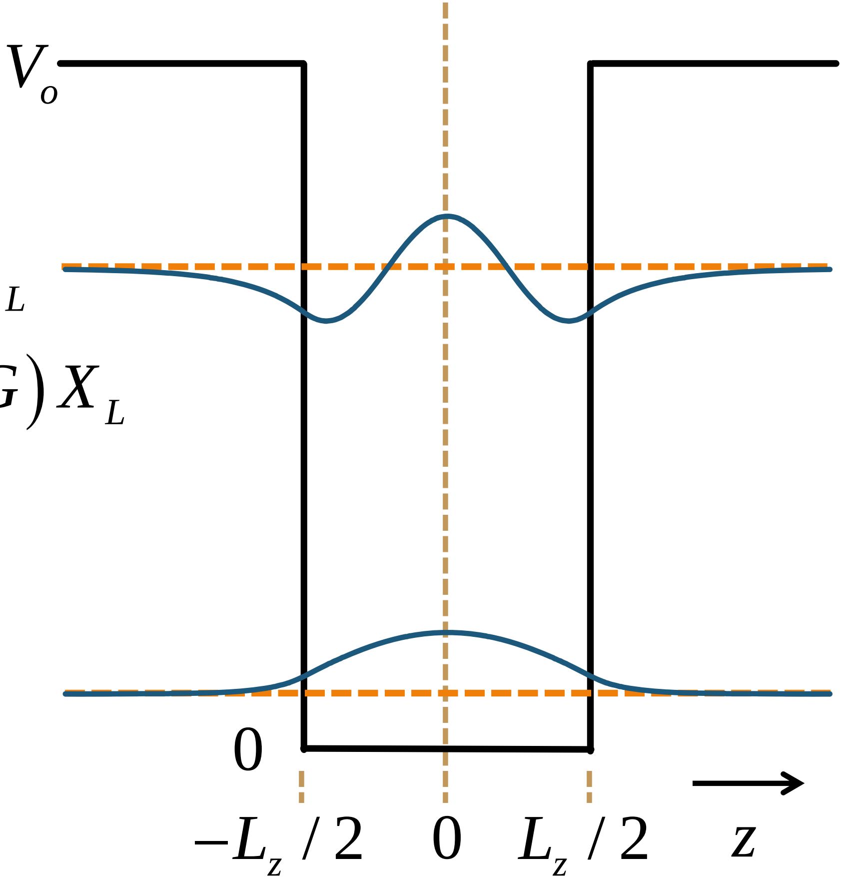
S_L and C_L cannot both be 0

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

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

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

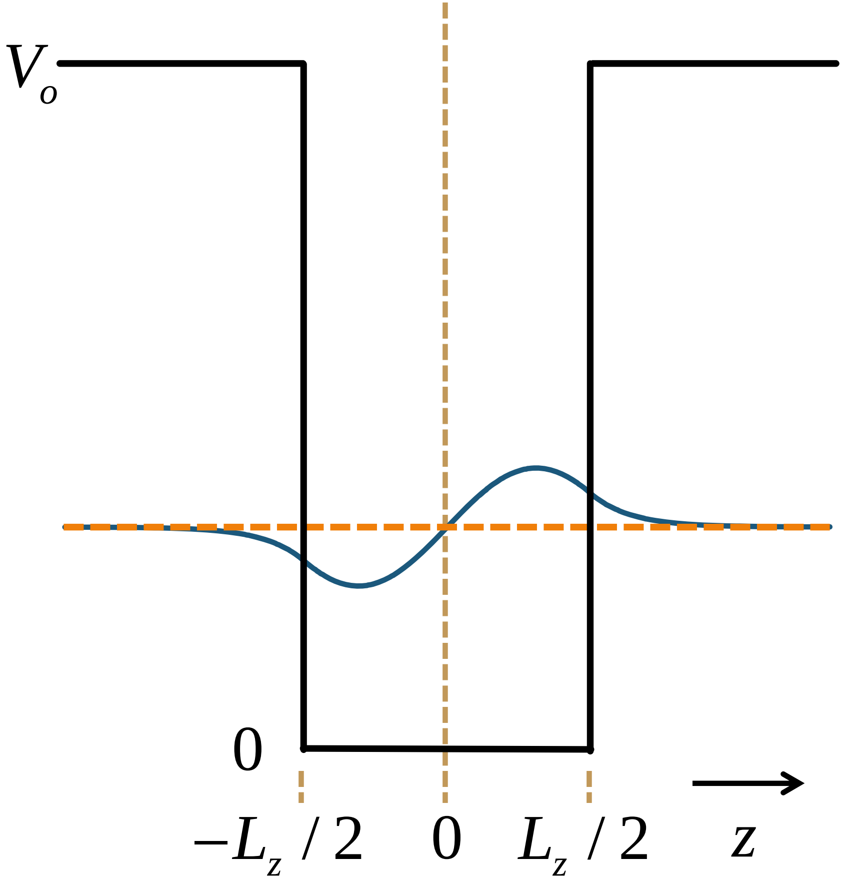
S_L and C_L cannot both be 0

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

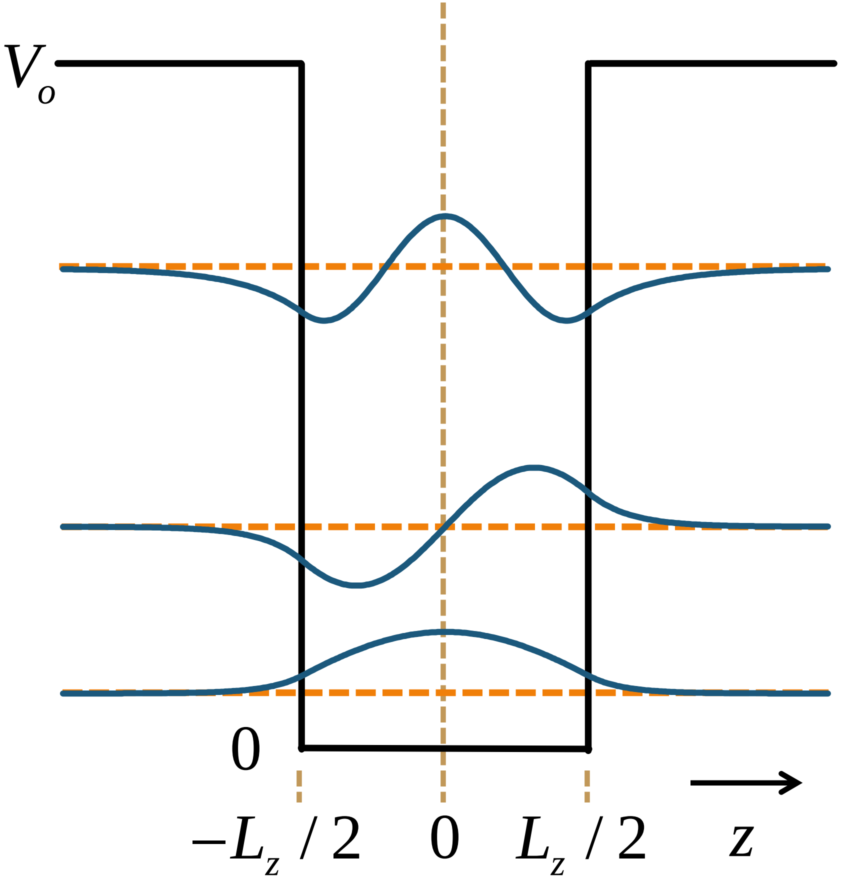
and hence for k and κ

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

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

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

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

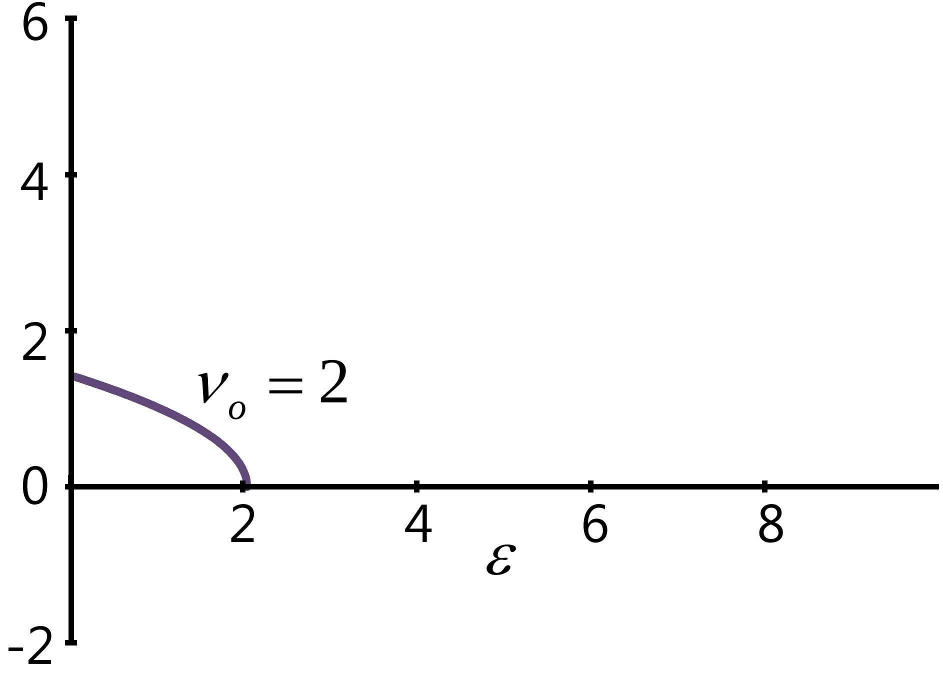
and $-\cot\left(kL_z/2\right) = \kappa/k$ becomes $-\cot\left[\left(\pi/2\right)\sqrt{\varepsilon}\right] = \sqrt{\left(v_o - \varepsilon\right)/\varepsilon}$

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

Graphical solution

Choose a specific well depth v_o and plot the curve

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



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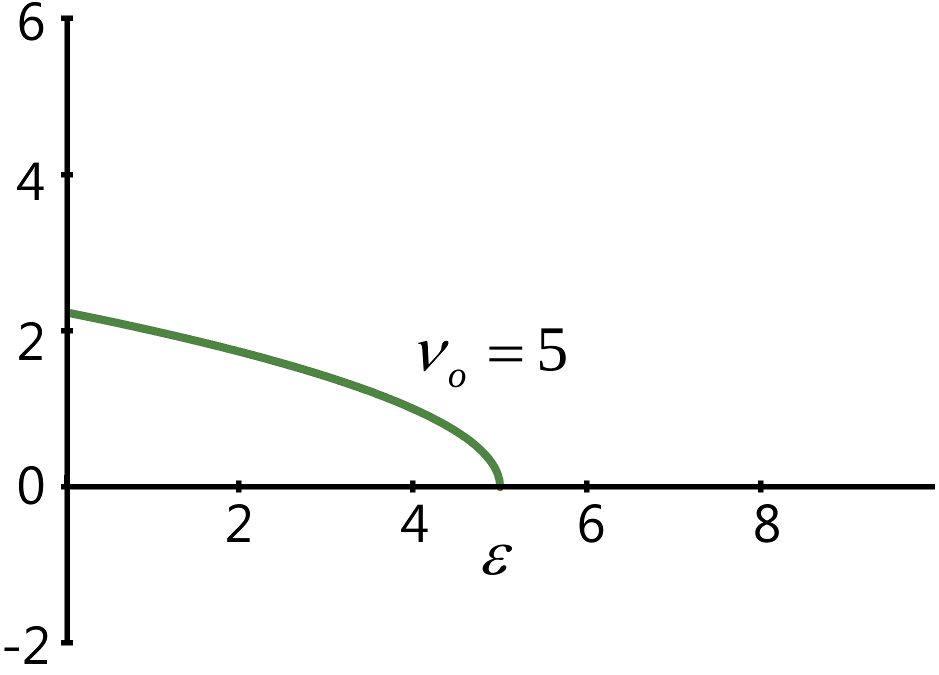

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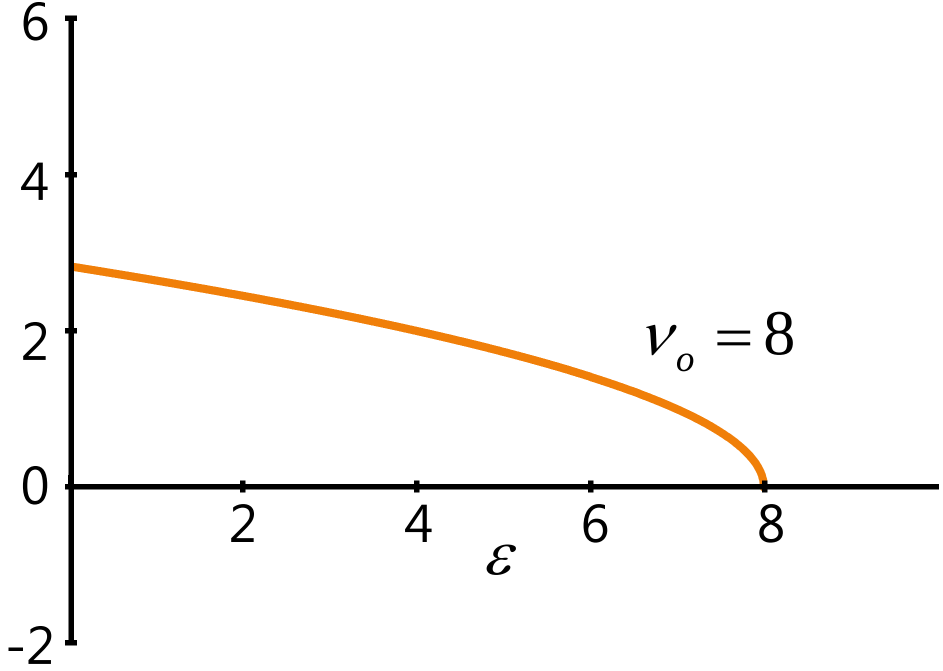


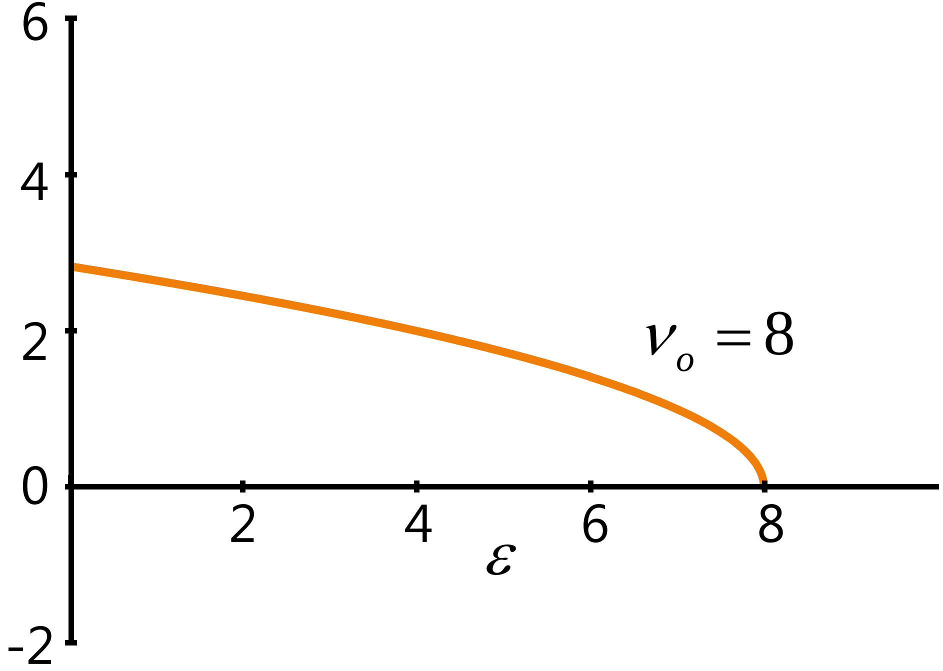
Graphical solution

Choose a specific well depth v_o

and plot the curve

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

Now add the curves



Graphical solution

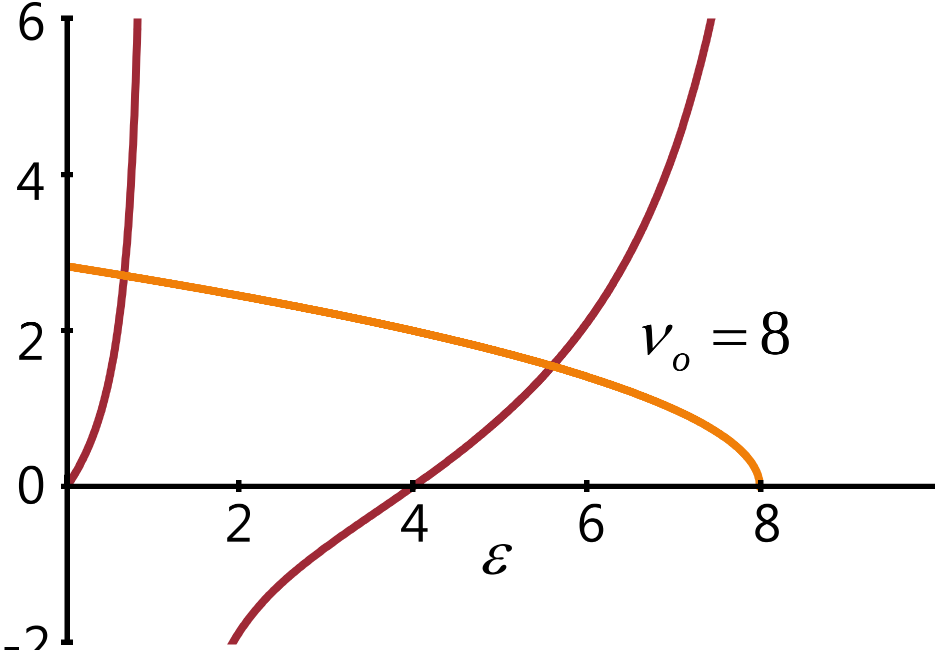
Choose a specific well depth v_o

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

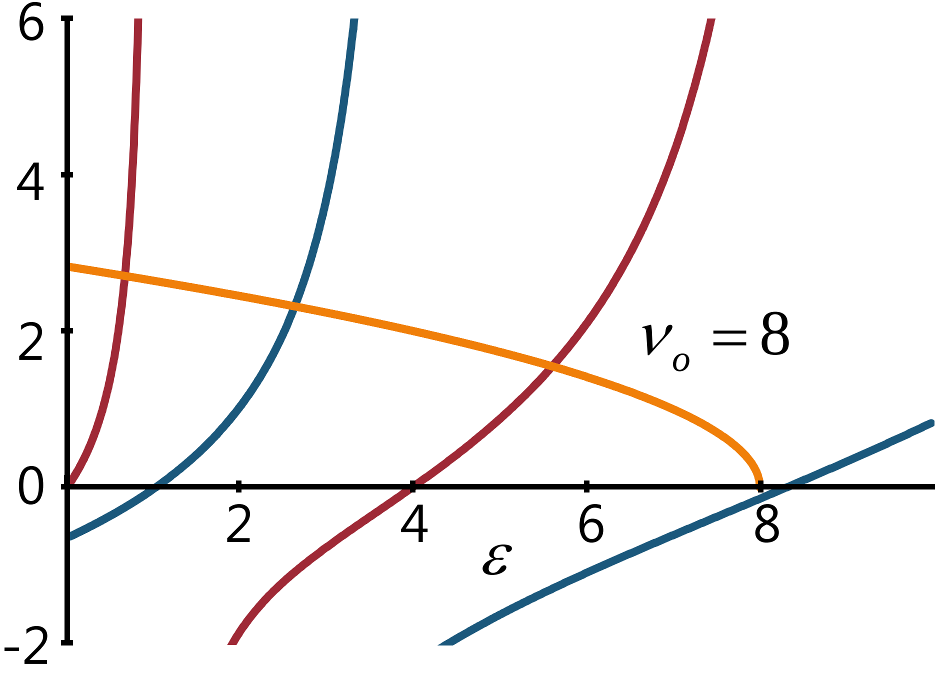
and plot the curve

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

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

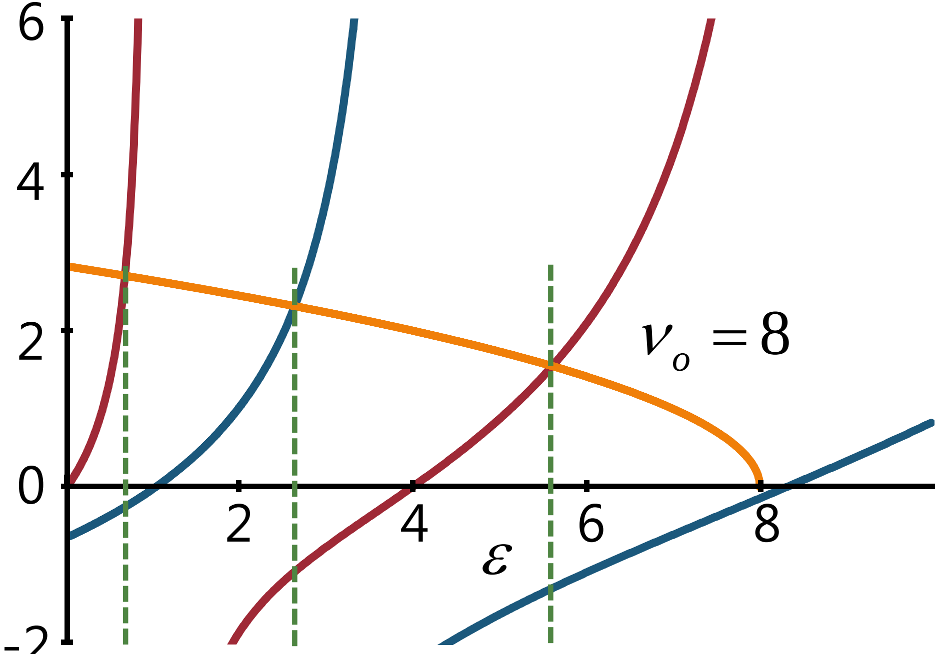
$$\sqrt{(v_o - \varepsilon)}$$

and

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

or

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



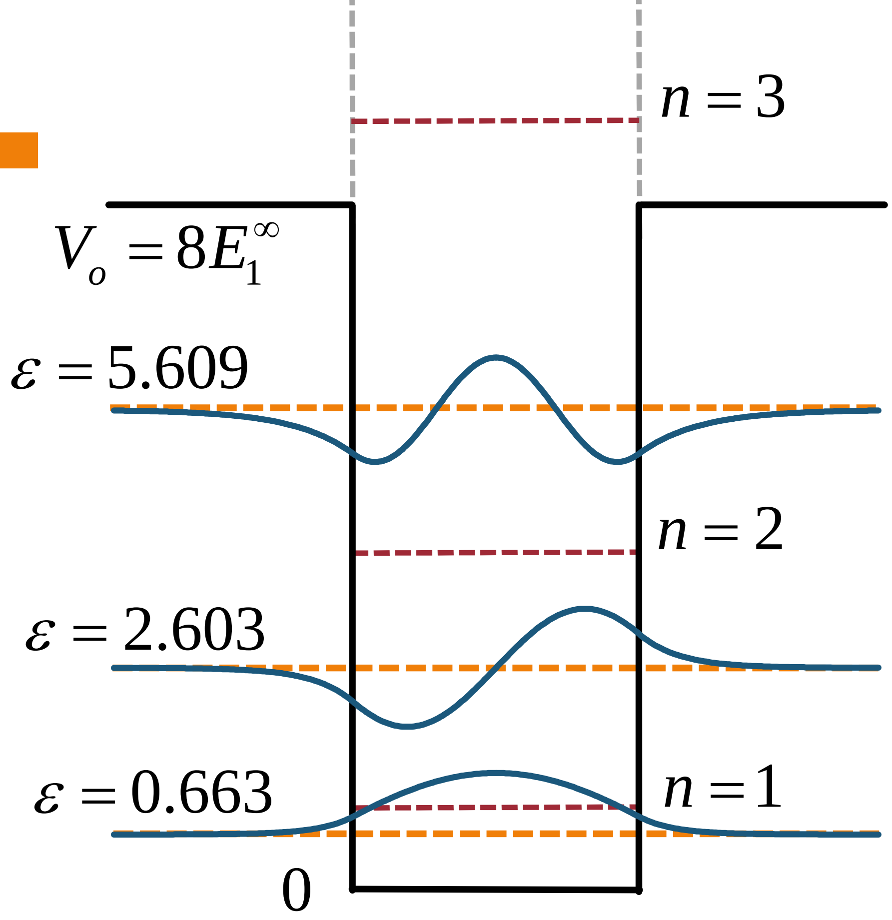
$\varepsilon = 0.663 \quad 2.603 \quad 5.609$

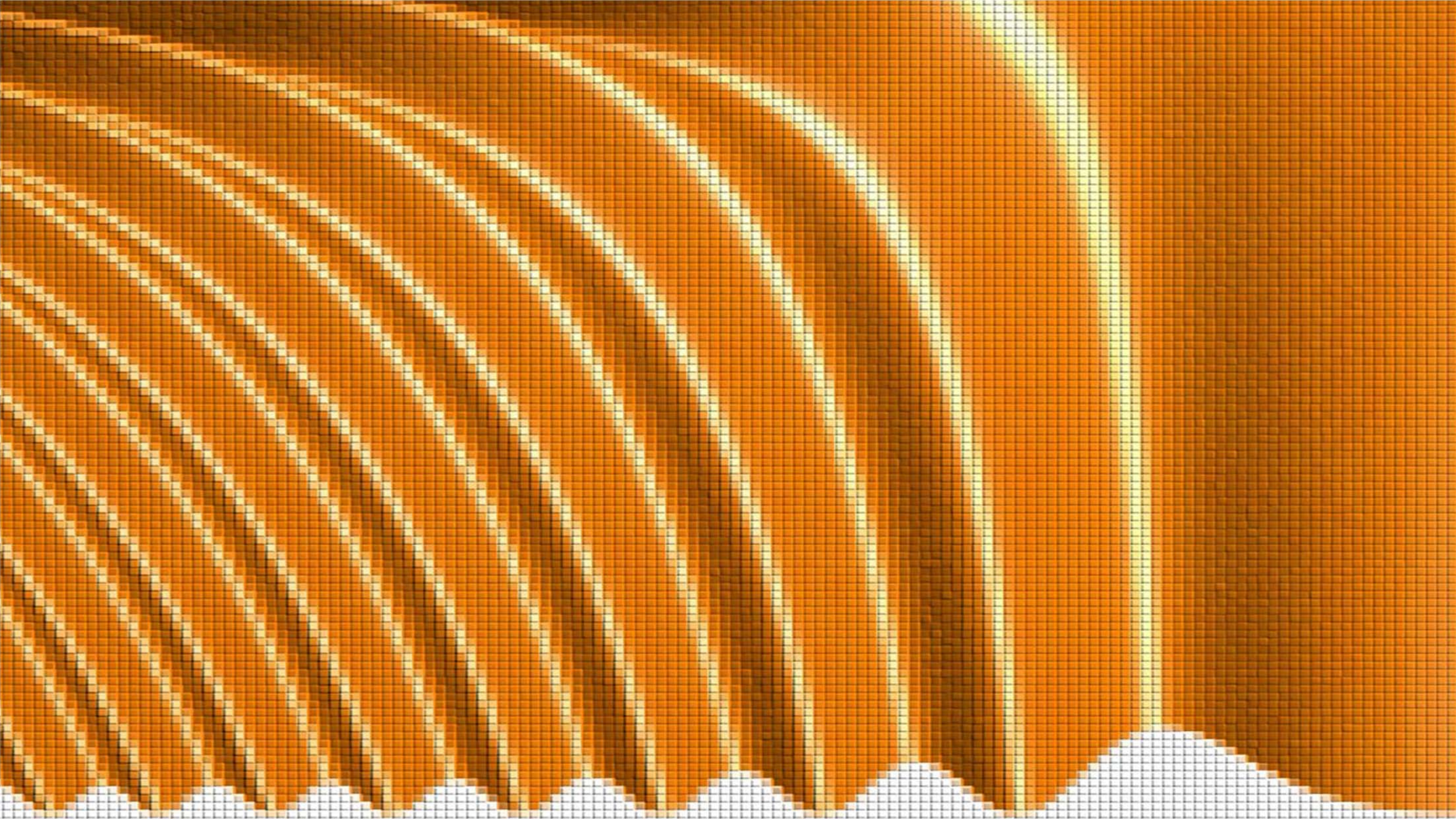
Solutions

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



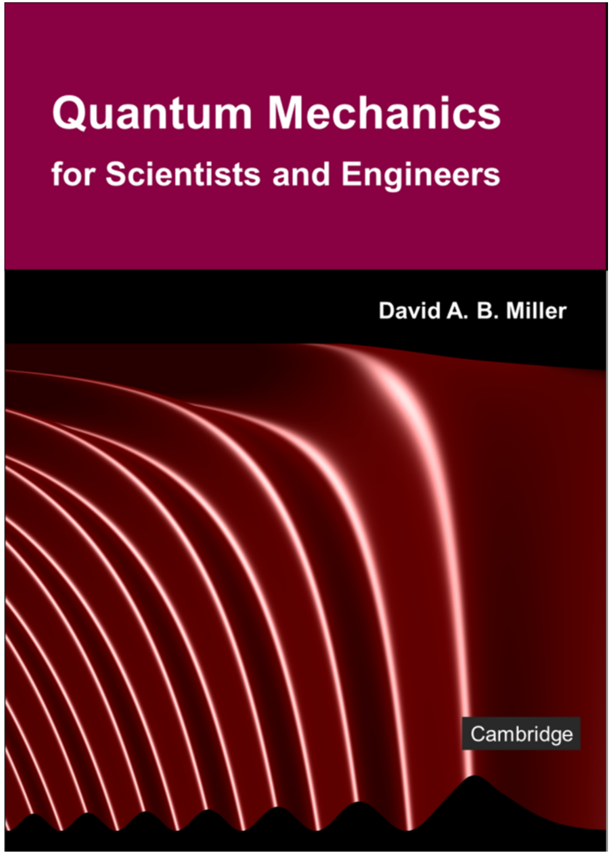


3.2 Finite well and harmonic oscillator

Slides: Video 3.2.4 The harmonic oscillator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.10



Particles in potential wells

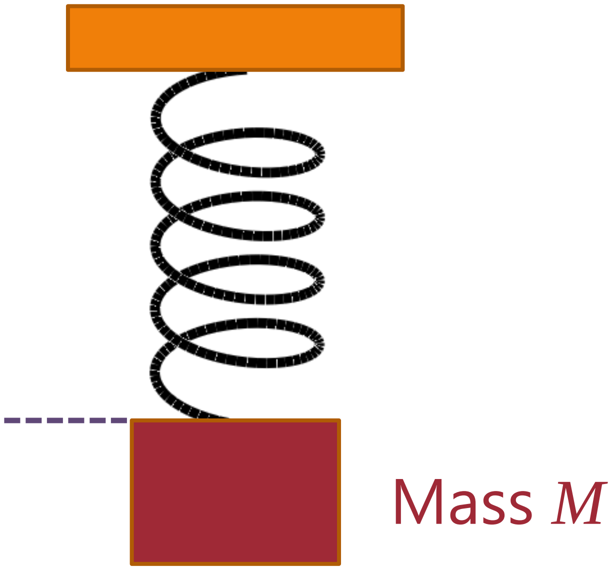
The harmonic oscillator

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

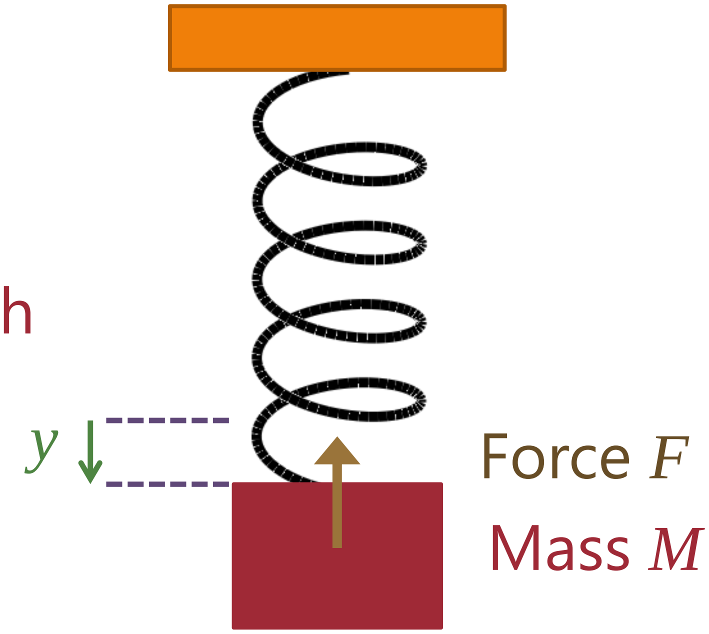
- proportional to the amount y by which it is stretched
  - For some "spring constant" K

$$F = -Ky$$

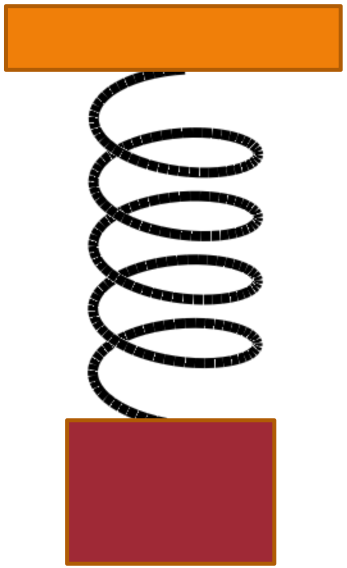
The minus sign is because this is "restoring"

- 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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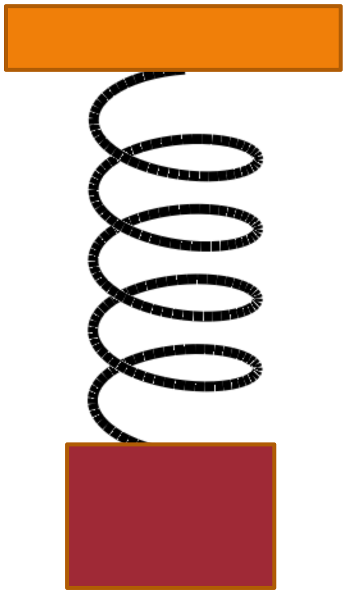
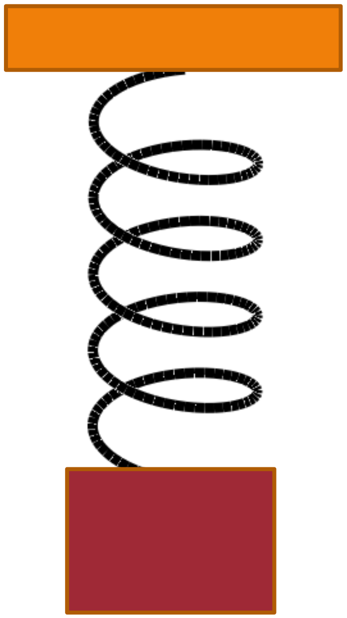


Mass on a spring



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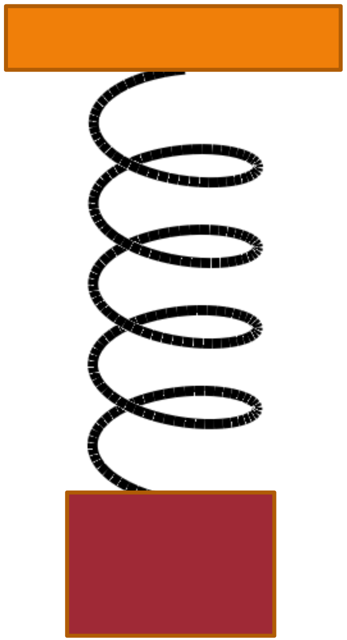
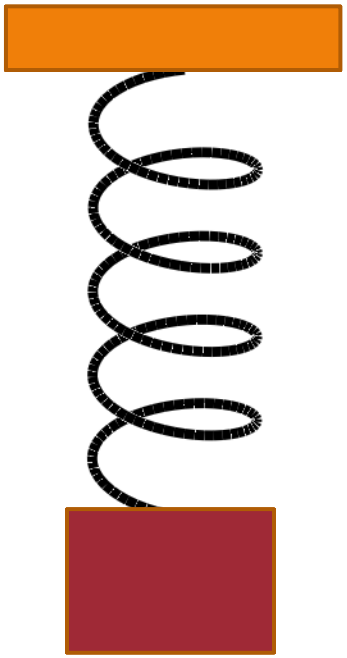


Mass on a spring



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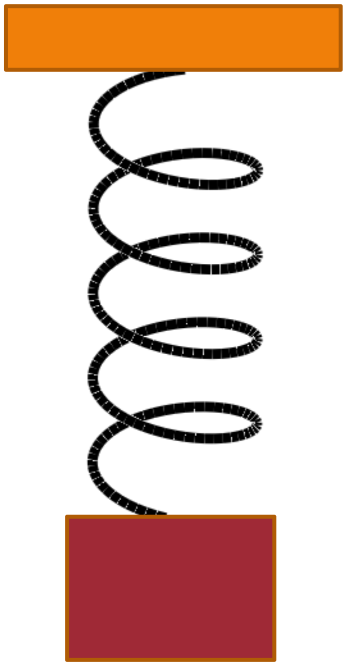

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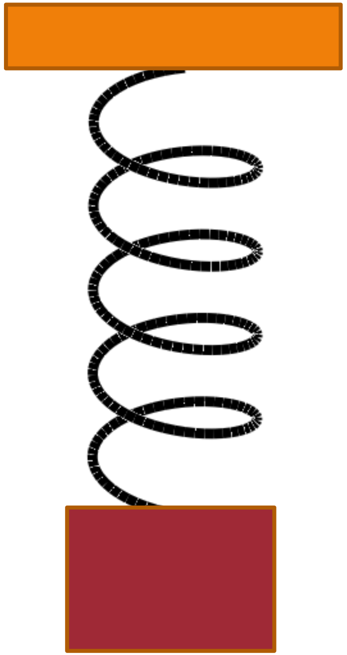


Mass on a spring

From Newton's second law

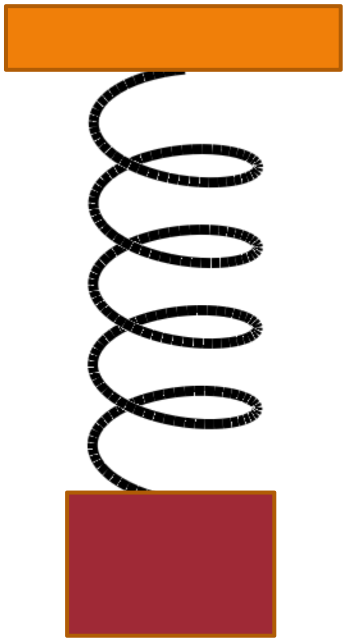
$$F = Ma = M\frac{d^2y}{dt^2} = -Ky$$

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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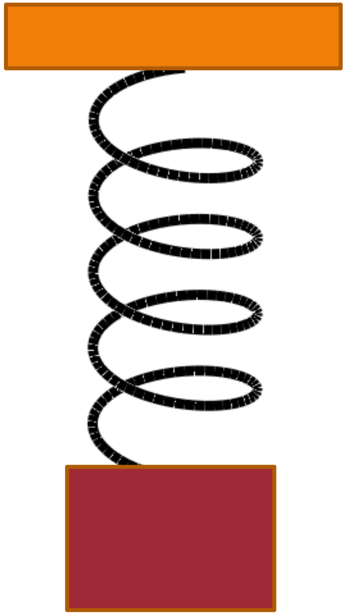

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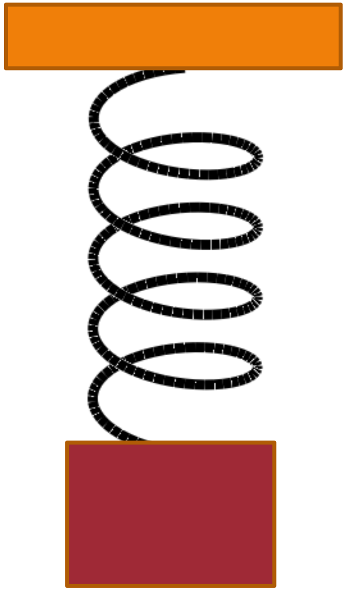

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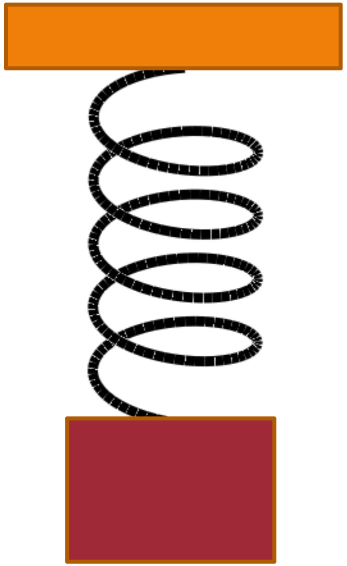

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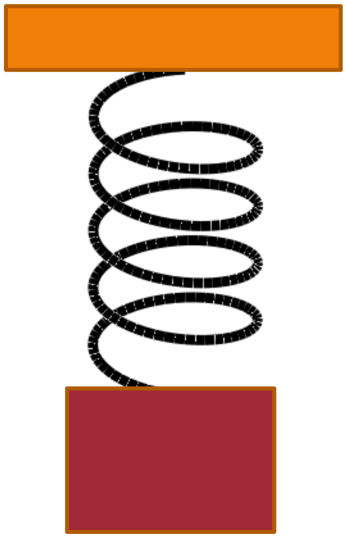

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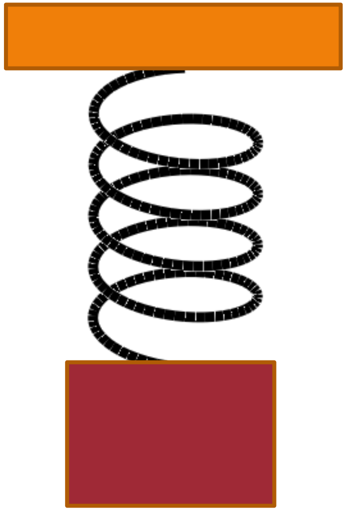

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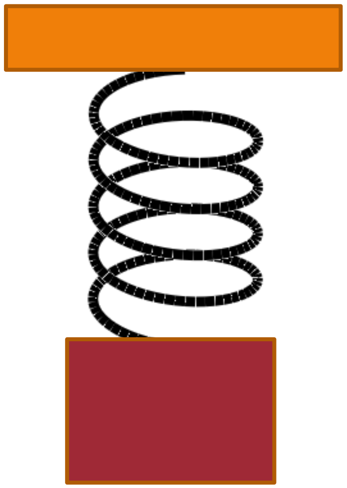

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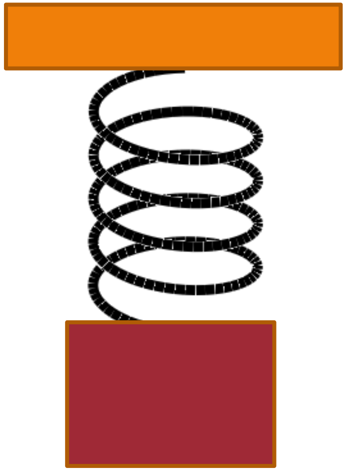

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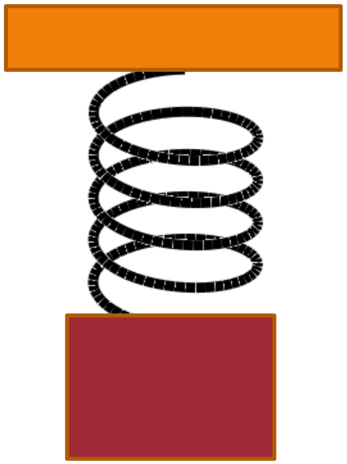

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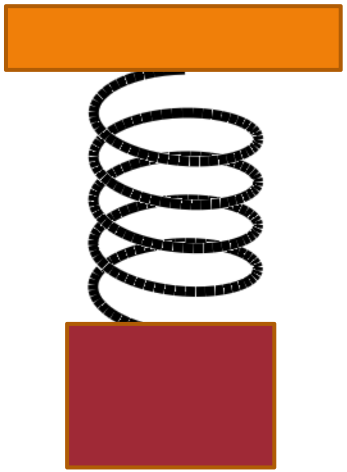

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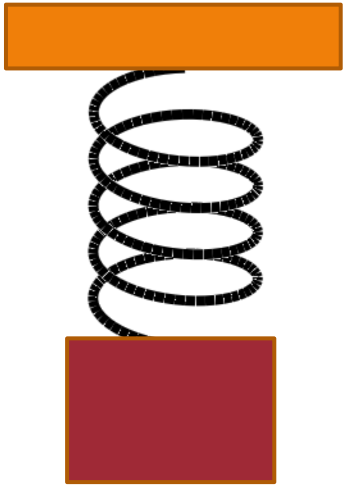

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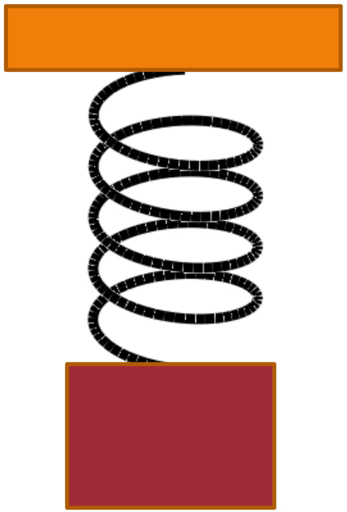

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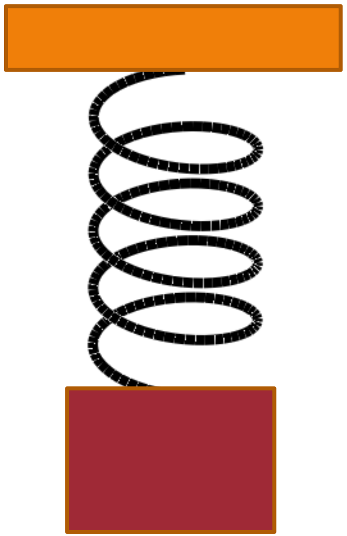

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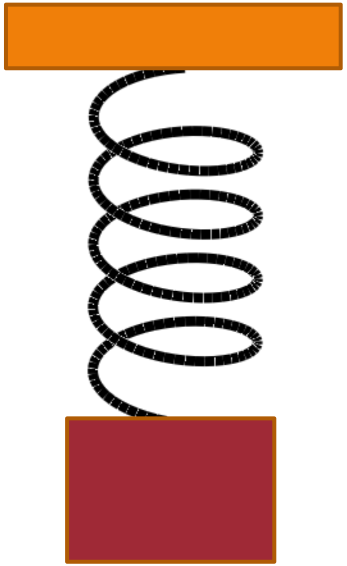
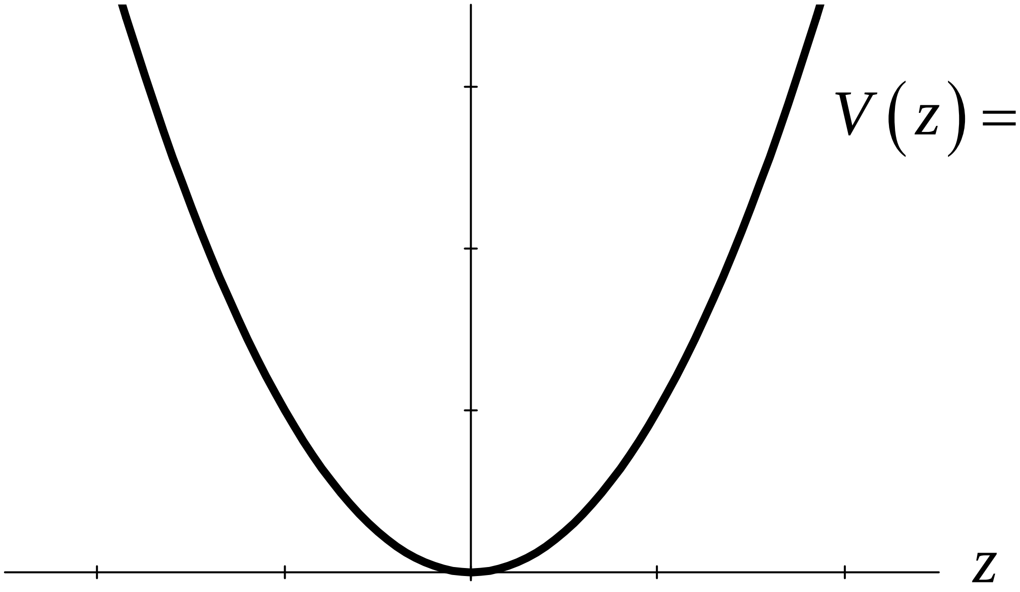
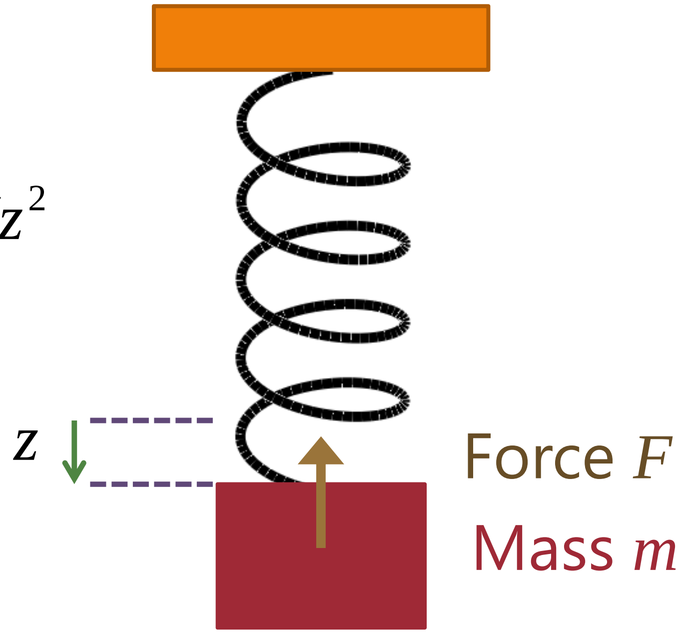


Potential energy



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



The potential from the restoring force F is

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

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

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

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

that is,

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

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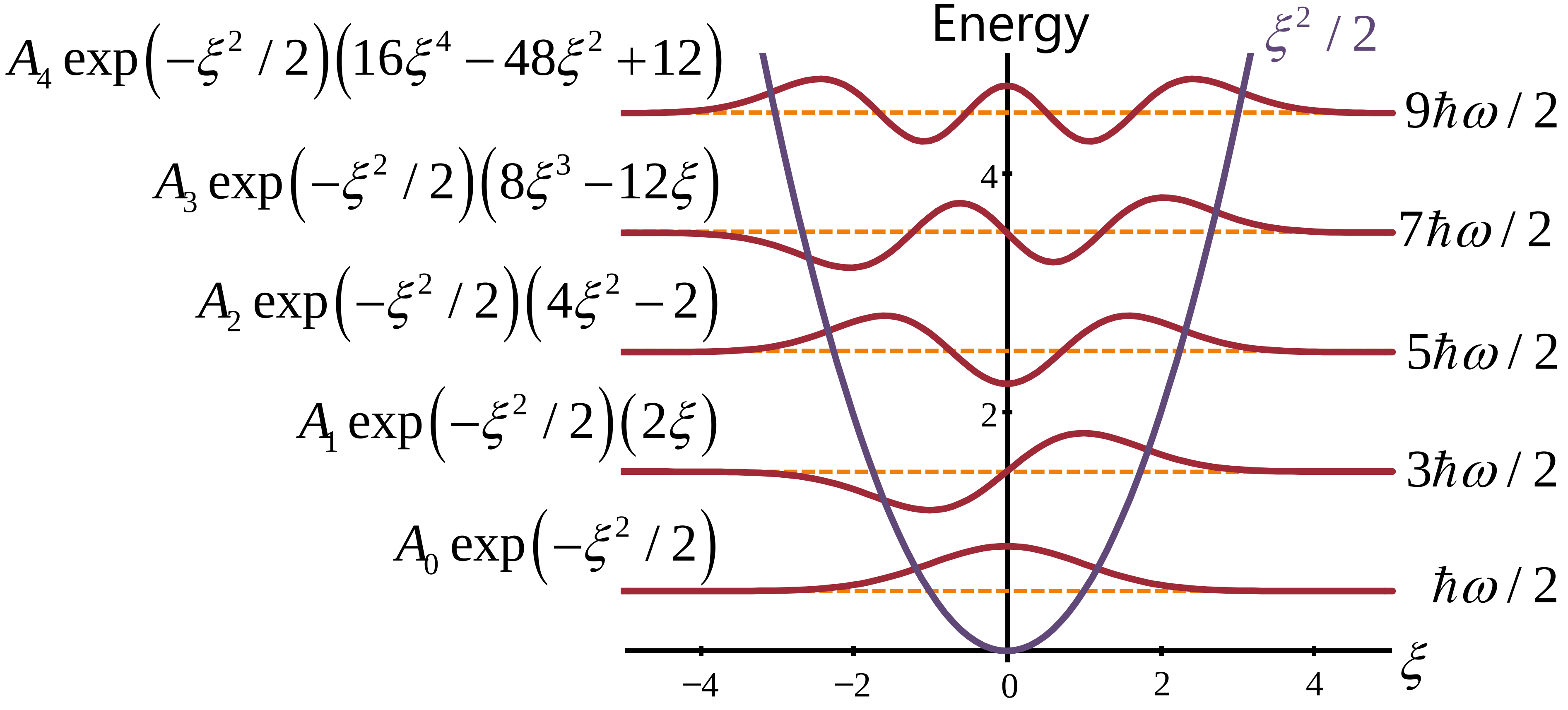
$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

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



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