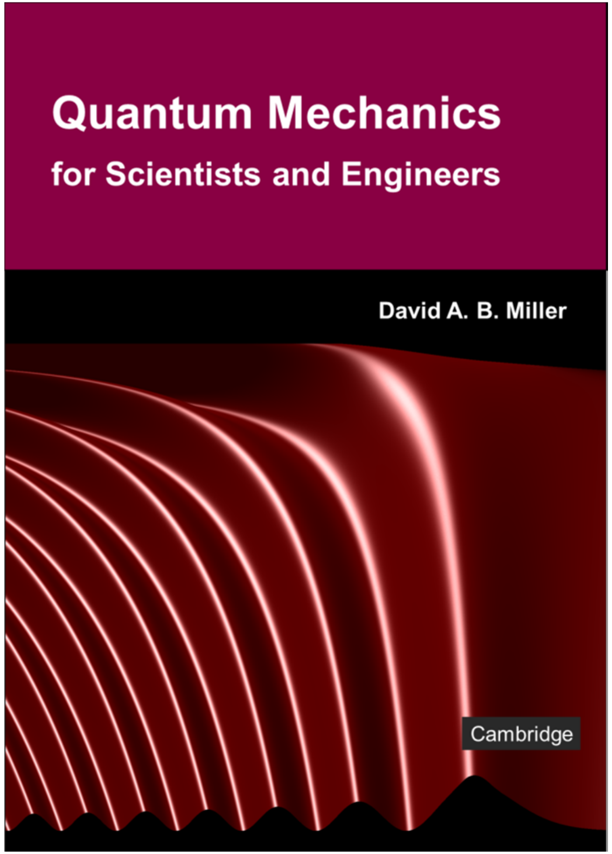
3.2 Finite well and harmonic oscillator

Slides: Video 3.2.4 The harmonic oscillator

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.10



Particles in potential wells

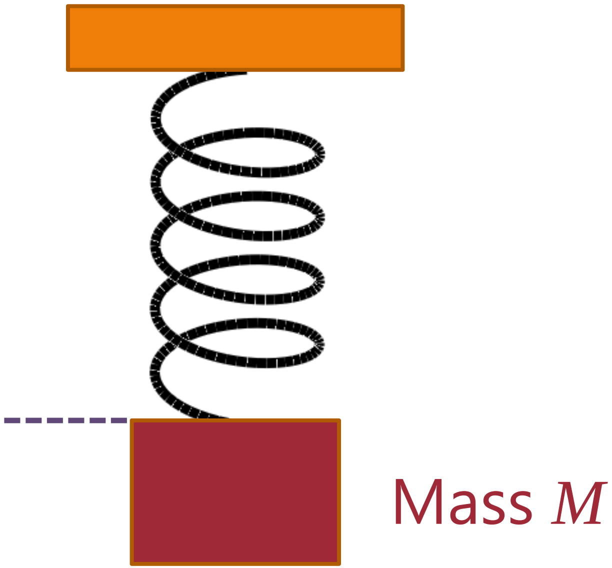
The harmonic oscillator

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

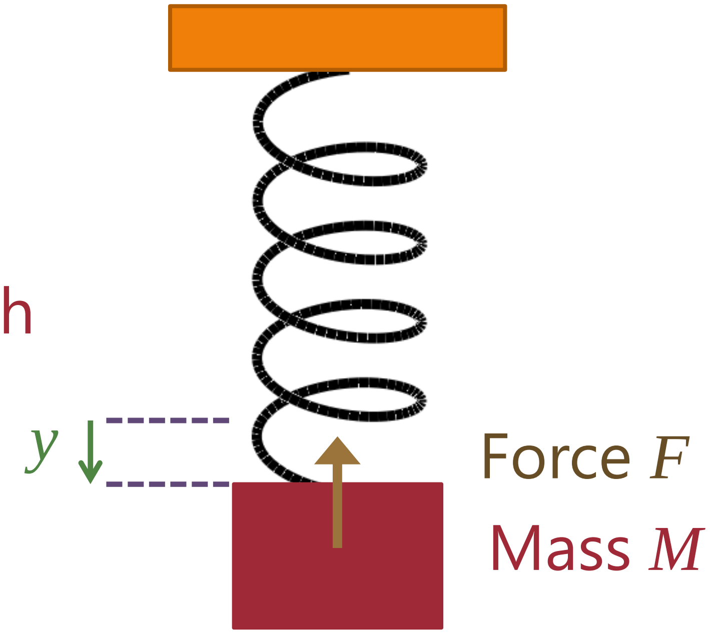
- proportional to the amount y by which it is stretched
  - For some "spring constant" K

$$F = -Ky$$

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

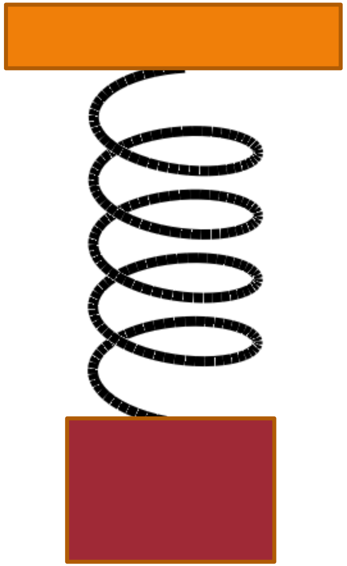
$$F = Ma = M\frac{d^2y}{dt^2} = -Ky$$

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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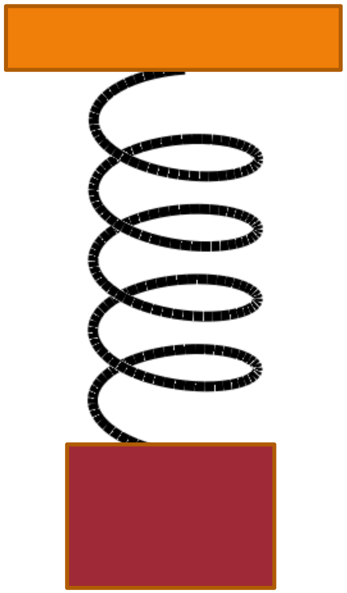

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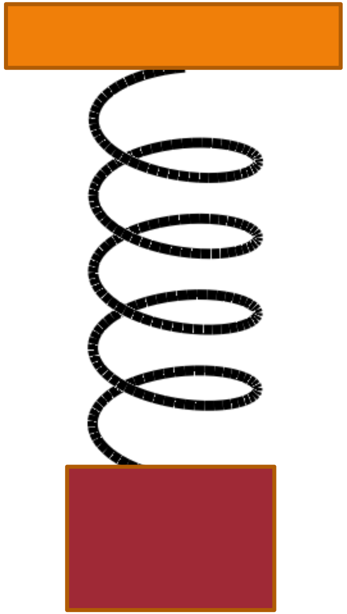

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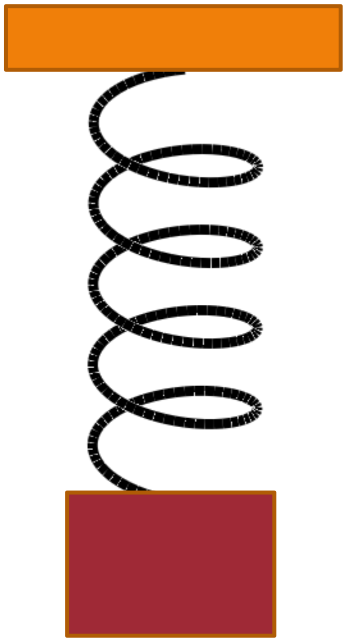

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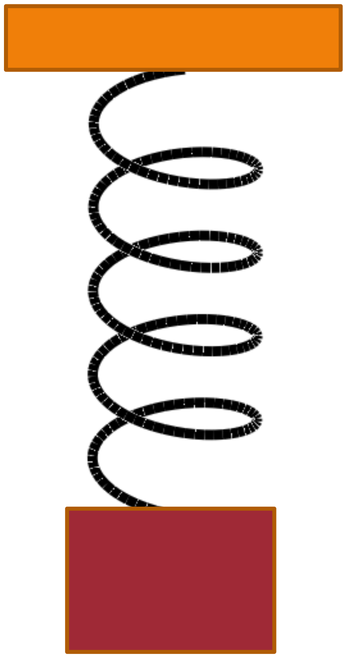

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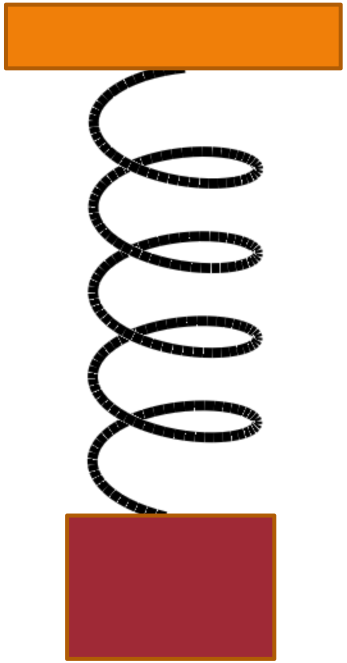

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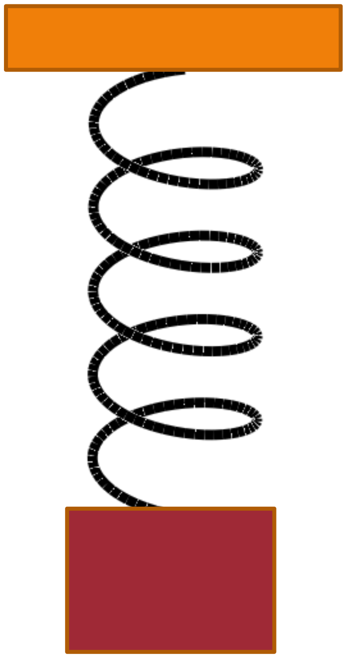

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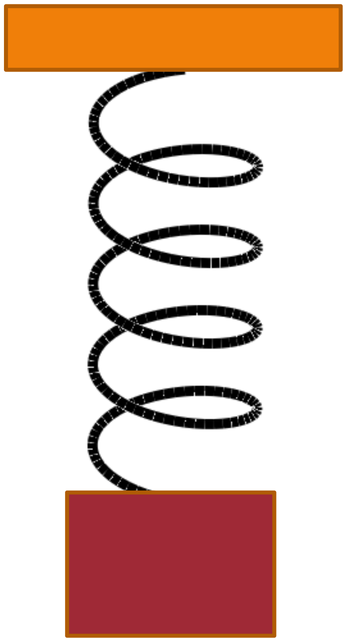

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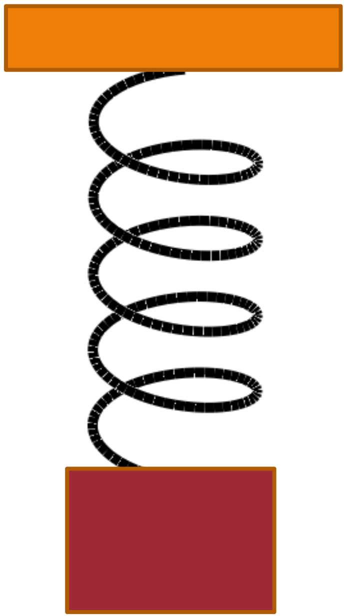

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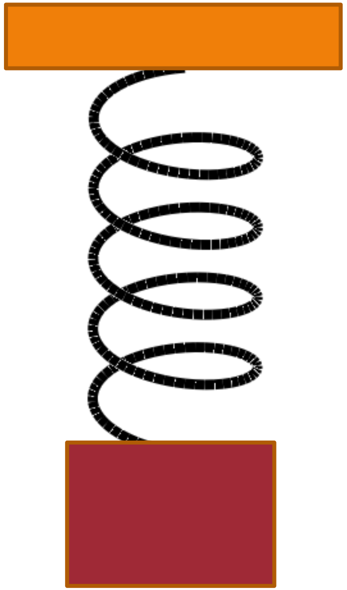

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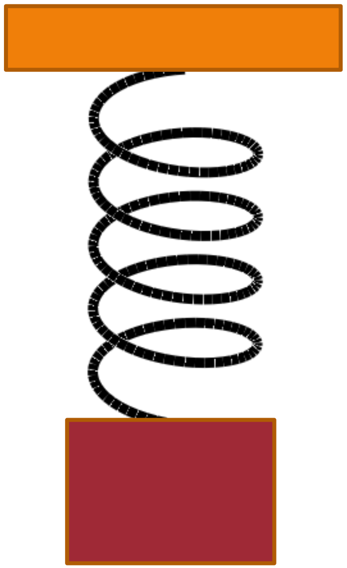

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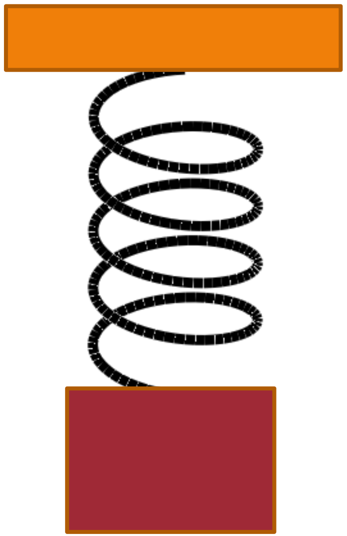

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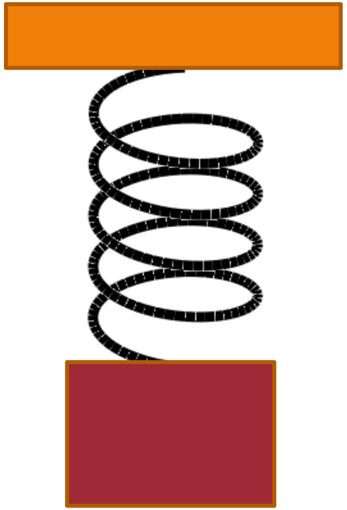

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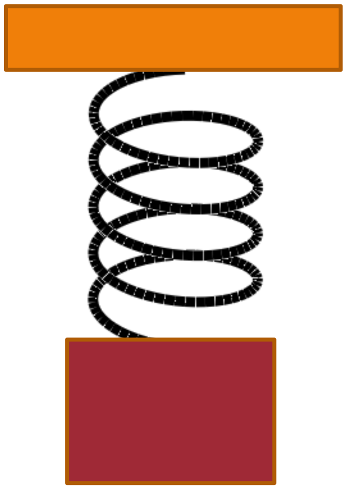

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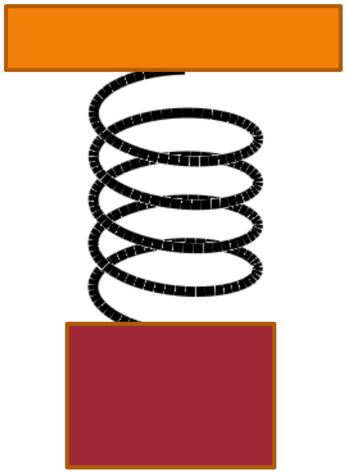

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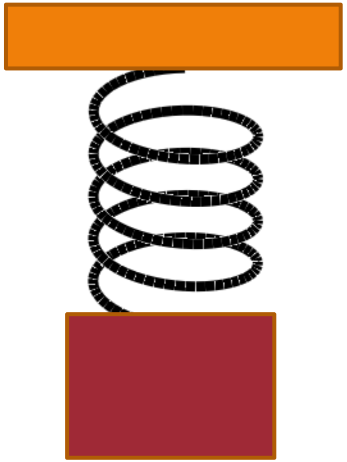

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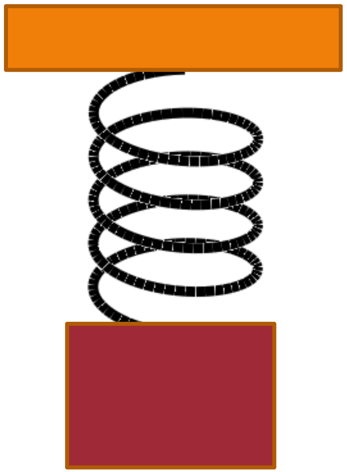

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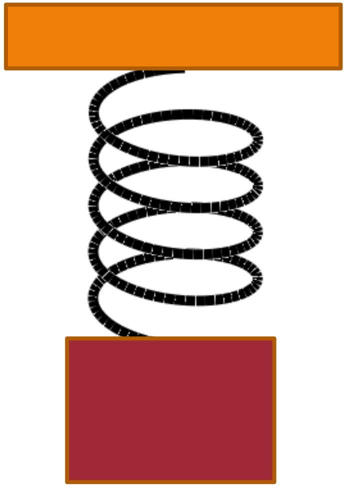

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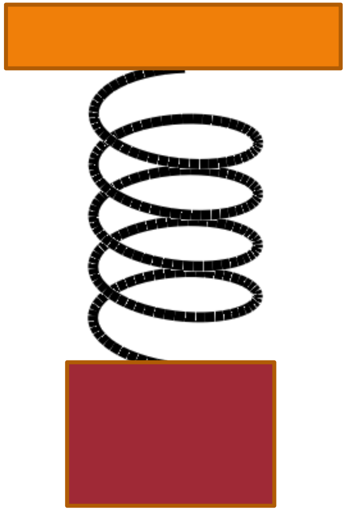

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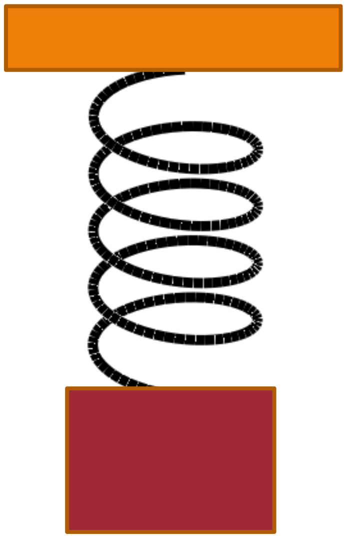

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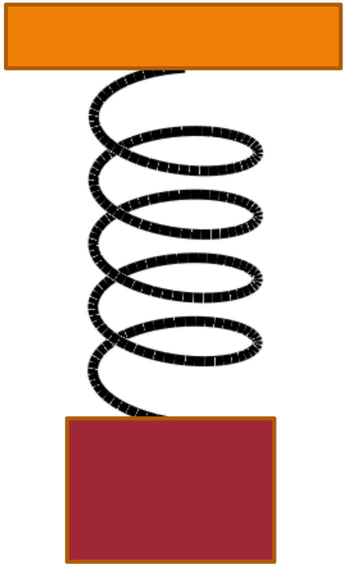
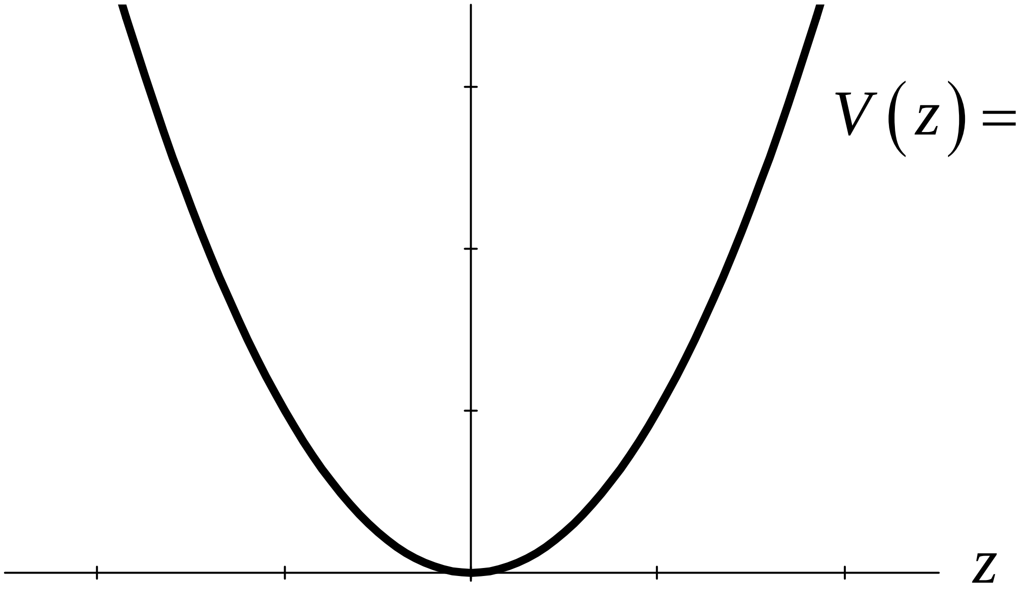
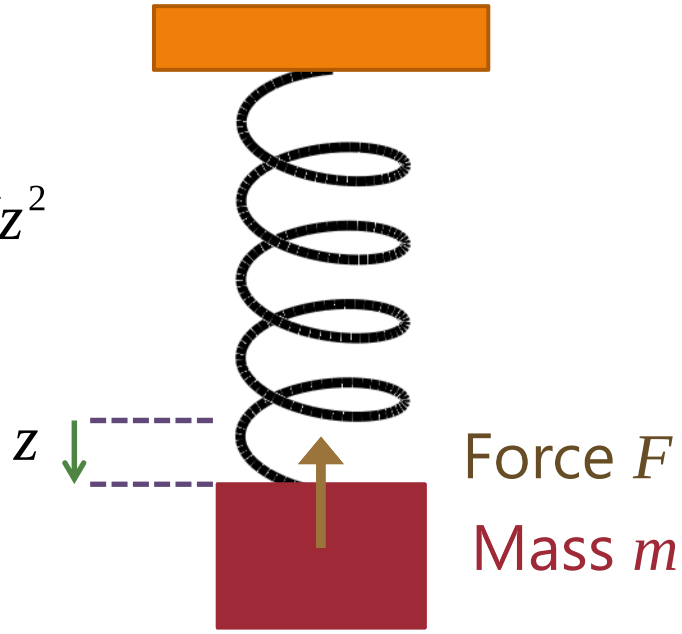


Potential energy



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



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,

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

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

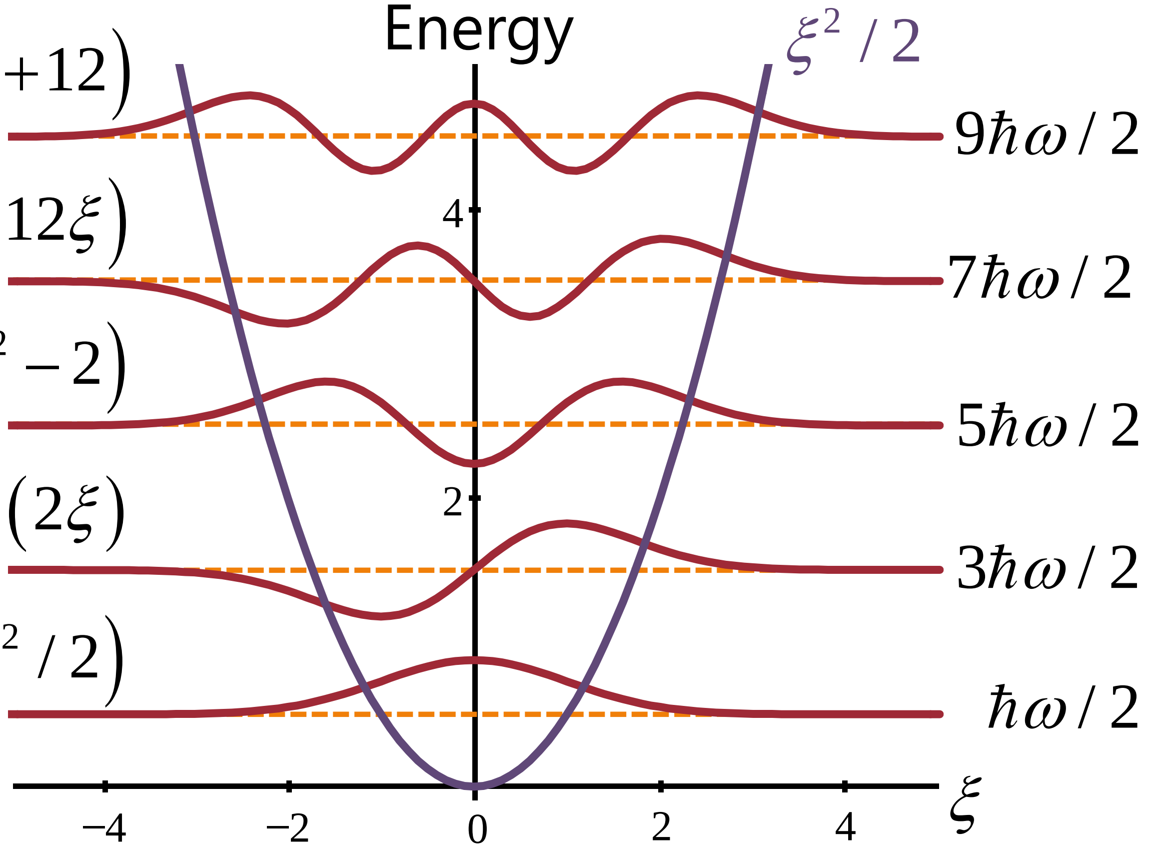
$$A_4 \exp\left(-\xi^2/2\right)\left(16\xi^4 - 48\xi^2 + 12\right)$$

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

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

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

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



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