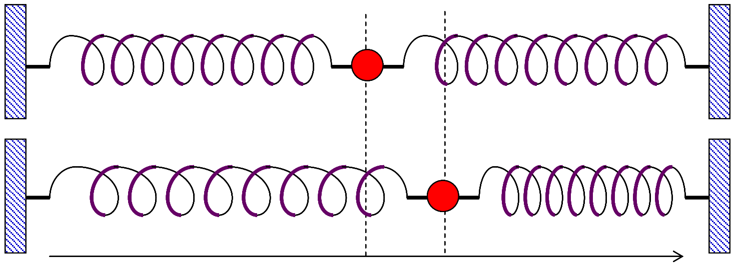
1-D Harmonic Oscillator

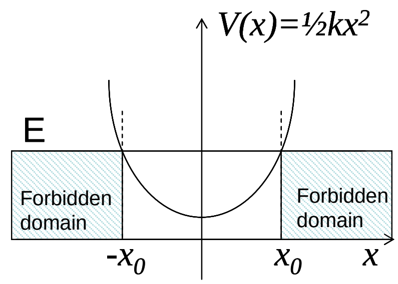
We saw the infinite potential well gives a clear function. Now we are studying the harmonic oscillator. It is very important for

- field theory
- lattice vibration of solid state
- heat transport and heat capacity
- Hydrogen atom electron energy level
- Electron going very fast along a pathway

You can expand V by a Taylor Series:

$$V(r) = \underset{=0}{V(\vec{r}_0)} + \underbrace{(\vec{r}-\vec{r}_0)V^{(1)}(\vec{r}_0)}_{\text{=0 at the equilibrium position V'=0}} + \underbrace{\tfrac{1}{2}(\vec{r}-\vec{r}_0)^2 V^{(2)}(\vec{r}_0)}_{\text{harmonic potential}} + \cdots + \tfrac{1}{n!}(\vec{r}-\vec{r}_0)^n V^{(n)}(\vec{r}_0)$$





$$F = -kx$$

$$m\frac{\partial^2 x}{\partial t^2} = -kx \qquad \omega_0^2 = \frac{k}{m}$$

$$\frac{d}{dt}\left(\tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\omega_0^2 x^2\right) = 0$$

$$\left.\begin{array}{l} E = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}kx^2 \\ H = \frac{p^2}{2m} + \frac{k}{2}x^2 \end{array}\right\} \text{The classical mechanics Hamiltonian}$$

We will learn that in Quantum Mechanics, the electron can also exist in the forbidden region. Solve Schrödinger equation:

$$\left.\begin{array}{l} H\varphi = E\varphi \\ \left(\frac{p^2}{2m} + \frac{k}{2}x^2\right)\varphi = E\varphi \end{array}\right\} \text{The quantum mechanics Hamiltonian}$$

It turns out that this math is also good in near future 2^{nd} quantized quantum field theory. (OK, Dr. Shen, we believe you…)

The Annihilation and Creation Operators

$a \equiv \frac{\beta}{\sqrt{2}}\left(x + \frac{ip}{m\omega_0}\right)$ Annihilation Operator

$a_+ \equiv \frac{\beta}{\sqrt{2}}\left(x - \frac{ip}{m\omega_0}\right)$ Creation Operator

$a \neq a_+$ not a Hermitian Operator

$\beta^2 \equiv \frac{m\omega_0}{\hbar}$

Showing that the Annihilation and Creation Operators do not commute:

Use this relation: $\left[x, p\right] = i\hbar$ to show that $\left[a, a_+\right] = 1$

$$\left[a, a_+\right] = aa_+ - a_+a$$

$$= \frac{\beta}{\sqrt{2}}\left(x + \frac{ip}{m\omega_0}\right)\frac{\beta}{\sqrt{2}}\left(x - \frac{ip}{m\omega_0}\right) - \frac{\beta}{\sqrt{2}}\left(x - \frac{ip}{m\omega_0}\right)\frac{\beta}{\sqrt{2}}\left(x + \frac{ip}{m\omega_0}\right)$$

$$= \frac{\beta^2}{2}\left[\left(\cancel{x^2} - \frac{ixp}{m\omega_0} + \frac{ipx}{m\omega_0} + \cancel{\left(\frac{p}{m\omega_0}\right)^2}\right) - \left(\cancel{x^2} + \frac{ixp}{m\omega_0} - \frac{ipx}{m\omega_0} + \cancel{\left(\frac{p}{m\omega_0}\right)^2}\right)\right]$$

$$= \frac{\beta^2}{2}\frac{i}{m\omega_0}\left[\left(px - xp\right) + \left(px - xp\right)\right]$$

$$= \frac{\beta^2}{2}\frac{i}{m\omega_0}2\left[p, x\right] = -\frac{i\beta^2}{m\omega_0}\left[x, p\right] = -\frac{i\beta^2}{m\omega_0}i\hbar = \frac{\beta^2\hbar}{m\omega_0} = 1$$

Note: $\beta^2 \equiv \frac{m\omega_0}{\hbar}$

$$\hat{a}_+\hat{a} = \hat{a}\hat{a}_+ + 1$$

$\hat{N} = \hat{a}_+\hat{a} \leftarrow$ eigenfunction of N let's you solve the Hamiltonian totally

$$\hat{x} = \frac{\left(\hat{a} + \hat{a}_+\right)}{\sqrt{2}\beta} \qquad \hat{p} = \frac{m\omega_0}{i}\frac{\left(\hat{a} - \hat{a}_+\right)}{\sqrt{2}\beta}$$

$$\hat{H} = \hbar\omega_0\left(\hat{a}_+\hat{a} + \tfrac{1}{2}\right) = \hbar\omega_0\left(\hat{N} + \tfrac{1}{2}\right)$$

$$\hat{N}\varphi_n = n\varphi_n = \hat{a}_+\hat{a}\varphi_n$$

n is only a number

$\hat{a}\varphi_n$ is also a state function.

At home prove that $\hat{N}$ is Hermitian. Let's look at the property of this technique developed by many scientists.

$$\hat{N}\hat{a}\varphi_n = \hat{a}_+\hat{a}\hat{a}\varphi_n = \left(\hat{a}\hat{a}_+ - 1\right)\hat{a}\varphi_n = \hat{a}\left[\hat{N} - 1\right]\varphi_n = \hat{a}\left(n-1\right)\varphi_n = \left(n-1\right)\hat{a}\varphi_n$$

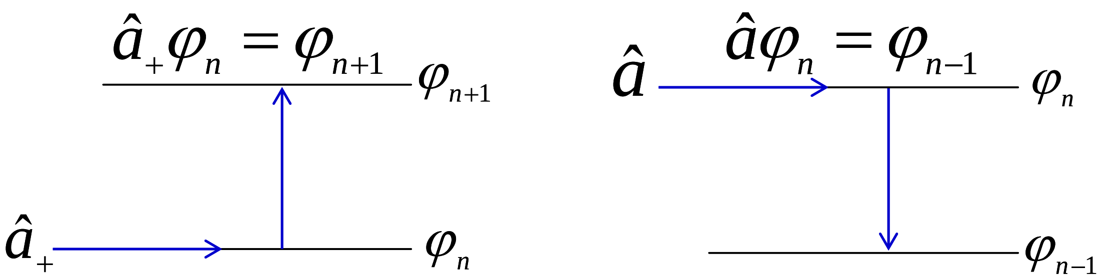
$$\hat{N}\hat{a}\varphi_n = \left(n-1\right)\hat{a}\varphi_n$$

$\hat{a}\varphi_n = \varphi_{n-1}$ the $\hat{a}$ operating on φ_n changes into another eigenfunction

At home show that

$$\hat{N}\hat{a}_+\varphi_n = \left(n+1\right)\hat{a}_+\varphi_n$$

$$\hat{a}_+\varphi_n = \varphi_{n+1}$$



$$\langle H \rangle \geq 0$$

$$\hat{H} = \tfrac{\hat{p}^2}{2m} + \tfrac{k}{2}\hat{x}^2 = \hbar\omega\left(\hat{N} + \tfrac{1}{2}\right) = \underbrace{\hbar\omega\left(n + \tfrac{1}{2}\right)}_{\geq 0}$$

$\therefore n < 0$ is not allowed

Ground state - if we set: $a\varphi_m = 0 \Rightarrow a\varphi_{m-1} = 0$

m is the minimum allowed value of n

$m = 0$

$a\varphi_0 = 0 = \varphi_{-1}$ this is not allowed

Solve this problem for the eigenfunction.

Now we look at the eigenvalues of H.

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right) \qquad n = 0,1,2,3,..$$

The energy levels are quantized. The ground state is $E_0 = \frac{1}{2}\hbar\omega$ it is the minimum energy for the oscillator.

Figure 7.8 and 7.9 on page 197 are discussed. Application to molecular vibration spectrum is discussed. Find the peak emission energy as

$$h\nu = \hbar\omega_0 \underbrace{\left(n - n'\right)}_{=1,2,3,\ldots}$$

Summary - Today we solved:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{k}{2}\hat{x}^2 \Rightarrow E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

☼Homework: 7.4 understand this – the description in the book is not correct.