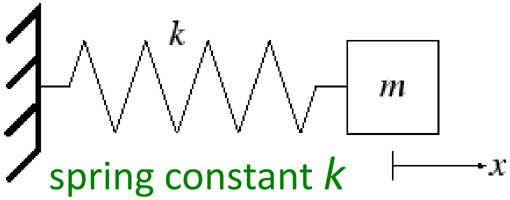
EE201/MSE207 Lecture 4

Harmonic oscillator

Important for optics (photons) and phonons, though they are massless particles. Also rare examples like electrons in a very smooth Q.Well.
Recently became important for NEMS.
Very important as a fundamental example, starting point for many problems.

Classical physics

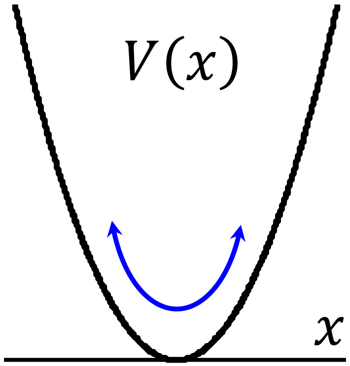


$$F = -kx \qquad \ddot{x} = \frac{F}{m} = -\frac{k}{m}x$$

$$x(t) = A\cos(\omega t + \varphi) \qquad \omega = \sqrt{k/m}$$

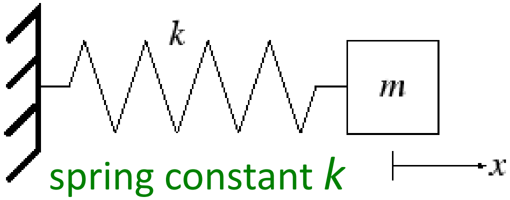
Potential energy $V(x) = \frac{kx^2}{2} = \frac{1}{2}m\omega^2 x^2$ $\left(F = -\frac{dV}{dx}\right)$

(by the way, $\bar{V} = \bar{T} = E/2$)



Harmonic oscillator

Classical physics



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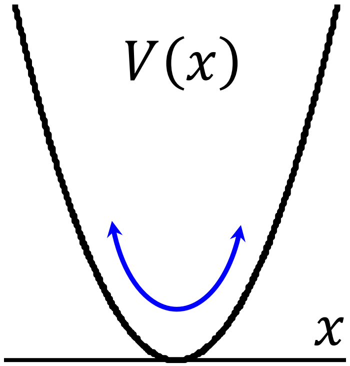


Quantum mechanics

TISE $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\,\psi = E\psi$$

Need to find energies and corresponding wavefunctions

Two ways to solve:

1) solve as a differential equation (Hermite polynomials, etc.)

2) solve using a trick: algebraic technique of ladder operators

We will consider only the second way (important for second quantization, similar for angular momentum, spin, etc.)

Ladder operators

(raising/lowering or creation/annihilation)

Define $$\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega\hat{x}) = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp\hbar\frac{\partial}{\partial x} + m\omega x\right)$$

(hat means operator)

Idea why: $$\hat{H} = \frac{1}{2m}[\hat{p}^2 + (m\omega\hat{x})^2] \qquad \frac{\hat{H}}{\hbar\omega} = \frac{1}{2\hbar m\omega}[\hat{p}^2 + (m\omega\hat{x})^2]$$

$$a^2 + b^2 = (a+ib)(a-ib)$$

However, operators usually do not commute: $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

$$\hat{a}_{-}\hat{a}_{+} = \frac{1}{2\hbar m\omega}(i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x}) =$$

$$= \frac{1}{2\hbar m\omega}[\hat{p}^2 + (m\omega\hat{x})^2 - im\omega(\hat{x}\hat{p} - \hat{p}\hat{x})] = \frac{\hat{H}}{\hbar\omega} - \frac{i}{2\hbar}(\hat{x}\hat{p} - \hat{p}\hat{x})$$

What is $\hat{x}\hat{p} - \hat{p}\hat{x}$? This is called commutator, $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

Commutator $[\hat{x}, \hat{p}]$

$$(\hat{x}\hat{p} - \hat{p}\hat{x}) f(x) = x(-i\hbar)\frac{\partial f}{\partial x} - (-i\hbar)\frac{\partial}{\partial x}[x\, f(x)] = i\hbar\, f(x)$$

Therefore $\boxed{[\hat{x}, \hat{p}] = i\hbar}$

Now back to calculation of $\hat{a}_-\hat{a}_+$

$$\left.\begin{aligned} \hat{a}_-\hat{a}_+ &= \frac{\hat{H}}{\hbar\omega} - \frac{i}{2\hbar}(\hat{x}\hat{p} - \hat{p}\hat{x}) = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \\ \text{Similarly} \qquad \hat{a}_+\hat{a}_- &= \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \end{aligned}\right\} \quad \boxed{[\hat{a}_-, \hat{a}_+] = 1}$$

TISE can be written as $\hbar\omega\,(\hat{a}_+\hat{a}_- + 1/2)\psi = E\,\psi$

or as $\hbar\omega\,(\hat{a}_-\hat{a}_+ - 1/2)\psi = E\,\psi$

Lemma If $\psi(x)$ satisfies TISE with energy E, then $\hat{a}_+\psi$ also satisfies TISE, with energy $E+\hbar\omega$.

(This is why $\hat{a}_+$ is called raising operator)

Proof

$$\hat{H}(\hat{a}_+\psi) = \hbar\omega(\hat{a}_+\hat{a}_- + {}^1\!/_2)(\hat{a}_+\psi) = \hbar\omega(\hat{a}_+\hat{a}_-\hat{a}_+ + {}^1\!/_2\,\hat{a}_+)\psi$$

$$= \hbar\omega\hat{a}_+\underbrace{(\hat{a}_-\hat{a}_+ + {}^1\!/_2)}_{\frac{\hat{H}}{\hbar\omega}+\frac{1}{2}+\frac{1}{2}}\psi = \hat{a}_+\left(\hat{H}+\hbar\omega\right)\psi = \hat{a}_+(E+\hbar\omega)\psi =$$

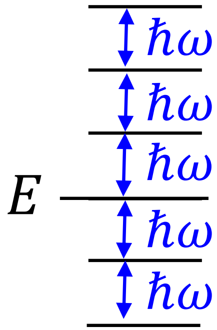
$$= (E+\hbar\omega)(\hat{a}_+\psi)$$

Q.E.D.

Lemma 2 If $\psi(x)$ satisfies TISE with energy E, then $\hat{a}_-\psi$ also satisfies TISE, with energy $E-\hbar\omega$. (similar proof)

Now main trick

If we have one solution $\psi(x)$, we can construct many other solutions (ladder of solutions)



Process of going down should stop somewhere ($E \geq 0$)

Then $\hat{a}_-\psi_0 = 0$ (further derivation is simple)

Ground state of harmonic oscillator

$$\hat{a}_-\psi_0 = 0 \quad \Rightarrow \quad \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0(x) = 0 \quad \Rightarrow \quad \frac{d\psi_0}{\partial x} = -\frac{m\omega}{\hbar}x\psi_0$$

Solution $\psi_0(x) = A\exp\left(-\frac{m\omega}{2\hbar}\,x^2\right)$

Find A from normalization $\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}\,x^2\right)}$

ground state

What is its energy? $\hat{H} = \hbar\omega(\hat{a}_+\hat{a}_- + 1/2)$ $\hat{H}\psi_0 = \frac{\hbar\omega}{2}\psi_0$

$\boxed{E_0 = \frac{1}{2}\hbar\omega}$ (“zero-point” energy, vacuum energy)

Now can find all stationary states by repeatedly applying $\hat{a}_+$ to the ground state

Stationary states of harmonic oscillator

$$\psi_n(x) = A_n(\hat{a}_+)^n \exp\left(-\frac{m\omega}{2\hbar}\,x^2\right) \qquad \boxed{E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega} \qquad n = 0, 1, 2, \ldots$$

A_n is normalization constant

Useful relations:

$$\begin{cases} \hat{a}_+\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}(x) \\ \hat{a}_-\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x) \end{cases}$$

therefore

$$\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0$$

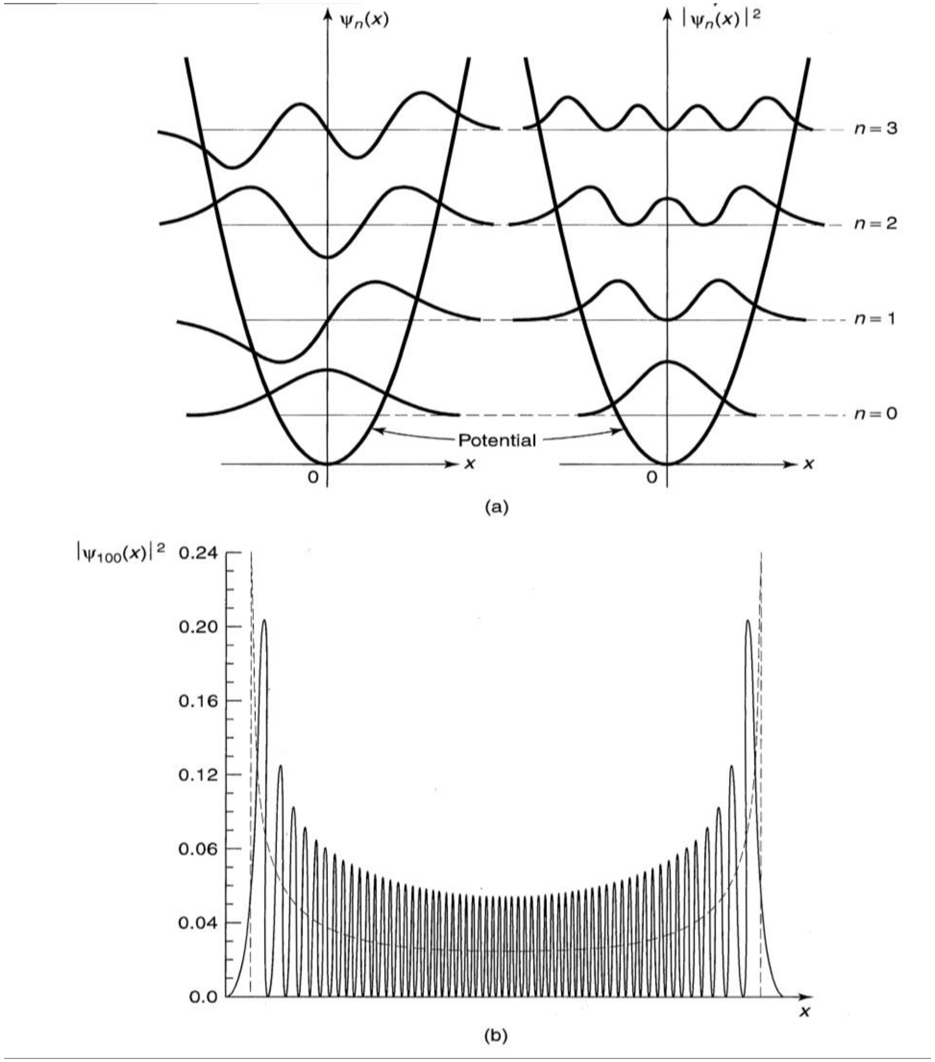
A few lowest levels:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}\,x^2\right)$$

$$\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\,x \exp\left(-\frac{m\omega}{2\hbar}\,x^2\right)$$

$$\psi_2(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(\sqrt{2}\frac{m\omega}{\hbar}x^2 - \frac{\sqrt{2}}{2}\right) \exp\left(-\frac{m\omega}{2\hbar}\,x^2\right)$$

Stationary states of harmonic oscillator



(a)

(b)

Fig. 2.7 from Griffiths' book

General stationary states for harmonic oscillator

$$\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n \psi_0 \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Explicitly

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) \exp\left(-\frac{\xi^2}{2}\right)$$

$$\xi = \sqrt{\frac{m\omega}{\pi\hbar}}\, x$$

$H_n(\xi)$ – Hermite polynomials

General solution of SE

$$\boxed{\Psi(x,t) = \sum_{n=0}^{\infty} c_n\, \psi_n(x) \exp[-i(n+1/2)\omega t]}$$

$$\sum_{n=0}^{\infty} |c_n|^2 = 1$$

Free particle

$V(x) = 0$ TISE $$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{dx^2} = E\psi$$

solution: $$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$$ $$\boxed{k = \frac{\sqrt{2mE}}{\hbar}}$$

k – “wave vector”, $k = \dfrac{2\pi}{\lambda}$

with time dependence:

$$\Psi(x,t) = A\exp\left[ik\left(x - \frac{\hbar k}{2m}t\right)\right] + B\exp\left[-ik\left(x + \frac{\hbar k}{2m}t\right)\right]$$

propagates to the right

with velocity $v_{ph} = \dfrac{\hbar k}{2m}$

propagates to the left with the same velocity

interesting that classically $v_{\text{classical}} = \sqrt{\dfrac{2E}{m}} = \dfrac{\hbar k}{m}$ (twice larger)

(will discuss later, difference between phase and group velocities)

Not normalizable! What to do? Construct a wave packet.

Wave packet

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)\exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right]dk$$

$k > 0$ to the right
$k < 0$ to the left

energy is not well-defined

At $t = 0$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)\,e^{ikx}dk$$

just a Fourier transform

Remind Fourier transform:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(k)\,e^{ikx}dk \qquad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)\,e^{-ikx}dx$$

So if we know $\Psi(x,0)$, then can find $\phi(k)$, and then know $\Psi(x,t)$

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)\,e^{-ikx}dx$$

Normalization:

$$\int_{-\infty}^{\infty}|\Psi(x,0)|^2\,dx = 1$$

is equivalent to

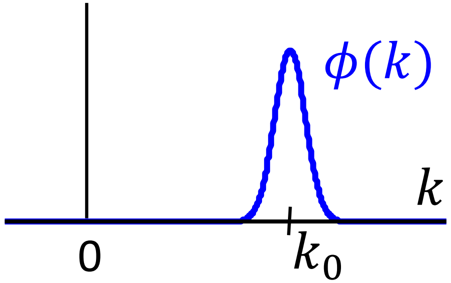
$$\int_{-\infty}^{\infty}|\phi(k)\,|^2\,dk = 1$$

$\phi(k)$ is like wavefunction in *k*-space

Phase and group velocities

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)\exp[i(kx-\omega t)]\,dk \qquad \omega=\frac{\hbar k^2}{2m}$$

Assume that $\phi(k)$ is concentrated around k_0, then



$$\omega(k)\approx\omega_0+\frac{d\omega}{dk}(k-k_0)=\omega_0+\omega'\Delta k$$

$$\Psi(x,t)\approx\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k_0+\Delta k)\exp[i(k_0+\Delta k)x-i(\omega_0+\omega'\Delta k)t]\,d\Delta k$$

$$=\frac{1}{\sqrt{2\pi}}\exp\left[ik_0\underbrace{\left(x-\frac{\omega_0}{k_0}t\right)}_{\text{phase velocity: } v_{ph}=\omega_0/k_0}\right]\int_{-\infty}^{\infty}\phi(k_0+\Delta k)\exp[i\Delta k\underbrace{(x-\omega' t)}_{\text{group velocity: } v_{gr}=\omega'=d\omega/dk}]\,d\Delta k$$

In our case
$\omega=\hbar k^2/(2m)$

$$v_{gr}=\frac{d\omega}{dk}=\frac{\hbar k}{m}=v_{\text{classical}}$$

$$v_{ph}=\frac{\omega}{k}=\frac{\hbar k}{2m}$$

So, in quantum case
$v_{gr}=2v_{ph}$
(shape faster than ripples)

(For waves on water $v_{ph}=2v_{gr}$)

Another normalization

Actually, it is difficult to work with wavepackets, so in practice people usually work with extended waves

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}}\, \mathrm{e}^{ikx}$$

This function satisfies “normalization”

$$\boxed{\int_{-\infty}^{\infty} \psi_k^*(x)\, \psi_{k'}(x)\, dx = \delta(k - k')}$$

Some properties of delta-function $\delta(x)$

$$\int_{-\infty}^{\infty} f(x)\, \delta(x)\, dx = f(0)$$

$$\int_{-\infty}^{\infty} f(x)\, \delta(x - a)\, dx = f(a)$$

$$\boxed{\int_{-\infty}^{\infty} e^{iax}\, dx = 2\pi\, \delta(a)}$$

(from Fourier transform theorem)