The Harmonic Oscillator

The Classical Harmonic Oscillator

$$F_x = -kx = m\frac{d^2x}{dt^2} \quad , \quad x = A\sin(\pi 2\nu t + b) \qquad \nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$
$$= -\frac{dV}{dx}$$

$$V = \frac{1}{2}kx^2 = 2\pi^2\nu^2 m x^2 = 2\pi^2\nu^2 m A^2 \sin^2(2\pi\nu t + b)$$
$$T = \frac{1}{2}m(\frac{dx}{dt})^2 = 2m\pi^2\nu^2 A^2\cos^2(2\pi\nu t + b)$$
$$E = T + V = \frac{1}{2}kA^2 = 2\pi^2\nu^2 m A^2$$

$$t = \frac{1}{2\pi\nu}\left[\sin^{-1}(\frac{x}{A}) - b\right], \quad \frac{dt}{dx} = \frac{1}{2\pi\nu}\frac{1}{A}\frac{1}{\sqrt{1-(\frac{x}{A})^2}} \quad , \quad dt = \frac{1}{2\pi\nu A}\frac{1}{\sqrt{1-(\frac{x}{A})^2}}dx$$

the probability that the particle is found between $x \sim x+dx$, $2\nu dt = \frac{1}{\sqrt{1-(\frac{x}{A})^2}}\frac{1}{2\pi\nu A}dx$

The Quantum Harmonic Oscillator

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \quad --- (1)$$

let $u = \sqrt{\frac{m\omega}{\hbar}}x$, $du = \sqrt{\frac{m\omega}{\hbar}}dx$, $\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{d\alpha}$, $\frac{d^2}{dx^2} = \sqrt{\frac{m\omega}{\hbar}}\frac{d^2}{d\alpha^2}$

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

$$2E\psi = \hbar\omega(-\frac{d^2}{du^2} + u^2)\psi \quad , \quad \frac{d^2\psi}{du^2} = -\underbrace{\frac{2E}{\hbar\omega}}_{K}\psi + u^2\psi \quad , \quad \frac{d^2\psi}{du^2} = (u^2 - K)\psi$$

for u very large (mean x is very large)

$$\frac{d^2\psi}{du^2} \approx u^2\psi \quad , \quad \text{then } \psi(u) \approx Ae^{-\frac{u^2}{2}} + \underbrace{Be^{\frac{u^2}{2}}}_{\text{not normalizable}} = h(u)e^{-\frac{u^2}{2}}$$

$$\frac{d\psi}{du} = (\frac{dh}{du} - uh)e^{-\frac{u^2}{2}} \qquad \frac{d^2\psi}{du^2} = \left[\underbrace{\frac{d^2h}{du^2} - 2u\frac{dh}{du} + (K-1)h}_{=0}\right]e^{-\frac{u^2}{2}}$$

$$h(u) = a_0 + a_1u + a_2u^2 + \cdots = \sum_{j=0}^{\infty}a_ju^j \qquad \frac{dh}{du} = a_1 + 2a_2u + 3a_3u^2 + \cdots = \sum_{j=0}^{\infty}ja_ju^{j-1}$$
$$\frac{d^2h}{du^2} = 2a_2 + 2\cdot 3a_3u + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}u^j$$

$$\Rightarrow \sum_{j=0}^{\infty}\left[\underbrace{(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j}_{=0}\right]u^j = 0 \quad , \quad a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)}a_j$$

$$a_2 = \frac{1-K}{2}a_0 \qquad a_4 = \frac{5-K}{12}a_2 = \frac{(5-K)(1-K)}{24}a_0$$
$$a_3 = \frac{3-K}{6}a_1 \qquad a_5 = \frac{7-K}{20}a_3 = \frac{(7-K)(3-K)}{120}a_1$$

$$\Rightarrow h(u) = h_{even}(u) + h_{odd}(u)$$

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for large j, $a_{j+2} \approx \frac{2}{j} a_j$

$$a_j = \frac{a_2}{(\frac{j-2}{2})!} = \frac{1-K}{2} \frac{1}{(\frac{j-2}{2})!} \Rightarrow h(u) = \sum a_j u^j \approx c \sum \frac{1}{(\frac{j}{2})!} u^j \approx c \sum \frac{1}{j!} u^{2j} \approx c e^{u^2}$$

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$$\approx \frac{c}{(\frac{j}{2})!} \qquad \Rightarrow \psi = h e^{-\frac{u^2}{2}} = \sum a_j u^j e^{-\frac{u^2}{2}} = c e^{u^2} e^{-\frac{u^2}{2}} = c e^{\frac{u^2}{2}}$$

can't normall.

let $a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j$, $2j+1-K=0$, $K = 2j+1 = 2n+1$

$2j+1-K = 0$

$$\Rightarrow a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j$$

if $n=0$, $h(u) = a_0$ $\quad \psi_0 = a_0 e^{-\frac{u^2}{2}}$

if $n=1$, $a_0 = 0$ $\quad h(u) = a_1 u$ $\quad \psi_1(u) = a_1 u e^{-\frac{u^2}{2}}$

if $n=2$ $\quad h_2(u) = a_0(1-2u^2)$ $\quad \psi_2(u) = a_0(1-2u)^2 e^{-\frac{u^2}{2}}$

$$\Rightarrow \psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(u) e^{-\frac{u^2}{2}} \qquad H_n(u) = (-1)^n e^{u^2} \frac{d^n}{du^n} e^{-u^2}$$

Hermite polynomials

$K = \frac{2E}{\hbar\omega} = 2n+1$, $E_n = \hbar\omega(n+\frac{1}{2})$ $\quad n = 0, 1, 2 \cdots$

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Vibration of Diatomic Molecules

occurs at the minimum in $U(R)$ curve $=0$

U: electronic energy $= U(R) = \frac{U(R_e)}{0!} + \frac{U'(R_e)(R-R_e)}{1!} + \frac{\overset{k}{U''(R_e)}(R-R_e)^2}{2!} + \frac{U'''(R_e)(R-R_e)^3}{3!} + \cdots$

$\approx \frac{1}{2}k(R-R_e)^2 = \frac{1}{2}kx^2$

$E_{vib} \approx (v+\frac{1}{2})h\nu_e$ $\quad \nu_e = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ $\quad \mu = \frac{m_1 m_2}{m_1+m_2}$ $\quad k = \left.\frac{d^2U}{dR^2}\right|_{R=R_e}$

ν_e: equilibrium (or harmonic) vibrational frequency

$E_{vib} = (v+\frac{1}{2})h\nu_e - (v+\frac{1}{2})^2 h\nu_e x_e$ ← more accurate

$\nu_e x_e$: anharmonicity constant

$\nu_{light} =$

Proof $\int_{-\infty}^{\infty} f^*(\hat{a}_+ g)\,dx = \int_{-\infty}^{\infty} (\hat{a}_- f)^* g\,dx$

$$\begin{cases} \hat{a}_+ \psi_n = C_n \psi_{n+1} \\ \hat{a}_- \psi_n = d_n \psi_{n-1} \end{cases}$$

$$\int_{-\infty}^{+\infty} f^*(x) [\hat{a}_+ g(x)]\,dx$$
$$= \int_{-\infty}^{+\infty} f^*(x)\left(-i \frac{\hbar}{i}\frac{d}{dx} + m\omega x\right) g\,dx$$
$$= \int_{-\infty}^{+\infty} f^* \left(-\hbar \frac{dg}{dx}\right) dx = -\hbar\left(f^* g\Big|_{-\infty}^{+\infty} - \int \frac{df^*}{dx} g\,dx\right)$$
$$= \int \hbar \frac{df^*}{dx} \cdot g\,dx$$
$$\Rightarrow \int_{-\infty}^{+\infty} \Big[\underbrace{\left(i \frac{\hbar}{i}\frac{d}{dx} + m\omega x\right)}_{\hat{a}_-} f\Big]^* g\,dx$$
$$= \int_{-\infty}^{+\infty} (\hat{a}_- f)^* g\,dx$$

$$H = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right) = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)$$
$$H\psi_n = E_n\psi_n, \quad \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\psi_n = E_n\psi_n = \left(n+\frac{1}{2}\right)\hbar\omega\psi_n$$

$$\begin{rcases} \hat{a}_+\hat{a}_-\psi_n = n\psi_n \\ \hat{a}_-\hat{a}_+\psi_n = (n+1)\psi_n \end{rcases}$$

$$\int_{-\infty}^{+\infty} (\hat{a}_+\psi_n)^*(\hat{a}_+\psi_n)\,dx = \int_{-\infty}^{+\infty} (C_n\psi_{n+1})^*(C_n\psi_{n+1})\,dx = |C_n|^2 \int_{-\infty}^{+\infty} |\psi_{n+1}|^2 dx = |C_n|^2 = 1$$
$$= \int_{-\infty}^{+\infty} (\hat{a}_-\hat{a}_+\psi_n)^*\psi_n\,dx = \int_{-\infty}^{+\infty} (n+1)\psi_n^*\psi_n\,dx = n+1, \quad C_n = \sqrt{n+1}$$

$$\int_{-\infty}^{+\infty} (\hat{a}_-\psi_n)^*(\hat{a}_-\psi_n)\,dx = \int_{-\infty}^{+\infty} (d_n\psi_{n-1})^*(d_n\psi_{n-1})\,dx = |d_n|^2 \int_{-\infty}^{+\infty} |\psi_{n-1}|^2 dx = |d_n|^2 = 1$$
$$= \int_{-\infty}^{+\infty} (\hat{a}_+\hat{a}_-\psi_n)^*\psi_n\,dx = \int_{-\infty}^{+\infty} n\psi_n^*\psi_n\,dx = n, \quad d_n = \sqrt{n}$$

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

$\psi_1 = \hat{a}_+\psi_0$ $\quad \hat{a}_+\psi_1 = \sqrt{2}\psi_2, \quad \psi_2 = \frac{1}{\sqrt{2}}\hat{a}_+\psi_1$

$\hat{a}_+\psi_2 = \sqrt{3}\psi_3 \quad \psi_3 = \frac{1}{\sqrt{3}}\hat{a}_+\psi_2 = \frac{1}{\sqrt{3}}\frac{1}{\sqrt{2}}(\hat{a}_+)^2\psi_1$

$$= \frac{1}{\sqrt{3}}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{1}}(\hat{a}_0)^3\psi_0$$

$$\Rightarrow \psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0(x), \quad E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$
$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n|0\rangle$$

$$\langle x\rangle = \langle n|x|n\rangle = \int_{-\infty}^{+\infty} \psi_n^*(x)\, x\, \psi_n(x)\,dx$$

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$$\int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx = \delta_{mn}$$

$$= \frac{1}{n}\int_{-\infty}^{+\infty} \psi_m^* \, n \, \psi_n \, dx = \frac{1}{n}\int_{-\infty}^{+\infty} \underbrace{\psi_m^* \, \hat{a}_+}_{f^*} \, \underbrace{\hat{a}_- \psi_n}_{g} \, dx = \frac{1}{n}\int_{-\infty}^{+\infty} (\hat{a}_- \psi_m)^* (\hat{a}_- \psi_n) \, dx$$

$$= \frac{1}{n}\int_{-\infty}^{+\infty} (\hat{a}_+ \hat{a}_- \psi_m)^* \psi_n \, dx = \frac{1}{n}\int_{-\infty}^{+\infty} m \, \psi_m^* \psi_n \, dx$$

$$\Rightarrow \int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx = \frac{m}{n}\int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx, \quad (m-n)\underbrace{\int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx}_{\text{must be } 0 \text{ if } m \neq n} = 0$$

$$\begin{cases} \hat{a}_+ = \frac{1}{\sqrt{2m\hbar\omega}}(-ip + m\omega x) \\ \hat{a}_- = \frac{1}{\sqrt{2m\hbar\omega}}(+ip + m\omega x) \end{cases}, \quad x = \frac{1}{2m\omega}\sqrt{2m\hbar\omega}\,(\hat{a}_+ + \hat{a}_-) = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}_+ + \hat{a}_-)$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi_n^* \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}_+ + \hat{a}_-)\,\psi_n \, dx = \sqrt{\frac{\hbar}{2m\omega}}\left(\int_{-\infty}^{+\infty} \psi_n^* \underbrace{\hat{a}_+ \psi_n}_{\sqrt{n+1}\,\psi_{n+1}} dx + \int_{-\infty}^{+\infty} \psi_n^* \underbrace{\hat{a}_- \psi_n}_{\sqrt{n}\,\psi_{n-1}} dx\right)$$

$$= 0$$

$$x^2 = \frac{\hbar}{2m\omega}(\hat{a}_+ + \hat{a}_-)(\hat{a}_+ + \hat{a}_-) = \frac{\hbar}{2m\omega}\left[(\hat{a}_+)^2 + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+ + (\hat{a}_-)^2\right]$$

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega}\int_{-\infty}^{+\infty} \psi_n^* \left[(\hat{a}_+)^2 + \underbrace{\hat{a}_+\hat{a}_-}_{\sqrt{n}\sqrt{n}} + \underbrace{\hat{a}_-\hat{a}_+}_{\sqrt{n+1}\sqrt{n+1}} + (\hat{a}_-)^2\right]\psi_n \, dx = \frac{\hbar}{2m\omega}(2n+1)$$

$$\langle V \rangle = \langle \tfrac{1}{2} m\omega^2 x^2 \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle$$

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

$$= \frac{1}{2} E_n$$

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Analytic method

$\frac{\hbar\omega}{2}\left(-\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2}+\frac{m\omega x^2\psi}{\hbar}\right)$

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

$$\frac{d^2}{dx^2}=\sqrt{\frac{m\omega}{\hbar}}\frac{d^2}{d\xi^2}$$

$$E\psi=\frac{\hbar\omega}{2}\left(-\frac{d^2}{d\xi^2}+\xi^2\right)\psi,\quad \underbrace{\boxed{\frac{2E\psi}{\hbar\omega}}}_{K}=\left(-\frac{d^2}{d\xi^2}+\xi^2\right)\psi$$

$$\frac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi \quad \text{when } \xi \text{ very large} \quad \frac{d^2\psi}{d\xi^2}\simeq\xi^2\psi,\ \psi(\xi)=Ae^{-\frac{\xi^2}{2}}+\underbrace{Be^{\frac{\xi^2}{2}}}_{\text{not normalizable}}$$

$$\Rightarrow \psi(\xi)\simeq Ae^{-\frac{\xi^2}{2}},\quad \psi(\xi)=h(\xi)e^{-\frac{\xi^2}{2}}$$

$$\frac{d\psi}{d\xi}=\left(\frac{dh}{d\xi}-\xi h\right)e^{-\frac{\xi^2}{2}} \qquad \frac{d^2\psi}{d\xi^2}=\left[\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(\xi^2-1)h\right]e^{-\frac{\xi^2}{2}}$$

$\frac{dh}{d\xi}e^{-\frac{\xi^2}{2}}-\xi he^{-\frac{\xi^2}{2}}$

$=\frac{d^2h}{d\xi^2}e^{-\frac{\xi^2}{2}}+\frac{dh}{d\xi}(-\xi)e^{-\frac{\xi^2}{2}}-he^{-\frac{\xi^2}{2}}-\frac{dh}{d\xi}\xi e^{-\frac{\xi^2}{2}}-\xi h(-\xi)e^{-\frac{\xi^2}{2}}$

$$\Rightarrow \frac{d^2\psi}{d\xi^2}=\left[\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(\xi^2-1)h\right]e^{-\frac{\xi^2}{2}}=(\xi^2-K)\psi$$

$$\Rightarrow \frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(K-1)h=0$$

$$h(\xi)=a_0+a_1\xi+a_2\xi^2+\cdots=\sum_{j=0}^{\infty}a_j\xi^j \qquad \frac{dh}{d\xi}=\sum_{j=0}^{\infty}ja_j\xi^{j-1}$$

$j(j-1)a_j\xi^{j-2}$

$$\frac{d^2h}{d\xi^2}=\sum(j+1)(j+2)a_{j+2}\xi^j$$

$$\Rightarrow \sum_{j=0}^{\infty}\underbrace{\left[(j+1)(j+2)a_{j+2}-2ja_j+(K-1)a_j\right]}_{=0}\xi^j=0,\quad a_{j+2}=\frac{(2j+1-K)}{(j+1)(j+2)}a_j \quad \text{recursion formula}$$

$$\text{for large } j,\ a_{j+2}\approx\frac{2}{j}a_j \qquad a_j\approx\frac{C}{(\frac{j}{2})!}$$

$a_5=\frac{2}{5}a_3=\frac{2}{5}\frac{2}{3}a_1$

$a_3=\frac{2}{1}a_1 \quad a_4=\frac{2}{2}a_2$

$a_2=\frac{-2(n)}{2}a_0$

$a_2=-a_0$

$$\Rightarrow h(\xi)=C\sum\frac{1}{(\frac{j}{2})!}\xi^j\approx C\sum\frac{1}{j!}\xi^{2j}\approx Ce^{\xi^2},\ \psi(\xi)=Ce^{\xi^2}e^{-\frac{\xi^2}{2}}=Ce^{\frac{\xi^2}{2}}$$

for physically acceptable solutions, let $K=2n+1$, then $a_{j+2}=\frac{-2(n-j)}{(j+1)(j+2)}a_j$

if $j=0$ $\quad n=0$ $\quad a_1=0$ to kill h_{odd} $\quad$ then $a_2=0$ $\quad h_0(\xi)=a_0$ $\quad \psi_0(\xi)=a_0e^{-\xi^2/2}$

if $j=1$ $\quad n=1$ $\quad a_0=0$ $\quad$ then $a_3=0$ $\quad h_1(\xi)=a_1\xi$ $\quad \psi_1(\xi)=a_1e^{-\frac{\xi^2}{2}}$ $\quad a_3=\frac{3-3}{2\times3}a_1$

if $j=0$ $\quad n=2$ $\quad$ then $a_2=-2a_0$ $\quad h_2(\xi)=a_0(1-2\xi^2)$

$j=2$ $\quad n=2$ $\quad a_4=0$ $\quad \psi_2(\xi)=a_0(1-2\xi^2)e^{-\frac{\xi^2}{2}}$

Hermite polynomials $H_n(x)=(-1)^ne^{x^2}\frac{d^n}{dx^n}e^{-x^2}$

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

$\psi(x=0)=0,\quad A+B=0$

$Ae^{ika}+Be^{-ika}=0$

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Free Particle

$V(x)=0$ everywhere

$\frac{d^2\psi}{dx^2}=-k^2\psi$

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi,\quad \frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi,\quad \psi(x)=Ae^{ikx}+Be^{-ikx}\qquad k=\frac{\sqrt{2mE}}{\hbar}$

a free particle can carry any energy $\qquad E=\frac{\hbar^2k^2}{2m}$

$$\Psi(x,t)=Ae^{ikx}e^{-i\frac{\hbar^2k^2}{2m\hbar}t}+Be^{-ikx}e^{-i\frac{\hbar^2k^2}{2m\hbar}t}$$

$$=Ae^{ik(x-\frac{\hbar k}{2m}t)}+Be^{-ik(x-\frac{\hbar k}{2m}t)}$$

phase velocity $V_p=\frac{\hbar k}{2m}$

$$=Ae^{i(kx-\frac{\hbar k^2}{2m})t}\qquad k=\pm\sqrt{\frac{2mE}{\hbar}}$$

$V_c=\frac{\hbar k}{m}=2V_p=\sqrt{\frac{2E}{m}}$

classical

$(e^{-ik\infty}-e^{+ik\infty})(e^{ik\infty}-e^{-ik\infty})\qquad e^{k^2\infty^2}-e^{-k^2\infty^2}-e^{-k^2\infty^2}+e^{k^2\infty^2}$

$\int_{-\infty}^{+\infty}\psi_k^*(x)\psi_k(x)\,dx=|A|^2\int_{-\infty}^{+\infty}e^{-ikx}e^{ikx}\,dx=\infty.$ this function isn't normalizable

a free particle cannot exist in a stationary state

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\underbrace{\phi(k)}_{C_n}\underbrace{e^{i(kx-\frac{\hbar k^2}{2m}t)}}_{\Psi_n(x,t)}dk$$

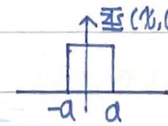
Plancherel's theorem 2.19

$$\boxed{\begin{gathered}f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}dk\\ \Updownarrow\\ F(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(x)e^{-ikx}dx\end{gathered}}$$

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

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

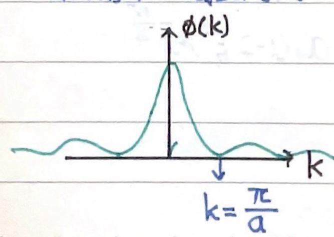
For example



$$\Psi(x,0)\begin{cases}\frac{1}{\sqrt{2a}}, & -a<x<a\\ 0, & \text{otherwise}\end{cases}$$

$$\phi(k)=\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{+a}e^{-ik}dx=\frac{1}{2\sqrt{\pi a}}\frac{1}{-i\hbar}e^{-i\hbar x}\Big|_{-a}^{a}=\frac{1}{\sqrt{\pi a}}\frac{\sin(ka)}{k}$$

$$\Psi(x,t)=\frac{1}{\pi\sqrt{2a}}\int_{-\infty}^{+\infty}\frac{\sin(ka)}{k}e^{i(kx-\frac{\hbar k^2}{2m}t)}dk$$



when $a\uparrow\quad \sigma_p\downarrow$

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