

Free particle, harmonic oscillator, Schrodinger equation

Free Particle

$$L = \frac{1}{2} m \dot{x}^2 \quad \text{Lagrangian}$$

$$i \leftrightarrow a$$

$$f \leftrightarrow b$$

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \int \dots \int dx_1 \dots dx_{N-1} \left(\frac{2\pi i \epsilon}{m} \right)^{-\frac{N}{2}} \exp \left[\frac{im}{2\epsilon} \sum_{i=1}^N (x_i - x_{i-1})^2 \right]$$

Gaussian integrals $\int e^{-ax^2} dx$ or $\int e^{-ax^2 + bx} dx$

Integral of a gaussian is a gaussian. Integration can be done variable after variable

$$K(b, a) = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \exp \left[\frac{im (x_b - x_a)^2}{2\hbar (t_b - t_a)} \right]$$

final result

Calculation is carried out as follows. Notice first

$$\int_{-\infty}^{+\infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{1}{2}} \exp \left[\frac{i m}{2 \hbar \epsilon} \left[(x_2 - x_1)^2 + (x_1 - x_0)^2 \right] \right] dx_1$$

$$= \sqrt{\frac{m}{2\pi i \hbar \cdot 2\epsilon}} \exp \left[i \frac{m}{2 \hbar (2\epsilon)} (x_2 - x_0)^2 \right]$$

Next we multiply this result by

$$x_0 = x_a, \quad t_a = t_0$$

$$x_N = x_b, \quad t_b = t_N$$

$$\frac{\sqrt{m}}{\sqrt{2\pi i \hbar \epsilon}} \exp \left[\frac{i m}{2 \hbar \epsilon} (x_3 - x_2)^2 \right]$$

and integrate now over x_2 to get:

$$\left(\frac{m}{2\pi i \hbar 3\epsilon} \right)^{\frac{1}{2}} \exp \left[i \frac{m}{2 \hbar \cdot 3\epsilon} (x_3 - x_0)^2 \right]$$

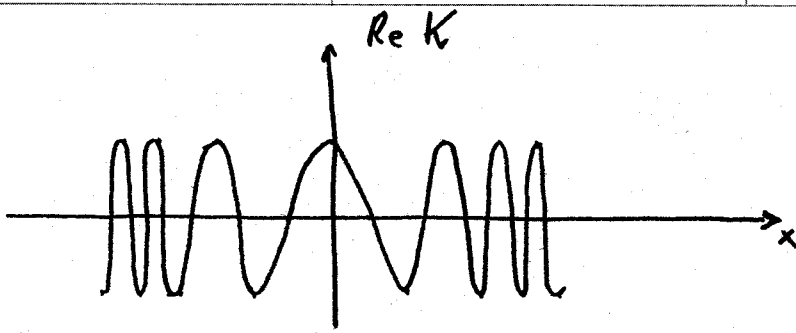
This established a recursion which, after $N-1$ steps, gives

$$\left(\frac{m}{2\pi i \hbar N \cdot \epsilon} \right)^{\frac{1}{2}} \exp \left[i \frac{m}{2 \hbar N \cdot \epsilon} (x_N - x_0)^2 \right]$$

which is identical to the announced result

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2 + \beta x} dx = e^{\frac{\beta^2}{4\alpha}} \left(\frac{\pi}{\alpha} \right)^{\frac{1}{2}} \quad \text{Gaussian}$$

even if α and β are complex
 $\text{Re } \alpha > 0$ guarantees convergence



$$a = (0, 0)$$

$$b = (x, t)$$

$$K(x, t; 0, 0) = \left(\frac{m}{2\pi i \hbar t} \right)^{\frac{1}{2}} e^{\frac{imx^2}{2\hbar t}}$$

For large x , rapidly oscillating real and imaginary parts (90° out of phase) when looked at for fixed t .

wavelength of oscillation

$$2\pi = \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t} = \frac{m x \lambda}{\hbar t} + \frac{m \lambda^2}{2\hbar t}$$

$$\lambda = \frac{2\pi \hbar}{m \left(\frac{x}{t} \right)} \quad x \gg \lambda \quad \uparrow \text{negligible}$$

From classical viewpoint a particle which moves from origin to x in time t has velocity $\frac{x}{t}$ and momentum $m \frac{x}{t}$.

From QM viewpoint, if motion can be adequately described by classical momentum $p = m \frac{x}{t}$, then amplitude varies in space with wavelength $\lambda = \frac{h}{p}$ (de Broglie)

More generally:

$$K \sim \exp \left[\frac{i}{\hbar} S_{cl}(b, a) \right]$$

amplitude of particle to arrive at point b

we want to show that amplitude varies rapidly in space with wavelength $\lambda = \frac{h}{p}$

if $S_{cl} \gg \hbar$, phase varies rapidly as a function of end point b

$$k = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial x_b}$$

change in phase per unit displacement (wave number)

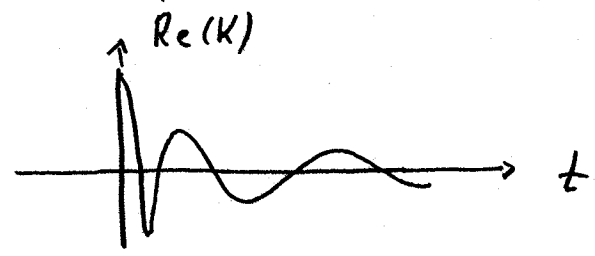
$$\rightarrow p = \hbar k$$

$$p = \frac{\partial L}{\partial \dot{x}} \quad \left. \frac{\partial L}{\partial \dot{x}} \right|_{x=x_b} = \frac{\partial S_{cl}}{\partial x_b} \quad k = \frac{2\pi}{\lambda}$$

$$\delta S = \int_{t_a}^{t_b} \delta x \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right] dt$$

$$p = \frac{h}{\lambda} \quad \text{de Broglie}$$

Next, we look at time dependence of K:



both frequency and amplitude change

For large t

$$2\pi = \frac{m x^2}{2\hbar t} - \frac{m x^2}{2\hbar (t+T)} = \frac{m x^2}{2\hbar t^2} \left(\frac{T}{1 + \frac{T}{t}} \right)$$

T period of oscillation

$$\omega = \frac{2\pi}{T}$$

$$\omega \approx \frac{m}{2\hbar} \left(\frac{x}{t} \right)^2$$

↓

$$\text{Energy} = \hbar \omega$$

more generally: $\omega = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial t} \rightarrow \omega = \frac{E}{\hbar}$

$$E = L - \dot{x} p$$

$$L(x_b) - \dot{x}_b \left(\frac{\partial L}{\partial \dot{x}} \right)_{x=x_b} = \frac{\partial S_{cl}}{\partial t_b}$$

(1) If the amplitude K varies as e^{ikx} , we say particle has momentum $\hbar k$

(2) If amplitude K has a definite frequency $-e^{-i\omega t}$ we say energy is $\hbar \omega$

By substitution for free particle:

$$-\frac{\hbar}{i} \frac{\partial K(b,a)}{\partial t_b} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(b,a)}{\partial x_b^2}$$

required to show
in 242

$$t_b > t_a$$

wave function:

$$\psi(x', t') = \int_{-\infty}^{+\infty} K(x', t'; x, t) \psi(x, t) dx$$

Using the equation for K ,

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad \text{Schrödinger Eq. !}$$

required to
show in 242

Harmonic Oscillator

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

$$K_{L(b,a)} = \left(\frac{m\omega}{2\pi i \hbar \sin \omega T} \right)^{\frac{1}{2}} \exp \left\{ \frac{i m \omega}{2 \hbar \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2 x_a x_b \right] \right\}$$

$$T = t_b - t_a$$

the exponent has the form $e^{\frac{i}{\hbar} S_{cl}}$

$$S_{cl} = \frac{m\omega}{2 \sin \omega T} \left[(x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right]$$

required to show in 242

Proof comes from recursive integration

Schrödinger Equation

$$\psi(x, t+\epsilon) = \int_{-\infty}^{+\infty} \frac{1}{A} \left\{ \exp \left[\frac{i}{\hbar} \frac{m(x-y)^2}{2\epsilon} \right] \right\} \cdot$$

↙ rapidly oscillates for large $y-x$

$$\times \left\{ \exp \left[-\frac{i}{\hbar} \epsilon V \left(\frac{x+y}{2}, \epsilon t \right) \right] \right\} \psi(y, t) dy$$

$y = x + \eta$ substitution, expect large contribution for small η only

$$\psi(x, t+\epsilon) = \int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{i m \eta^2}{2\hbar \epsilon}} e^{-\frac{i \epsilon}{\hbar} V \left[\frac{x+\eta}{2}, t \right]} \psi(x+\eta, t) d\eta$$

integral contributes in $0 \leq |\eta| \leq \sqrt{\frac{\hbar \epsilon}{m}}$ range

$$\psi(x,t) + \epsilon \frac{\partial \psi}{\partial t} = \int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \left[1 - \frac{i\epsilon}{\hbar} V(x,t) \right]$$

power series $\times \left[\psi(x,t) + \eta \frac{\partial \psi}{\partial x} + \frac{1}{2} \eta^2 \frac{\partial^2 \psi}{\partial x^2} \right] d\eta$

$$\frac{1}{A} \int_{-\infty}^{+\infty} e^{\frac{im\eta^2}{2\hbar\epsilon}} d\eta = \frac{1}{A} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}}$$

$$A = \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}} \text{ was chosen before !}$$

$$\int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \cdot \eta d\eta = 0$$

$$\int_{-\infty}^{+\infty} \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} \cdot \eta^2 d\eta = \frac{i\hbar\epsilon}{m}$$

Therefore $\psi + \epsilon \frac{\partial \psi}{\partial t} = \psi - \frac{i\epsilon}{\hbar} V\psi - \frac{\hbar\epsilon}{2im} \frac{\partial^2 \psi}{\partial x^2}$

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x,t) \psi(x,t)$$

Schrödinger Eq. !