Free Particle and Oscillator ; Schrodinger eq.

Free Particle

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

$$i \leftrightarrow a$$
$$f \leftrightarrow b$$

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

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

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

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

Next we multiply this result by

$$x_0 = x_a, \; t_a = t_0$$
$$x_N = x_b \quad t_b = t_N$$

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

and integrate now over x_2 to get:

$$\left(\frac{m}{2\pi i \hbar \, 3\varepsilon}\right)^{\frac{1}{2}} \exp\left[i\frac{m}{2\hbar \cdot 3\varepsilon} (x_3-x_0)^2\right]$$
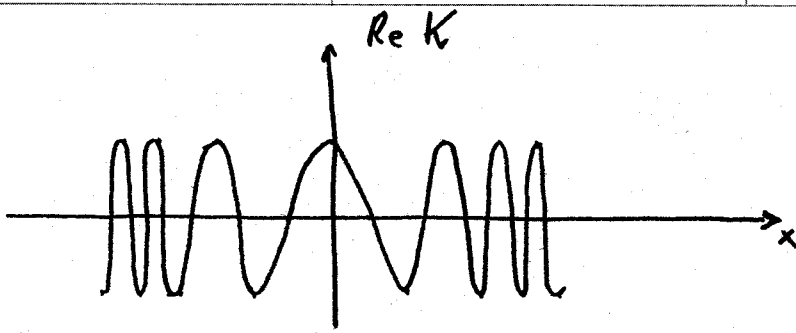
This established a recursion which, after $N-1$ steps, gives

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

which is identical to the announced result

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

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

Re K

$a = (0,0)$

$b = (x, t)$

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

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

wavelength of oscillation :

$$2\pi = \frac{m(x+\lambda)^2}{2\hbar t} - \frac{m x^2}{2\hbar t} = \frac{m x \lambda}{\hbar t} + \underbrace{\frac{m \lambda^2}{2\hbar t}}_{\substack{x \gg \lambda \\ \text{negligible}}}$$

$$\lambda = \frac{2\pi \hbar}{m\left(\frac{x}{t}\right)}$$

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 $\lambda = \frac{\hbar}{p}$

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

$$k = \frac{1}{\hbar} \frac{\partial S_{cl}}{\partial x_b} \qquad \text{change in phase per unit displacement}$$
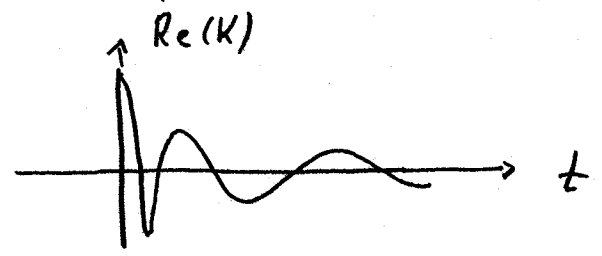
$$\rightarrow p = \hbar k \qquad \text{(wave number)}$$

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

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

$$p = \frac{\hbar}{\lambda} \qquad \text{de Broglie}$$

Next, we look at time dependence of K:

$Re(K)$

t

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

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

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

$$\downarrow$$

$$Energy = \hbar \omega$$

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

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

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

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

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

5.

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 hw 2

$$t_b > t_a$$

wave function:

$$\psi(x_1', t') = \int_{-\infty}^{+\infty} K(x', t'; x, t)\, \psi(x, t)\, dx$$

Using the equation for K,

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

required to show in hw2

Harmonic Oscillator

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

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

$$T = t_b - t_a$$

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

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

reqired to show in hw 2

Proof comes from recursive integration

Schrödinger Equation

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

rapidly oscillates for large $y-x$

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

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

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

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

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

power series

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

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

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

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

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

Therefore

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

$$\downarrow$$

$$\boxed{ -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x,t) \psi(x,t) \\ \text{Schrödinger Eq. !} }$$