Schrödinger Equation, Propagator Trace

We have seen that the free particle propagator amplitude has the form

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

Using this form, we can easily show that the wavefunction (which is the probability amplitude of the particle) satisfies the Schrödinger equation.

Same observation can be made about harmonic oscillator

General argument will then follow.

By substitution for free particle :

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

$$t_b > t_a$$

wave function :

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

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. !

Harmonic Oscillator

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

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

$$T = t_b - t_a$$

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

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

Proof comes from recursive integration

Schrödinger Equation

rapidly oscillates for large $y-x$

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

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

$y = x + \eta$ 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

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

power series

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

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

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

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

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

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

$$\downarrow$$

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

Schrödinger Eq. !

We did not have to restrict V to be time independent:

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

$$\downarrow$$

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \qquad \text{Hamilton operator}$$

$$\frac{d}{dt}\left(\int \psi^* \psi \, dx\right) = 0 \qquad \text{derivation is conventional}$$

conservation of probability

Stationary states of definite energy:

$$\psi(x,t) = e^{-\frac{i}{\hbar}Et}\,\phi(x)$$

$$H\phi = E\phi \qquad \text{eigenvalue equation}$$

$$\psi = \underbrace{c_1\, e^{-\frac{i}{\hbar}E_1 t}\cdot \phi_1(x)}_{\psi_1} + \underbrace{c_2\, e^{-\frac{i}{\hbar}E_2 t}\,\phi_2(x)}_{\psi_2}$$

linear combination is also a solution

$$\int_{-\infty}^{+\infty} \phi_n^*(x)\,\phi_m(x)\,dx = \delta_{nm}$$

orthonormal stationary states
(f.e. oscillator eigenstates)

$$f(x) = \sum_{n=1}^{\infty} a_n \phi_n(x) \qquad \text{for arbitrary function}$$

$$\int_{-\infty}^{+\infty} \phi_m^*(x) f(x)\,dx = \sum_{n=1}^{\infty} a_n \int_{-\infty}^{+\infty} \phi_m^* \phi_n\,dx = a_m$$

$$f(x) = \sum_{n=1}^{\infty} \phi_n(x) \int_{-\infty}^{+\infty} \phi_n^*(y) f(y)\,dy =$$

$$= \int_{-\infty}^{+\infty} \left[\sum_{n=1}^{\infty} \phi_n(x)\,\phi_n^*(y) \right] f(y)\,dy$$

$$\downarrow$$

$$\delta(x-y) = \sum_{n=1}^{\infty} \phi_n(x)\,\phi_n^*(y)$$

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \, e^{-\frac{i}{\hbar} E_n t} \phi_n(x)$$

Let $f(x) = \psi(x,t_1) = \sum_{n=1}^{\infty} c_n \, e^{-\frac{i}{\hbar} E_n t_1} \phi_n(x) = \sum_{n=1}^{\infty} a_n \phi_n(x)$

be the wavefunction at $t = t_1$

$$\downarrow$$

$$c_n = a_n \, e^{+\frac{i}{\hbar} E_n t_1}$$

$$\psi(x,t_2) = \sum_{n=1}^{\infty} a_n \, e^{\frac{i}{\hbar} E_n (t_1 - t_2)} \phi_n(x)$$

$$\psi(x,t_2) = \sum_{n=1}^{\infty} \phi_n(x) \, e^{-\frac{i}{\hbar} E_n (t_2 - t_1)} \int_{-\infty}^{+\infty} \phi_n^*(y) f(y) \, dy$$

$$= \int_{-\infty}^{+\infty} \sum_{n=1}^{\infty} \phi_n(x) \phi_n^*(y) \, e^{-\frac{i}{\hbar} E_n (t_2 - t_1)} f(y) \, dy$$

On the other hand:

$$\psi(x,t_2) = \int_{-\infty}^{+\infty} K(x, t_2 ; y, t_1) f(y) \, dy$$

By comparison:

$$K(x_2,t_2;x_1,t_1) = \sum_{n=1}^{\infty} \phi_n(x_2)\phi_n^*(x_1)\, e^{-\frac{i}{\hbar}E_n(t_2-t_1)} \quad \text{for } t_2>t_1$$

$$= 0 \quad \text{for } t_2 < t_1 \text{ by definition}$$

With the choice $t_1=0$, $t_2=t$, we find:

$$\underbrace{\int_{-\infty}^{+\infty} dx\, K(x,t;x,0)}_{\mathrm{Tr}\,K} = \sum_{n=1}^{\infty} \underbrace{\int_{-\infty}^{+\infty} dx\, \phi_n^*(x)\phi_n(x)}_{1}\; e^{-\frac{i}{\hbar}E_n t}$$

$$\mathrm{Tr}\,K = \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}E_n t}$$

The fourier transform of $\mathrm{Tr}\,K(t)$ will provide the spectrum