0.1 Lecture V

0.2 Wavepackets

Consider the 1D system for a particle whose hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{1}$$

The Schrodinger Eq. in Hilbert space has the form

$$i\hbar \frac{\partial|\Psi(t)>}{\partial t} = \hat{H}|\Psi(t)> \tag{2}$$

and the formal solution

$$|\Psi(t)>= \exp(-i/\hbar \hat{H} t)|\Psi(0)> \tag{3}$$

(Question. Can you prove this?). We take the inner product with ket $|x>$

$$\begin{aligned} &< x|\Psi(t)>=< x|\exp(-i\frac{\hat{H}}{\hbar}t)|\Psi(0)>= \\ &\int dp \; < x|\exp(-i\frac{\hat{H}}{\hbar}t)|p>< p|\Psi(0)> \end{aligned} \tag{4}$$

If we assume that $V(x) = 0$(i.e. a free particle) using $< x|\exp(-i\frac{\hat{H}}{\hbar}t)|p>=$ $\exp(-i\frac{p^2}{2m\hbar}t) < x|p>$ and $< p|\Psi(0)>= \int dx' < p|x'>< x'|\Psi(0)>$, we get

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp \int dx' \exp(-i\frac{p^2}{2m\hbar}t) \exp(i\frac{p}{\hbar}(x-x'))\Psi_0(x') \tag{5}$$

where we defined $\Psi(x,t) =< x|\Psi(t)>$, and $\Psi_0(x) =< x|\Psi(0)>$. We can re-write the above expression in the form

$$\Psi(x,t) = \int dx' K(xt;x't')\Psi(x',t') \tag{6}$$

where in our case we set $t' = 0$ and

$$K(xt;x't') = \frac{1}{\sqrt{2\pi\hbar}} \int dp \exp(-i\frac{p^2(t-t')}{2m\hbar}) \exp(i\frac{p}{\hbar}(x-x')) \tag{7}$$

is called the propagator for a free particle. It can also be expressed as the probability amplitude

$$< x|\exp(-i\hat{H}t)|x' > \tag{8}$$

whose square gives the probability density for a particle to be found in the vicinity of x at time t, provided that the system is described by probability amplitude $\Psi_0(x)$ at t=0. **Proof:**

$$\begin{aligned}
< x|\exp(-i\hat{H}t)|x' > &= \\
\int dp \int dp' \exp(-i\frac{p^2}{2m\hbar}t) < p|p' >< x|p >< p'|x' > &= \\
\frac{1}{2\pi\hbar}\int dp \int dp' \delta(p'-p) \exp(-i\frac{p^2}{2m\hbar}t) \exp(i\frac{p}{\hbar}(x-x')) &= \\
\frac{1}{2\pi\hbar}\int dp \exp(-i\frac{p^2}{2m\hbar}t) \exp(i\frac{p}{\hbar}(x-x')) &= \\
K(xt : x'0) &
\end{aligned} \tag{9}$$

We can perform the integral to get an explicit expression for the free particle propagator (see text)

$$K(xt; x't') = \sqrt{\frac{m}{2\pi i\hbar t}} \exp(\frac{im(x-x')^2}{2\hbar t}) \tag{10}$$

Gaussian wavepackets

We now make some assumptions regarding the initial condition, $\Psi_0(x) \equiv \Psi(x, t=0)$. We define a gaussian wavepacket

$$\Psi_0(x) = \frac{1}{a^{1/4}(2\pi)^{1/4}} \exp(i\frac{p_0}{\hbar}x) \exp(-x^2/4a^2) \tag{11}$$

Using this we can find the expectation value

$$< \hat{x} >= \int \Psi_0^*(x) x \Psi(x) = 0 \tag{12}$$

and the variance $< \Delta x >^2 = < x^2 > - < x >^2$, but

$$< \hat{x}^2 >= \int \Psi_0^*(x) x^2 \Psi(x) = a^2 \tag{13}$$

and so $<\Delta x>= a$. Also

$$< \hat{p} >= -i\hbar \int dx \Psi_0^*(x) \frac{\partial \Psi(x)}{\partial x} = p_0 \tag{14}$$

We find (can you show this?) $< \hat{p}^2 > - < \hat{p} >^2 = \hbar^2/4a^2$ or

$$\Delta p = \hbar/2a \tag{15}$$

The Gaussian wavepacket has the interesting property that

$$\Delta x \, \Delta p = \hbar/2. \tag{16}$$

It gives the minimum uncertainty in both $\hat{x}$, $\hat{p}$ when simultaneous measurements are made. Using the the Gaussian wavepacket we calculate the wavepacket at some time $t > 0$. Hence

$$\begin{aligned} \Psi(x,t) &= \int dx' K(xt; x'0) \Psi_0(x') \\ & \int dx' \sqrt{\frac{m}{2\pi i \hbar t}} \exp(\frac{im(x-x')t}{2\hbar t}) \\ & \times \frac{1}{a^{1/4}(2\pi)^{1/4}} \exp(i\frac{p_0}{\hbar}x) \exp(-x^2/4a^2) \end{aligned} \tag{17}$$

evaluating this integral (see text) we get

$$\begin{aligned} \Psi(x,t) &= \frac{1}{a^{1/2}(2\pi)^{1/4}(1+it/\tau)^{1/2}} \exp[i\frac{\tau}{t}(\frac{x}{2a})^2] \\ & \times \ \exp[-\frac{(i\tau/4a^2t)(x-p_0t/m)^2}{1+it/\tau}] \\ \tau \equiv \frac{2ma^2}{\hbar} & \end{aligned} \tag{18}$$

We calculate the probability density

$$\begin{aligned} P(x,t) = |\Psi(x,t)|^2 &= \frac{1}{a\sqrt{2\pi}(1+t^2/\tau^2)^{1/2}} \\ & \exp[-\frac{(x-p_0t/m)^2}{2a^2(1+t^2/\tau^2)}] \end{aligned} \tag{19}$$

this looks like a wavepacket but now with a new width

$$a(1+t^2/\tau^2)^{1/2} \tag{20}$$

and the center of symmetry has shifted to the value $x = p_0/m\,t$. The normalization factor changes so the $\int dx P(x,t) = 1$ at all times.

Consider what happens if we let the parameter $\hbar \to 0$. This is called the classical limit, and as $\hbar \to 0$ we get

$$P(x,t) = \frac{1}{a\sqrt{2\pi}} \exp[-\frac{(x - p_0 t/m)^2}{2a^2}]. \tag{21}$$

This is exactly what one would get, in classical mechanics, if we had some uncertainty in the position of the particle, given by a Gaussian at $t = 0$, and we looked we considered calssical propagation. We get the same uncertainty at time t, as at $t = 0$ or $\Delta x(t) = \Delta x(0)$. Also, if we let $a \to 0$ we find

$$P(x,t) = \delta(x - p_0 t/m) \tag{22}$$

the particle moves on a classical trajectory.

If $\hbar \neq 0$ we find the uncertainty Δx increases in time according to

$$\Delta x(t) = \Delta x(0)(1 + t^2/\tau^2)^{1/2} \tag{23}$$

Feynman Path Integral

Up to now we considered the propagator for a free particle. When $\hat{V} \neq 0$, it is much more difficult to obtain a closed form for the propagator, and only a few cases are available for closed form analytic representation. However, there is an alternative representation for the propagator $K(xt; x't')$ for arbitrary $\hat{V}$ that is called the Feynman path integral representation of the propagator. We have,

$$K(xt; x't') =< x| \exp(-i\frac{\hat{H}}{\hbar}(t - t'))|x' > . \tag{24}$$

Lets call the total time interval $\tau \equiv (t - t')$ and we define a small time interval $\Delta t \equiv (t - t')/N$ where N is some large integer. We can then write the above amplitude as

$$\begin{aligned} < x| \exp(-i\frac{\hat{H}}{\hbar}(t \quad - \quad t_1)) \exp(-i\frac{\hat{H}}{\hbar}(t_1 - t_2)) \exp(-i\frac{\hat{H}}{\hbar}(t_2 - t_3))... \\ \exp(-i\frac{\hat{H}}{\hbar}(t_{N-1} \quad - \quad t'))|x > \end{aligned} \tag{25}$$

which we can also express as

$$
\begin{aligned}
\int dx_1 \int dx_2 ... \int dx_{N-1} \quad \times \\
< x|\exp(-i\frac{\hat{H}}{\hbar}(t-t_1))|x_1 >< x_1|\exp(-i\frac{\hat{H}}{\hbar}(t_1-t_2))|x_2 > \quad \times \\
< x_{N-1}|\exp(-i\frac{\hat{H}}{\hbar}(t_{N-1}-t'))|x >
\end{aligned}
\tag{26}
$$

Now $\exp(-i\frac{\hat{H}}{\hbar}\Delta\tau) \neq \exp(-i\frac{\hat{H}_0}{\hbar}\Delta\tau)\exp(-i\frac{\hat{V}}{\hbar}\Delta\tau)$, where $\hat{H}_0 \equiv \hat{p}^2/2m$ because $[\hat{H}_0, \hat{V}] \neq 0$, however, if Δt is sufficiently small then we can replace the inequalty with $\approx$. In the limit $\Delta t \to 0$ we are allowed the express the exponents as the products

$$
\begin{aligned}
\int dx_1 \int dx_2 ... \int dx_{N-1} \times \\
< x|\exp(-i\frac{\hat{H}_0}{\hbar}(t-t_1))|x_1 > \exp[-i\frac{V(x_1)}{\hbar}(t-t_1] \times \\
< x_1|\exp(-i\frac{\hat{H}_0}{\hbar}(t_1-t_2))|x_2 > \exp[-i\frac{V(x_2)}{\hbar}(t_1-t_2)]... \times \\
< x_{N-1}|\exp(-i\frac{\hat{H}_0}{\hbar}(t_{N-1}-t'))|x' > \exp[-i\frac{V(x')}{\hbar}(t_{N-1}-t')]
\end{aligned}
\tag{27}
$$

Using the expression for the free propagator, we get for the above expression

$$
\begin{aligned}
(\sqrt{\frac{m}{2\pi i\hbar\Delta t}})^{N-1} \int dx_1 \int dx_2 ... \int dx_{N-1} \times \\
\exp(\frac{im(x_1-x)^2}{2\hbar(t-t_1)})\exp[-i\frac{V(x_1)}{\hbar}(t-t_1)] \times \\
\exp(\frac{im(x_2-x_1)^2}{2\hbar(t_1-t_2)})\exp[-i\frac{V(x_2)}{\hbar}(t_1-t_2)]... \times \\
\exp(\frac{im(x'-x_{N-1})^2}{2\hbar(t_{N-1}-t')})\exp[-i\frac{V(x')}{\hbar}(t_{N-1}-t')]
\end{aligned}
\tag{28}
$$

Consider the classical Lagrangian for a particle in $1D$.

$$
\mathcal{L}(x) = \frac{m\dot{x}^2}{2} - V(x) \tag{29}
$$

Consider the action

$$
\int_{t_a}^{t_b} dt\, \mathcal{L} = m\frac{(x_b-x_a)^2}{t_b-t_a} - V(x_a)(t_b-t_a) \tag{30}
$$

where we defined $x_a \equiv x(t_a)$, $x_b \equiv x(t_b)$ and we took $t_b - t_a$ to be an infitesimal interval. We therefore recognize that the product of factors can be expressed as

$$(\sqrt{\frac{m}{2\pi i\hbar\Delta t}})^{N-1} \int dx_1 \int dx_2 ... \int dx_{N-1} \times$$
$$\exp(\frac{i}{\hbar}\int_{t_1}^{t} dt_1 \mathcal{L}(x_1)] \; \exp[\frac{i}{\hbar}\int_{t_2}^{t_1} dt_2 \mathcal{L}(x_2)] \, ... \exp[\frac{i}{\hbar}\int_{t'}^{t_{N-1}} dt_{N-1}\mathcal{L}(x')] \quad (31)$$

Or

$$(\sqrt{\frac{m}{2\pi i\hbar\Delta t}})^{N-1} \int dx_1 \int dx_2 ... \int dx_{N-1} \times$$
$$\exp(\frac{i}{\hbar}\Big[\Big[\int_{t_1}^{t} dt_1 \mathcal{L}(x_1)] + \int_{t_2}^{t_1} dt_2 \mathcal{L}(x_2)] \, ... + \int_{t'}^{t_{N-1}} dt_{N-1}\mathcal{L}(x')]) \quad (32)$$

The above expression has the form of the path integral and thus

$$\begin{aligned} K(xt;x't') = \quad & Lim_{N\to\infty}\,(\sqrt{\tfrac{m}{2\pi i\hbar\Delta t}})^{N-1}\int dx_1 \int dx_2 ... \int dx_{N-1} \times \\ \exp(\frac{i}{\hbar} \quad & \Big[\int_{t_1}^{t} dt_1 \mathcal{L}(x_1)] + \int_{t_2}^{t_1} dt_2 \mathcal{L}(x_2) \, ... + \int_{t'}^{t_{N-1}} dt_{N-1}\mathcal{L}(x')]) \equiv \\ & \int_{x'}^{x} \mathcal{D}(x(t)) \exp\Big[i \int_{t'}^{t} \tfrac{dt}{\hbar} \mathcal{L}(x,\dot{x})\Big] \end{aligned} \quad (33)$$

Thus the propagator is expressed as a sum over all paths of the exponent of the action.

Homework

Consider a 1 D particle that is constrained to move in a container whose sides are located at $x = \pm L/2$.

(a) Find the time independent energy eigenstates for this system. The eigenstates must vanish at the boundaries of the container.

(b) Use the result of (a) to find the time-dependent functions corresponding to the energy eigenstates found in (a).

(c) Given an hamiltonian H, whose eigenstates are labeled $|n>$ with eigenvalue E_n. Show that the propagator

$$< x'|\exp(-i/\hbar \hat{H}(t-t')|x> = \sum_n u_n(x')^* u_n(x) \exp(-i/\hbar E_n(t-t')) \quad (34)$$

where $u_n(x) =< x|n >$.

(d) Use the results of part (a) and (c) to find an expression for the propagator $K(xt; x't')$. Simplify as much as you can.

(e) Suppose that at t=0, the particle is found in a Gaussian wavepacket of width $a = L/8$, and is characterized by $< p >= p_0$. Use the result of part (d) to find an expression for the probability amplitude $\Psi(x, t)$ for any time $t > 0$.