Ph 12b Quantum Physics
9 February 2010
The free particle

Note Title 2/6/2010

Fourier series and the Fourier transform:

Consider periodic functions on the interval $[-\frac{L}{2}, \frac{L}{2}]$. We denote $\psi(x) = \langle x|\psi\rangle$: the wave function evaluated at position x is the inner product of state vector $|\psi\rangle$ with (improper) position eigenstate $|x\rangle$. Position eigenstates with distinct eigenvalues are orthogonal, and eigenstates have "continuum" normalization

$$\langle y|x\rangle = \delta(x-y)$$ where $\delta(x-y)$ is the Dirac δ function

can be interpreted as $\psi_x(y)$: the wave function of position eigenstate with eigenvalue x, regarded as a function of y. The completeness relation is: $\hat{I} = \int_{-L/2}^{L/2} dx\, |x\rangle\langle x|$.

The wave number operator is $\hat{k} = -i\frac{d}{dx}$ (and momentum operator is $\hat{p} = \hbar\hat{k}$). The orthonormal basis of $\hat{k}$ eigenstates is $\{|k_n\rangle, n \in \mathbb{Z}\}$

where $$\langle x|k_n\rangle = \frac{1}{\sqrt{L}} e^{ik_n x}$$ and $k_n = \frac{2\pi}{L} n$;

Thus $$\langle k_n|k_m\rangle = \delta_{nm}.$$

These eigenstates are complete:
$$\sum_{n=-\infty}^{\infty} |k_n\rangle\langle k_n| = \hat{I}$$

Here $\hat{I}$ denotes the identity operator acting on Hilbert space

$\mathcal{H} = \{$ square integrable periodic functions on $[-\frac{L}{2}, \frac{L}{2}]\}$.

Completeness implies

$$\psi(x) = \langle x | \psi \rangle = \sum_{n=-\infty}^{\infty} \langle x | k_n \rangle \langle k_n | \psi \rangle$$

where $\langle x | k_n \rangle = \frac{1}{\sqrt{L}} e^{i k_n x}$, and

$$\langle k_n | \psi \rangle = \int_{-L/2}^{L/2} dx \, \frac{1}{\sqrt{L}} e^{-i k_n x} \psi(x).$$

Thus the completeness relation is just a succinct way to express the Fourier Theorem for periodic functions.

Furthermore,

$$\delta(x-y) = \langle y | x \rangle = \langle y | \hat{I} | x \rangle = \sum_{n=-\infty}^{\infty} \langle y | k_n \rangle \langle k_n | x \rangle$$

$$= \frac{1}{L} \sum_{n=-\infty}^{\infty} e^{i k_n (x-y)}$$

is another, equivalent, way to express the Fourier theorem.

This identity relates two ways of writing a <u>distribution</u>, not a <u>function</u>. That is, the sum over n does not converge to any function, yet makes sense when we "smear" the sum by integrating it against a smooth periodic function.

We may obtain the Fourier theorem for functions on the real line by taking the formal limit $L \to \infty$. In this limit, our expression for $\delta(x-y)$ is regarded as the Riemann approximation to an integral

$$\delta(x-y) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \frac{2\pi}{L} e^{i k_n (x-y)} \xrightarrow[L \to \infty]{} \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{i k (x-y)}$$

(since $2\pi/L$ is the spacing $k_{n+1}-k_n$ between consecutive values of k_n). Therefore, on the real line we define momentum eigenstates with "continuum normalization" such that $\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx}$,

where

$$\delta(x-y) = \langle x|y\rangle = \int_{-\infty}^{\infty} dk\, \langle x|k\rangle\langle k|y\rangle \; ; \text{ that is,}$$

$$\int_{-\infty}^{\infty} dk\; |k\rangle\langle k| = \hat{I}$$

This completeness relation implies

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{\infty} dk \langle x|k\rangle\langle k|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int dk\, e^{ikx}\langle k|\psi\rangle$$

$$\tilde{\psi}(k) = \langle k|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-ikx}\psi(x),$$

which is the Fourier theorem for functions on $\mathbb{R}$.

Note that $\hat{I} = \int_{-\infty}^{\infty} dx\; |x\rangle\langle x|$

(completeness of position eigenstates) implies

$$\langle k'|k\rangle = \int_{-\infty}^{\infty} dx \langle k'|x\rangle\langle x|k\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = \delta(k-k')$$

To summarize: on real line, both position and momentum eigenstates obey continuum normalization,

$$\langle k'|k\rangle = \delta(k-k') \qquad \langle x'|x\rangle = \delta(x-x')$$

and completeness:

$$\hat{I} = \int_{-\infty}^{\infty} dk \; |k\rangle\langle k| = \int_{-\infty}^{\infty} dx \; |x\rangle\langle x|$$

where $\langle x | k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$, and

$\psi(x) = \langle x|\psi\rangle$, $\quad \tilde{\psi}(k) = \langle k|\psi\rangle$

are Fourier transforms of one another.

The free-particle "propagator":

For a free particle in one dimension, with Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{P}^2 = \frac{\hbar^2}{2m}\hat{K}^2,$$

the wave-number eigenstates are also energy eigenstates. The time evolution operator is

$$\hat{U}(t) = \exp(-i\hat{H}t/\hbar) = \int_{-\infty}^{\infty} dk \; |k\rangle e^{-i\omega_k t}\langle k|$$

where $\omega_k = E_k/\hbar = \dfrac{\hbar k^2}{2m}$.

We may express the wavefunction $\psi(x,t)$ in terms of the initial wavefunction $\psi(x,0)$ at time zero as follows:

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|\hat{U}(t)|\psi(0)\rangle$$

$$= \int_{-\infty}^{\infty} dx' \; \langle x|\hat{U}(t)|x'\rangle\langle x'|\psi(0)\rangle \qquad \text{(using completeness of position eigenstates)}$$

$$= \int_{-\infty}^{\infty} dx' \; \psi(x',0) \; K(x',x;t)$$

where $K(x',x;t) = \langle x|\hat{U}(t)|x'\rangle$

(I would have preferred to define $\langle x|\hat{U}|x'\rangle = K(x,x';t)$, reversing x and x' in argument of K, but I am following Liboff's notation here.)

Thus, $K(x',x;t)$ is the amplitude for a particle that is at position x' at time 0 to arrive at position x at time t. It is called the "Green function" or "propagator" for the free particle, and it encodes the general solution to the time-dependent Schrödinger equation.

To find an explicit formula for $K(x',x;t)$, we plug in our expansion of $\hat{U}(t)$ in the wave-number eigenstate basis:

$$K(x',x;t) = \int_{-\infty}^{\infty} dk \, \langle x|k\rangle e^{-i\omega_k t} \langle k|x'\rangle$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \, e^{ik(x-x')} e^{-i\omega_k t}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \, e^{ik(x-x')} e^{-i\hbar k^2 t/2m}$$

For $t=0$, this expression becomes

$\delta(x'-x) = \langle x|x'\rangle = \langle x|\hat{U}(0)|x'\rangle$, as expected.

For $t \neq 0$, the integral actually converges (though "conditionally," not "absolutely"). The integrand wiggles as a function of k, but wiggles faster and faster as $|k| \to \infty$. Thus the <u>area</u> under each positive or negative wiggle decreases as $|k|$ increases, and the integrand wiggles with decreasing amplitude as the limits of integration increase. (see plots of $\sin k^2$ and its integral on the preceding page.)

We can evaluate the k integral explicitly to find the function $K(x', x; t)$. The integral is Gaussian, and since we will often need to evaluate Gaussian integrals, let's derive a useful general formula for

$$\int_{-\infty}^{\infty} dx\, e^{iBx} e^{-\frac{1}{2}Ax^2},$$

where $\mathrm{Re}\, A > 0$

The argument of the exponential is:

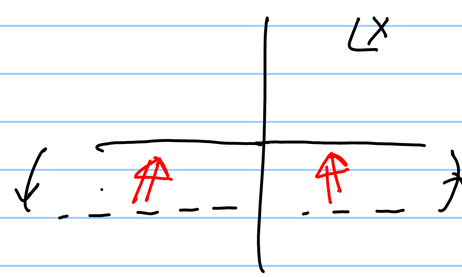
$$-\tfrac{1}{2}Ax^2 + iBx = -\tfrac{1}{2}A\left(x - i\tfrac{B}{A}\right)^2 - \tfrac{B^2}{2A}$$

(by completing the square).

Thus

$$\int_{-\infty}^{\infty} dx\, e^{iBx} e^{-\frac{1}{2}Ax^2} = e^{-B^2/2A} \int_{-\infty}^{\infty} dx\, \exp\left[-\tfrac{1}{2}A\left(x - iB/A\right)^2\right]$$

This integral converges for $\mathrm{Re}\, A > 0$. We can change variables, so $x - iB/A \to x$, but then the



integration contour is along a horizontal line parallel to the real axis. However, since the integrand is an analytic function, and the contribution from large $|x|$ is negligible, we may displace the contour back to the real axis without changing the integral, which becomes:

$$\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}Ax^2} = \sqrt{2\pi/A}$$

Thus we obtain:

$$\boxed{\int_{-\infty}^{\infty} dx\, e^{iBx} e^{-\frac{1}{2}Ax^2} = \sqrt{\frac{2\pi}{A}}\, e^{-B^2/2A}}$$

Now, the integral we want to do actually has $\mathrm{Re}\,A = 0$, but since the integral converges, we may evaluate it by taking the limit $\mathrm{Re}\,A \to 0$ from positive values. Writing $A = |A|e^{i\varphi}$, and

$$\sqrt{\frac{2\pi}{A}} = e^{-i\varphi/2}\sqrt{\frac{2\pi}{|A|}} \longrightarrow e^{\mp i\pi/4} \quad \text{as } A \to \pm i|A|$$

Hence $$\int_{-\infty}^{\infty} dx\, e^{iBx} e^{\pm iA'x^2} = e^{\pm i\pi/4}\sqrt{\frac{2\pi}{A'}}\, e^{-B^2/2A'},$$

for A' real and positive,

and $$\int_{-\infty}^{\infty} dx\, e^{iBx} e^{-iA'x^2} = e^{-i\pi/4}\sqrt{\frac{2\pi}{|A'|}}\, e^{-B^2/2A'}$$

for A' real and negative.

For shorthand, we'll just write this as $\sqrt{\frac{2\pi}{iA'}}\, e^{-B^2/2A'}$ for A' of either sign (using convention $1/\sqrt{i} = e^{-i\pi/4}$).

Thus, for example,

$$\int_{-\infty}^{\infty} dx \sin x^2 = \mathrm{Im}\int_{-\infty}^{\infty} dx\, e^{ix^2} = \mathrm{Im}\left(e^{i\pi/4}\sqrt{\pi}\right) = \sqrt{\pi/2}.$$

The Gaussian integral for the propagator is

$$K(x', x; t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-x')} e^{-i\hbar k^2 t/2m}.$$

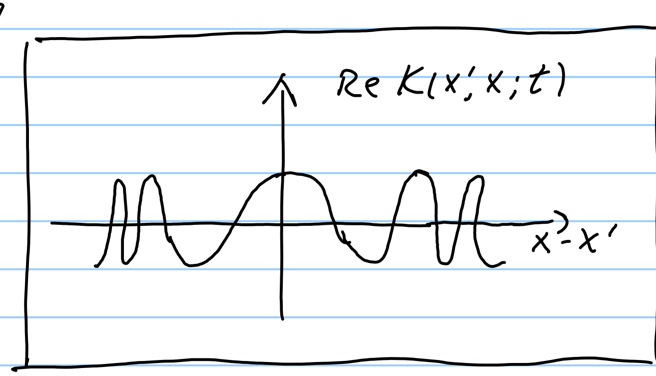
Hence $B = (x - x')$, $A' = \frac{\hbar t}{m} \Rightarrow$

$$\boxed{K(x', x; t) = \sqrt{\frac{m}{2\pi i\hbar t}}\, \exp\left[\frac{im(x-x')^2}{2\hbar t}\right]}$$

"Quantum diffusion":

Qualitatively, what does the propagator tell us about the quantum-mechanical free particle? The real and imaginary parts of

$$K(x';x;t) = \sqrt{\frac{m}{2\pi i\hbar t}}\exp\left[i\frac{m(x-x')^2}{2\hbar t}\right]$$



wiggle, and wiggle faster as $(x-x')$ increases. When we integrate the propagator against an initial waveform, we anticipate that destructive interference occurs for

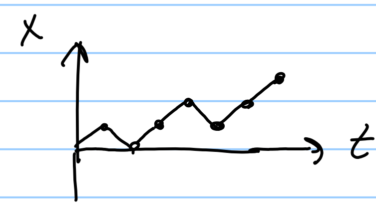
$$\frac{m(x-x')^2}{2\hbar t} \gtrsim 1,$$

so the typical distance the particle travels in time t is δx where:

$$(\delta x)^2 \simeq \frac{\hbar t}{m}.$$

The distance traveled increases with time t like $\sqrt{t}$, the characteristic behavior of a random walk.

E.g. suppose a particle moves distance Δx in each time step of width Δt, where it steps either to the left or the right, with the two directions chosen equiprobably.



Then the expected distance squared traveled in N steps is

$$\left\langle \left(\sum_{i=1}^{N} x_i\right)^2 \right\rangle = \left\langle \sum_{ij} x_i x_j \right\rangle = \left\langle \sum_i x_i^2 \right\rangle = N\langle x_i\rangle^2 = N(\Delta x)^2,$$

where $x_i = \pm\Delta x$, and the x_i's are independent and identically distributed, each with mean zero. (You may be familiar with the equivalent statement: if you flip a coin N times, the typical excess of tails over heads (or heads over tails) is about $\sqrt{N}$.)

Likewise, a free particle monitored for a short time Δt has quantum fluctuations in its position with a typical displacement

$$\Delta x^2 \sim \frac{\hbar}{m}\Delta t$$

(Hence $\hbar/m$ is the "quantum diffusion constant".)

We may view these fluctuations as a consequence of the uncertainty principle:

If the particle is localized within Δx, then its momentum uncertainty is $\Delta p \simeq \hbar/\Delta x$ and the corresponding velocity uncertainty is $\Delta v = \Delta p/m \simeq \frac{\hbar}{m\Delta x}$.

After time Δt, the resulting position uncertainty is

$$\Delta x + \Delta v \Delta t = \Delta x + \frac{\hbar \Delta t}{m \Delta x}$$

which attains its minimum when $\Delta x^2 \simeq \frac{\hbar}{m}\Delta t$

(Compare the discussion of the "standard quantum limit" for position measurement in homework #1.)

If we inspect the motion of a moving particle with better and better time resolution, the distance traveled decreases like Δt, but the fluctuations decrease more slowly, like $\sqrt{\Delta t}$. The trajectory seems to wiggle more and more as Δt gets smaller, so that the slope of the trajectory does not have a limit as $\Delta t \to 0$. The trajectory is continuous, but has no derivative; the particle's velocity is ill-defined. The particle has a "trajectory" only in a suitably averaged sense, for some nonzero time resolution Δt.

Example: Propagation of a Gaussian wave packet.

Suppose the initial state is a Gaussian wave packet centered at $x=0$:

$$\psi(x,0) = \frac{1}{(2\pi a^2)^{1/4}} e^{ik_0 x} e^{-x^2/4a^2}.$$

Probability distribution is:

$$P(x,0) = |\psi(x,0)|^2 = \frac{1}{(2\pi a^2)^{\frac{1}{2}}} e^{-x^2/2a^2}, \quad \text{so that}$$

$$\int_{-\infty}^{\infty} dx\, P(x,0) = 1, \quad \langle x^2 \rangle = \int_{-\infty}^{\infty} dx\, P(x,0) = a^2$$

The Fourier transform is also Gaussian

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

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a^2)^{1/4}} \int_{-\infty}^{\infty} dx\, e^{i(k_0-k)x} e^{-x^2/4a^2}$$

A Gaussian integral with $B = k_0 - k$, $A = \frac{1}{2a^2} \Rightarrow \frac{B^2}{2A} = a^2(k-k_0)^2$

$$\Rightarrow \tilde{\psi}(k,0) = \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a^2)^{1/4}} \sqrt{4\pi a^2}\, e^{-a^2(k-k_0)^2}$$

$$= \left(\frac{2a^2}{\pi}\right)^{1/4} e^{-a^2(k-k_0)^2}$$

$$\Rightarrow \tilde{P}(k,0) = |\tilde{\psi}(k,0)|^2 = \sqrt{\frac{2a^2}{\pi}}\, e^{-2a^2(k-k_0)^2} \Rightarrow \langle (k-k_0)^2 \rangle = \frac{1}{4a^2}.$$

Thus $\Delta x \Delta k = \frac{1}{2}$ — minimum uncertainty wave packet.

Now use propagator to compute $\psi(x,t)$:

$$\psi(x,t) = \int dx' \, \psi(x',0) \, K(x',x;t)$$

$$= \int dx' \frac{1}{(2\pi a^2)^{1/4}} e^{ik_0 x'} e^{-x'^2/4a^2} \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im(x'-x)^2}{2\hbar t}\right)$$

$$= \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar t}} \, e^{imx^2/2\hbar t} \int dx' \, e^{iBx'} e^{-\frac{1}{2}Ax'^2}$$

where $A = \frac{1}{2a^2} - \frac{im}{\hbar t} = \frac{1}{2a^2}\left(1 - i\frac{\tau}{t}\right)$, and $\tau = \frac{2ma^2}{\hbar}$,

$B = k_0 - \frac{mx}{\hbar t} = -\frac{m}{\hbar t}\left(x - \frac{\hbar k_0}{m} t\right)$

This is $v_g t$ where v_g is packet's group velocity

τ is characteristic time for packet to spread by an amount comparable to its initial width.

Using formula $\sqrt{\frac{2\pi}{A}} \, e^{-B^2/2A}$ for integral:

$$\psi(x,t) = \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{m}{2\pi i\hbar t}} \sqrt{2\pi} \sqrt{\frac{2a^2}{1 - i\tau/t}} \, e^{imx^2/2\hbar t}$$

$$\times \exp\left[-\left(\frac{m}{\hbar t}\right)^2 \left(x - \frac{\hbar k_0}{m} t\right)^2 \left(\frac{a^2}{1 - i\tau/t}\right)\right]$$

$$= \frac{1}{(2\pi a^2)^{1/4}} \sqrt{\frac{\tau}{it}} \frac{1}{\sqrt{1 - i\tau/t}} \, e^{imx^2/2\hbar t}$$

$$\times \exp\left[-\frac{1}{4a^2} \frac{\tau^2}{t^2} \frac{1}{1 - i\tau/t} \left(x - \frac{\hbar k_0}{m} t\right)^2\right]$$

$$= \frac{1}{(2\pi a^2)^{1/4}} \frac{1}{\sqrt{1 + it/\tau}} \, e^{imx^2/2\hbar t} \exp\left[-\frac{1}{4a^2}\left(x - \frac{\hbar k_0}{m} t\right)^2 \frac{1 + i\tau/t}{1 + t^2/\tau^2}\right].$$

(It is a useful exercise to check that this expression matches the formula for $\psi(x,0)$ in the limit $t \to 0$.)

The probability distribution for position at time t is

$$P(x,t) = |\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi a^2(1+t^2/\tau^2)}} \exp\left[- \frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{2a^2(1+t^2/\tau^2)} \right],$$

which is still a Gaussian distribution. We see that:

① The center of the wavepacket moves at the group velocity

$$v_g = \frac{\hbar k_0}{m} = \frac{\langle \hat{p} \rangle}{m}.$$

② The wave packet spreads due to "quantum diffusion".

Its width increases to

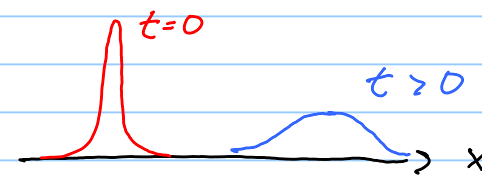
$$\Delta x^2 = a^2 \left(1 + t^2/\tau^2\right)$$

The spreading is not so important for $t \ll \tau = \frac{2ma^2}{\hbar}$.

But for $t \gg \tau$, $\Delta x \simeq \frac{at}{\tau} = \frac{\hbar}{2ma} t = (\Delta v) t$,

where the spread in velocity is

$$\Delta v = \frac{\hbar \Delta k}{m} = \frac{\hbar}{2ma}.$$



③ The uncertainty in momentum does not change, as

$$\tilde{\psi}(k,t) = e^{-i\omega_k t} \tilde{\psi}(k,0)$$

only the phase of $\tilde{\psi}(k,t)$ evolves, not its modulus.

Therefore, the wave packet does not maintain minimum uncertainty; rather

$$\Delta k = \frac{1}{2a}, \quad \Delta x = a\sqrt{1+t^2/\tau^2} \Rightarrow \Delta x \Delta k = \frac{1}{2}\sqrt{1+t^2/\tau^2}.$$

For minimum uncertainty, the coefficient of the quadratic term in the exponential of $\psi(x)$ and $\tilde{\psi}(k)$ must be real -- but here it has a nonzero imaginary part.

For the spreading Gaussian wave packet, the two contributions to the width (the initial width and the broadening due to momentum uncertainty) add in quadrature, like independent errors:

$$(\Delta x)_t^2 = (\Delta x)_0^2 + (\Delta v)^2 t^2 = (\Delta x)_0^2 + \left(\frac{\hbar t}{2m}\right)^2 (\Delta x)_0^{-2}.$$

The minimal width at time t is achieved by choosing $(\Delta x)_0^2 = \frac{\hbar t}{2m} \implies (\Delta x)_t^2 \geq \frac{\hbar t}{m}$.

If we monitor the position with time resolution Δt, we see fluctuations in position with

$$\frac{(\Delta x)^2}{\Delta t} \sim \frac{\hbar}{m} \quad \text{or} \quad \left(\frac{\Delta x}{\Delta t}\right) \sim \sqrt{\frac{\hbar}{m \Delta t}}$$

The particle's velocity does not have a smooth $\Delta t \to 0$ limit.