$|x\rangle$ and $|p\rangle$ representation

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(Date: November 20, 2014)

Here we are interested in the $|x\rangle$ representation and $|p\rangle$ representation of the ket $|\psi\rangle$, in the forms of the wave functions $\langle x|\psi\rangle$ and $\langle p|\psi\rangle$ in the one-dimensional system. The solution of the Schrodinger equation is given by such forms. We also introduce the transformation function $\langle x|p\rangle$ which plays an important role for the Fourier transform between the $|x\rangle$ representation and $|p\rangle$ representation. We also discuss the property of the Dirac delta function.

1. $|x\rangle$ representation

The wave function $\psi(x)$ in the $|x\rangle$ representation can be described by

$$\psi(x) = \langle x|\psi\rangle ,$$

or

$$\psi^*(x) = \langle x|\psi\rangle^* = \langle \psi|x\rangle ,$$

where

$|x'\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue x'.
$|x'\rangle$ is the state vector that a particle is located at $x = x$'.
$|\langle x|\psi\rangle|^2 dx$: probability of finding a particle between x and x+dx.

Note that

$$\hat{x}|x'\rangle = x'|x'\rangle ,$$

$$\langle x''|\hat{x}|x'\rangle = \langle x''|x'|x'\rangle = x'\langle x''|x'\rangle = x'\delta(x''-x') .$$

The eigenstate $|x\rangle$ obeys the orthonormality condition,

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

where $\delta(x''-x')$ is the Dirac delta function.

Using the closure relation:

$$\int_{-\infty}^{\infty} dx|x\rangle\langle x|dx = \hat{1},$$

the inner product can be rewritten as

$$\langle\psi|\varphi\rangle = \int_{-\infty}^{\infty} dx\langle\psi|x\rangle\langle x|\varphi\rangle dx = \int_{-\infty}^{\infty} dx\,\psi^*(x)\varphi(x)dx.$$

The state $|x\rangle$ is also rewritten as

$$|x\rangle = \left(\int_{-\infty}^{\infty} dx'|x'\rangle\langle x'|dx'\right)|x\rangle = \int_{-\infty}^{\infty} dx'|x'\rangle\langle x'|x\rangle = \int_{-\infty}^{\infty} dx'|x'\rangle\delta(x-x').$$

2. $|p\rangle$ representation

The wave function in the $|p\rangle$ representation is defined by

$$\psi(p) = \langle p|\psi\rangle.$$

$|p\rangle$**:** state that a particle has a linear momentum *p*.

$$\hat{p}|p'\rangle = p'|p'\rangle \qquad \langle p''|\hat{p}|p'\rangle = \langle p''|p'|p'\rangle = p'\langle p''|p'\rangle = p'\delta(p''-p').$$

$|\langle p|\psi\rangle|^2$: probability of finding a particle having a linear momentum between *p* and *p* +d*p*.

$$|p\rangle = \left(\int_{-\infty}^{\infty} dp'|p'\rangle\langle p'|\right)|p\rangle = \int_{-\infty}^{\infty} dp'|p'\rangle\langle p'|p\rangle = \int_{-\infty}^{\infty} dp'|p'\rangle\delta(p'-p) = |p\rangle,$$

$$\langle p'|p\rangle = \delta(p-p').$$

Closure relation:

$$\int_{-\infty}^{\infty} dp|p\rangle\langle p|dp = \hat{1}.$$

3. Transformation function

$|p'\rangle$ is the eigenket of $\hat{p}$ with the eigenvalue p',

$$\hat{p}|p'\rangle = p'|p'\rangle .$$

Note that in general, (**formula**)

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle . \tag{1}$$

(This formula will be discussed later in association with the translation operator). When $|\psi\rangle = |x'\rangle$ in Eq.(1), we get

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x') .$$

When $|\psi\rangle = |p\rangle$ in Eq.(1), we get

$$\begin{aligned}
\langle x|\hat{p}|p\rangle = p\langle x|p\rangle &= \int dx'\langle x|\hat{p}|x'\rangle\langle x'|p\rangle \\
&= \int dx'\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')\langle x'|p\rangle \\
&= \frac{\hbar}{i}\frac{\partial}{\partial x}\int dx'\delta(x-x')\langle x'|p\rangle \\
&= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle
\end{aligned}$$

or

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle . \tag{2}$$

using the property of the Dirac delta function.

((**Alternative method**))
Using the formula

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle ,$$

with $|\psi\rangle = |p\rangle$, we get

$$\langle x|\hat{p}|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle . \tag{3}$$

The solution of Eq.(2) is given by

$$\langle x | p \rangle = C \exp(\frac{ipx}{\hbar}),$$

where *C* is the constant which is determined from the normalization condition.

$$\langle x | x' \rangle = \int \langle x | p \rangle \langle p | x' \rangle dp = |C|^2 \int \exp(\frac{ipx}{\hbar}) \exp(-\frac{ipx'}{\hbar}) dp$$
$$= |C|^2 \int \exp[\frac{ip}{\hbar}(x - x')] dp = |C|^2 2\pi \delta(\frac{x - x'}{\hbar})$$

or

$$\langle x | x' \rangle = \delta(x - x') = |C|^2 2\pi \delta(\frac{x - x'}{\hbar}) = |C|^2 2\pi\hbar \delta(x - x'),$$

from the property of the Dirac delta function (we will discussed later)

or

$$|C| = \frac{1}{\sqrt{2\pi\hbar}}.$$

Here we choose a real number *C* given by

$$C = \frac{1}{\sqrt{2\pi\hbar}}.$$

The transformation function:

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp(\frac{ipx}{\hbar}), \qquad (4)$$

or

$$\langle p | x \rangle = \langle x | p \rangle^* = \frac{1}{\sqrt{2\pi\hbar}} \exp(-\frac{ipx}{\hbar}). \qquad (5)$$

((Property of the Hermite operator $\hat{p}$))

$$\langle \alpha | \hat{p} | \beta \rangle^* = \langle \beta | \hat{p}^+ | \alpha \rangle,$$

$$\langle\alpha|\hat{p}|\beta\rangle = \int\langle\alpha|x\rangle\langle x|\hat{p}|\beta\rangle dx$$
$$= \int\langle x|\alpha\rangle^* \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\beta\rangle dx$$
$$= -\int\langle x|\beta\rangle\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\alpha\rangle^* dx$$

$$\langle\alpha|\hat{p}|\beta\rangle^* = \int\langle x|\beta\rangle^* \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\alpha\rangle dx$$
$$= \int\langle\beta|x\rangle\langle x|\hat{p}|\alpha\rangle dx$$
$$= \langle\beta|\hat{p}|\alpha\rangle$$

Thus we have $\hat{p}^+ = \hat{p}$ (Hermitian operator).

4. Fourier transform

We can define the Fourier transform using the transformation function

$$\langle p|\psi\rangle = \int\langle p|x\rangle\langle x|\psi\rangle dx$$
$$= \int\langle x|p\rangle^*\langle x|\psi\rangle dx$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int\exp(-\frac{ipx}{\hbar})\langle x|\psi\rangle dx$$

and

$$\langle x|\psi\rangle = \int\langle x|p\rangle\langle p|\psi\rangle dp = \frac{1}{\sqrt{2\pi\hbar}}\int\exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp\,.$$

Using this Fourier transform, we can confirm the formula

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle\,.$$

In fact, we have

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int \frac{\hbar}{i}\frac{\partial}{\partial x}\exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int p\exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp$$
$$= \int p\langle x|p\rangle\langle p|\psi\rangle dp$$
$$= \int \langle x|\hat{p}|p\rangle\langle p|\psi\rangle dp = \langle x|\hat{p}|\psi\rangle$$

using the closure relation.

5. Summary

(1) Transformation function

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar},$$

or

$$\langle p|x\rangle = \langle p|x\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}.$$

(2) Fourier transform

$$\langle p|\psi\rangle = \int_{-\infty}^{\infty}\langle p|x\rangle\langle x|\psi\rangle dx = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\langle x|\psi\rangle dx,$$

and

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty}\langle x|p\rangle\langle p|\psi\rangle dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{ipx/\hbar}\langle p|\psi\rangle dp.$$

6. $|k\rangle$ space

Here we introduce *k*, as $p = \hbar k$

$$\langle p|p'\rangle = \delta(p-p')$$
$$= \delta[\hbar(k-k')]$$
$$= \frac{1}{\hbar}\delta(k-k') = \frac{1}{\hbar}\langle k|k'\rangle$$

Then we have the following relation

$$|p\rangle = \frac{1}{\sqrt{\hbar}}|k\rangle,$$

$$\langle x|p\rangle = \frac{1}{\sqrt{\hbar}}\langle x|k\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar},$$

or

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

and

$$\langle k|x\rangle = \langle x|k\rangle^* = \frac{1}{\sqrt{2\pi}}e^{-ikx}.$$

Fourier transform in the *x*-*k* space

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

and

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

7. Expectation value

$$\langle\hat{k}^n\rangle = \langle\psi|\hat{k}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|k\rangle\langle k|\hat{k}^n|\psi\rangle dk$$
$$= \int_{-\infty}^{\infty}\langle k|\psi\rangle^* k^n\langle k|\psi\rangle dk$$

$$\langle\hat{p}^n\rangle = \langle\psi|\hat{p}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|p\rangle\langle p|\hat{p}^n|\psi\rangle dp$$
$$= \int_{-\infty}^{\infty}\langle p|\psi\rangle^* p^n\langle p|\psi\rangle dp$$

where

$$\left\langle \hat{p}^n \right\rangle = \hbar^n \left\langle \hat{k}^n \right\rangle .$$

8. Another method to calculate $\left\langle \hat{p}^n \right\rangle$

$\left\langle \hat{p}^n \right\rangle$ can be evaluated in a different way;

$$\begin{aligned} \left\langle \hat{p}^n \right\rangle &= \langle \psi | \hat{p}^n | \psi \rangle \\ &= \int_{-\infty}^{\infty} \langle \psi | x \rangle \langle x | \hat{p}^n | \psi \rangle dx \\ &= \int_{-\infty}^{\infty} \langle x | \psi \rangle^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^n \langle x | \psi \rangle dx \end{aligned} \tag{1}$$

$$\begin{aligned} \left\langle \hat{x}^n \right\rangle &= \langle \psi | \hat{x}^n | \psi \rangle \\ &= \int_{-\infty}^{\infty} \langle \psi | x \rangle \langle x | \hat{x}^n | \psi \rangle dx \\ &= \int_{-\infty}^{\infty} \langle x | \psi \rangle^* x^n \langle x | \psi \rangle dx \end{aligned}$$

or

$$\begin{aligned} \left\langle \hat{x}^n \right\rangle &= \langle \psi | \hat{x}^n | \psi \rangle = \int_{-\infty}^{\infty} \langle \psi | p \rangle \langle p | \hat{x}^n | \psi \rangle dp \\ &= \int_{-\infty}^{\infty} \langle p | \psi \rangle^* \left(i\hbar \frac{\partial}{\partial p} \right)^n \langle p | \psi \rangle dp \end{aligned} \tag{2}$$

9. Proof of Eq.(1)

$$I = \int_{-\infty}^{\infty} \langle x | \psi \rangle^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^n \langle x | \psi \rangle dx ,$$

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n \langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n e^{ipx/\hbar}\langle p|\psi\rangle dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{i}{\hbar}p\right)^n e^{ipx/\hbar}\langle p|\psi\rangle dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} p^n e^{ipx/\hbar}\langle p|\psi\rangle dp$$

Then we have

$$I = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ip'x/\hbar}\langle p'|\psi\rangle^* dp' \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} p^n e^{ipx/\hbar}\langle p|\psi\rangle dp$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \int_{-\infty}^{\infty} dx e^{i(p-p')x/\hbar}\langle p'|\psi\rangle^* p^n \langle p|\psi\rangle$$

Note that

$$\int_{-\infty}^{\infty} dx e^{i(p-p')x/\hbar} = 2\pi\delta[\frac{1}{\hbar}(p-p')] = 2\pi\hbar\delta(p-p'),$$

we get

$$I = \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \langle p'|\psi\rangle^* p^n \langle p|\psi\rangle \delta(p-p') = \int_{-\infty}^{\infty} dp \langle p|\psi\rangle^* p^n \langle p|\psi\rangle .$$

10. Proof of Eq.(2)

$$\langle \hat{x}^n\rangle = \int_{-\infty}^{\infty} \langle p|\psi\rangle^* \left(i\hbar\frac{\partial}{\partial p}\right)^n \langle p|\psi\rangle dp ,$$

$$\left(i\hbar\frac{\partial}{\partial p}\right)^n \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(i\hbar\frac{\partial}{\partial p}\right)^n e^{-ipx/\hbar}\langle x|\psi\rangle dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(-i\hbar\frac{i}{\hbar}x\right)^n e^{-ipx/\hbar}\langle x|\psi\rangle dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} x^n e^{-ipx/\hbar}\langle x|\psi\rangle dx$$

$$\left\langle \hat{x}^n \right\rangle = \int_{-\infty}^{\infty} dp \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx'/\hbar} \left\langle x' \middle| \psi \right\rangle^* dx' \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} x^n e^{-ipx/\hbar} \left\langle x \middle| \psi \right\rangle dx$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \left\langle x' \middle| \psi \right\rangle^* x^n \left\langle x \middle| \psi \right\rangle \int_{-\infty}^{\infty} dp e^{ip(x'-x)/\hbar}$$

Note that

$$\int_{-\infty}^{\infty} dp e^{ip(x'-x)/\hbar} = 2\pi\hbar \delta(x - x') ,$$

$$\left\langle \hat{x}^n \right\rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \left\langle x' \middle| \psi \right\rangle^* x^n \left\langle x \middle| \psi \right\rangle \delta(x - x') = \int_{-\infty}^{\infty} dx \left\langle x \middle| \psi \right\rangle^* x^n \left\langle x \middle| \psi \right\rangle .$$

11. Mathematica

The FourierTransform is defined by

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

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

In Mathematica, we use the following command for the above Fourier transform.

Fourier transform of $\psi(x)$:

FourierTransform[ψ[x], x, k, FourierParameters→{0,-1}]:

Inverse Fourier transform of $\psi(k)$:

InverseFourierTransform[ψ[k], k, x, FourierParameters→{0,-1}]:

$\psi(p) = \left\langle p \middle| \psi \right\rangle$ can be calculated from $\psi(k) = \left\langle k \middle| \psi \right\rangle$ as

$$\psi(p) = \left\langle p \middle| \psi \right\rangle = \frac{1}{\sqrt{\hbar}} \left\langle k \middle| \psi \right\rangle = \frac{1}{\sqrt{\hbar}} \psi(k) ,$$

where

$$k = \frac{p}{\hbar} .$$

Note that

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ikx} \psi(x) dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-i\frac{px}{\hbar}} \psi(x) dx$$

$$= \frac{1}{\sqrt{\hbar}} \psi[k = \frac{p}{\hbar}]$$

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12. Exercise-1 (Gasirowicz, p.53)

Given that

$$\psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4} e^{-\frac{\alpha x^2}{2}},$$

calculate

(a) $\langle x^n \rangle = \langle \psi | \hat{x}^n | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^n \psi(x) dx$,

(b) $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$.

Solution

$$\langle x^n \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^n \psi(x) dx = \frac{[1 + (-1)^n]}{2\sqrt{\pi}} \alpha^{-n/2} \Gamma(\frac{n+1}{2}),$$

$$\langle x^2 \rangle = \frac{1}{2\alpha}, \qquad \langle \hat{x} \rangle = 0,$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\sqrt{\alpha}}.$$

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13. Exercise-2

Calculate the momentum space wave function for system described by the wave function

$$\psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4} e^{-\frac{\alpha x^2}{2}}.$$

calculate

(a) $$\langle p^n \rangle = \int_{-\infty}^{\infty} \psi^*(p) p^n \psi(p) dp = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{\hbar}{i}\right)^n \frac{\partial^n}{\partial x^n} \psi(x) dx$$

(b) $$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}.$$

$$\psi(k) = \langle k | \psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \langle x | \psi \rangle dx$$
$$= \frac{1}{\pi^{1/4}\sqrt{\hbar}} (\frac{1}{\alpha})^{3/4} \sqrt{\alpha} \exp(-\frac{p^2}{2\alpha\hbar^2})$$

$$\psi(p) = \langle p | \psi \rangle = \frac{1}{\sqrt{\hbar}} \langle k | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ikx} \langle x | \psi \rangle dx$$
$$= \frac{1}{\pi^{1/4}\sqrt{\hbar}} (\frac{1}{\alpha})^{3/4} \sqrt{\alpha} \exp(-\frac{k^2}{2\alpha})$$

$$\langle \hat{k}^n \rangle = \int_{-\infty}^{\infty} \langle k | \psi \rangle^* k^n \langle k | \psi \rangle dk$$
$$= \frac{1}{2\sqrt{\pi}} [1 + (-1)^n] \alpha^{n/2} \Gamma(\frac{1+n}{2})$$

$$\langle \hat{k}^2 \rangle = \frac{\alpha}{2},$$

$$\langle \hat{k} \rangle = 0,$$

$$\Delta p = \hbar \sqrt{\langle \hat{k}^2 \rangle - \langle \hat{k} \rangle^2} = \frac{\hbar\sqrt{\alpha}}{\sqrt{2}},$$

$$\Delta x \Delta p = \frac{\hbar}{2}.$$

((**Note**))

$$\langle \hat{p}^n \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{\hbar}{i}\right)^n \frac{\partial^n}{\partial x^n} \psi(x) dx \,,$$

$$\langle \hat{p}^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{\hbar}{i}\right)^2 \frac{\partial^2}{\partial x^2} \psi(x) dx = \frac{\alpha \hbar^2}{2} \,,$$

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{\hbar}{i}\right) \frac{\partial}{\partial x} \psi(x) dx = 0 \,.$$

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14. Exercise-3

Given the wave function

$$\psi(x) = \frac{N}{x^2 + a^2} \,.$$

(a) Calculate N needed to normalize $\psi(x)$:

(b) Calculate $\langle \hat{x}^n \rangle$. What values of n lead to convergent integrals?

(c) Calculate $\langle p^2 \rangle$ directly, and using the momentum space wave function.

(d) Use the definitions

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \,, \quad \text{and} \quad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \,.$$

to calculate $\Delta x \Delta p$ for this problem.

((Solution))

(a)

$$N = a^{3/2} \sqrt{\frac{2}{\pi}} \,, \qquad \psi(x) = \frac{a^{3/2} \sqrt{\frac{2}{\pi}}}{x^2 + a^2} \,.$$

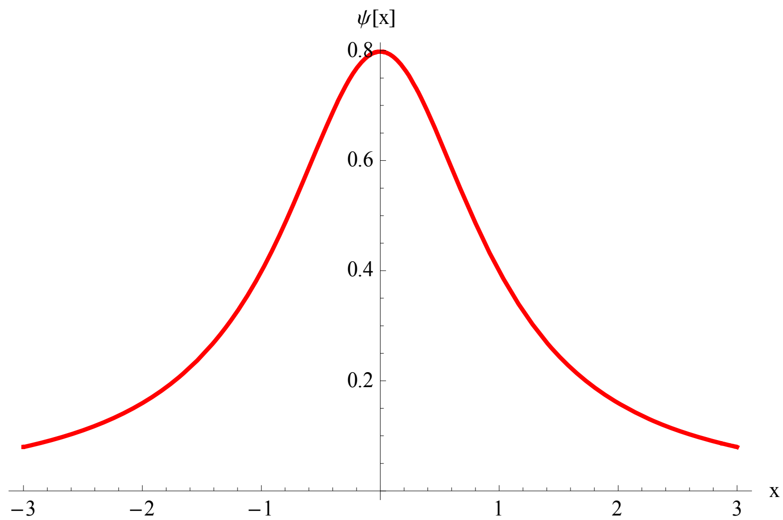

Fig. Plot of $\psi(x)$ as a function of *x*. $a = 1$.

(b)

$$\langle x^n \rangle = \langle \psi | \hat{x}^n | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^n \psi(x) dx$$
$$= -\frac{1}{2}[1+(-1)^n] a^n (n-1) \sec\left(\frac{n\pi}{2}\right)$$

only for n =1 and 2.

$$\langle x^2 \rangle = \langle \psi | \hat{x}^2 | \psi \rangle = a^2 ,$$

$$\langle x \rangle = \langle \psi | \hat{x} | \psi \rangle = 0 .$$

(c)

$$\psi(k) = \langle k | \psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \langle x | \psi \rangle dx$$
$$= \sqrt{a} e^{-ak} [e^{2ak} \Theta(-k) + \Theta(k)]$$

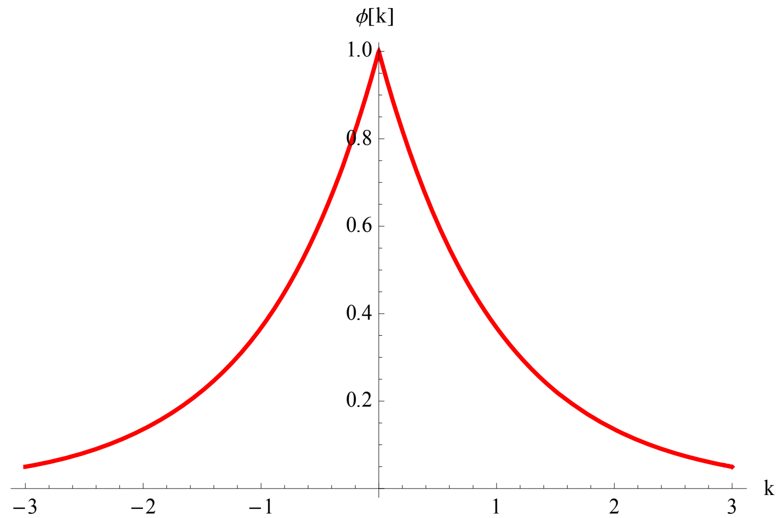

Fig. Plot of $\psi(k)$ as a function of k. $a = 1$.

$$\langle \hat{k}^n \rangle = \int_{-\infty}^{\infty} \langle k|\psi\rangle^* k^n \langle k|\psi\rangle dk$$

$$= \frac{1}{2^{1+n}}[1+(-1)^n]a^{-n}\Gamma(1+n)$$

$$\langle \hat{k}^2 \rangle = \frac{1}{2a^3},$$

$$\langle \hat{k} \rangle = 0.$$

(d)

$$\Delta x = a,$$

$$\Delta p = \hbar\sqrt{\langle \hat{k}^2 \rangle - \langle \hat{k} \rangle^2} = \frac{\hbar}{\sqrt{2}a}.$$

Then we have

$$\Delta x \Delta p = \frac{\hbar}{\sqrt{2}} > \frac{\hbar}{2}.$$

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15. ((LiBoff 5-53))

A free particle moving in one dimension is in the state

$$\langle x|\psi\rangle = \psi(x) = \int_{-\infty}^{\infty} e^{-\frac{a^2k^2}{2}} i\sin(ak) e^{ikx} dk \,.$$

(a) What values of momentum, $p_x = p$ of the particle will not be found?

(b) If the momentum of the particle in this state [$\langle x|\psi\rangle = \psi(x)$], in which momentum state is the particle most likely to be found? Hint: calculate $\langle p|\psi\rangle = \psi(p)$.

(c) If a = 2.1 Å, and the particle is an electron, what value of energy (in eV) will measurement find in the state described in part (b).

((**Solution**))

(a)

We note that

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

Comparing this with

$$\langle x|\psi\rangle = \psi(x) = \int_{-\infty}^{\infty} e^{-\frac{a^2k^2}{2}} i\sin(ak) e^{ikx} dk \,,$$

we get

$$\frac{1}{\sqrt{2\pi}}\langle k|\psi\rangle = e^{-\frac{a^2k^2}{2}} i\sin(ak) \,,$$

or

$$\langle k|\psi\rangle = \sqrt{2\pi} e^{-\frac{a^2k^2}{2}} i\sin(ak) \,.$$

Since $p = \hbar k$ and $|p\rangle = \frac{1}{\sqrt{\hbar}}|k\rangle$,

$$\langle p|\psi\rangle = \frac{1}{\sqrt{\hbar}}\langle k|\psi\rangle = \sqrt{\frac{2\pi}{\hbar}} e^{-\frac{a^2p^2}{2\hbar^2}} i\sin(\frac{ap}{\hbar}) \,,$$

$$|\langle p|\psi\rangle|^2 = \frac{2\pi}{\hbar} e^{-\frac{a^2p^2}{\hbar^2}} \sin^2(\frac{ap}{\hbar}) \,,$$

We will show a plot of the $P(\kappa) = e^{-\frac{a^2 p^2}{\hbar^2}} \sin^2(\frac{ap}{\hbar}) = e^{-\kappa^2} \sin^2 \kappa$ with $\kappa = \frac{ap}{\hbar}$ by using Mathematica below.

We find that $P(\kappa)$ becomes zero at $\kappa = 0$ ($p = 0$) and $\kappa = \pm\infty$ ($p = \pm\infty$).

(b)

$$\frac{dP(\kappa)}{d\iota} = 2e^{-\kappa^2} \sin\kappa(\cos\kappa - \kappa \sin\kappa)$$

When $\kappa = \frac{ap}{\hbar} = \pm 0.86033$, $P(\kappa)$ has a local maximum.

(c)

The energy of the free electron is given by

$$E(k) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^{22}}{2m}(\frac{0.86033}{a})^2 = 0.64 eV$$

where

a = 2.1Å=2.1x10^{-8} cm
m = 9.109381 x 10^{-28} g
$\hbar$ =1.05457 x 10^{-27} erg sec
1 eV = 1.602176 x 10^{-12} erg

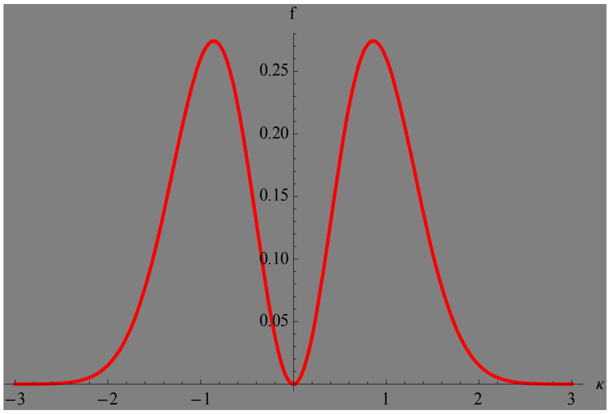
Note that we can calculate $\langle x|\psi\rangle$ using Mathematica

$$\langle x|\psi\rangle = \frac{1}{a}\sqrt{\frac{\pi}{2}}[-e^{-\frac{(x-a)^2}{2a^2}} + e^{-\frac{(x+a)^2}{2a^2}}].$$

((**Mathematica**))

```
Clear["Global`*"]; Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]};
f = Exp[-κ^2] Sin[κ]^2;
```

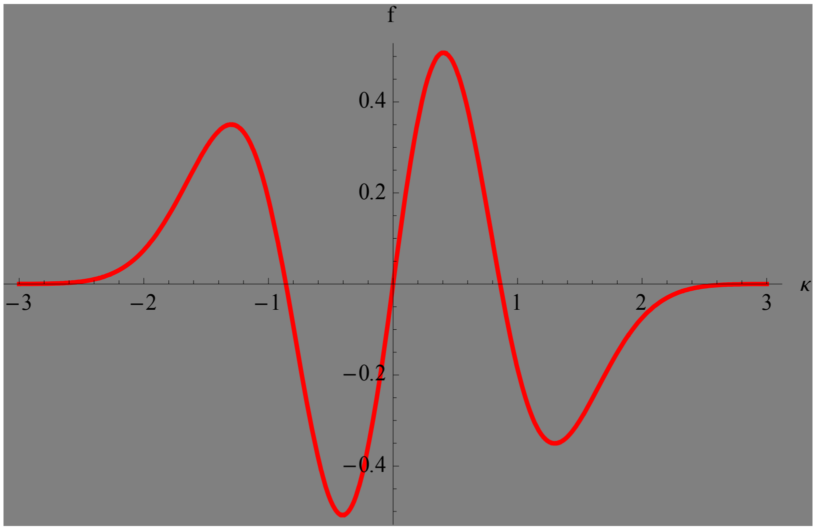
```
 Plot[f,{κ,-3,3},PlotStyle→{Hue[0],Thick},Background→GrayLevel[0.5],
AxesLabel→{"κ","f"}]
```




```
 g1=D[f,κ]//Simplify
```

$2\, e^{-\kappa^2} \text{Sin}[\kappa]\, (\text{Cos}[\kappa] - \kappa\, \text{Sin}[\kappa])$

```
Plot[g1, {κ, -3, 3}, PlotStyle → {Hue[0], Thick},
 Background → GrayLevel[0.5], AxesLabel → {"κ", "f"}]
```




```
h1 = Cos[κ] - κ Sin[κ]; FindRoot[h1 == 0, {κ, 0, 1}]
```

{κ → 0.860334}

```
FindRoot[h1 == 0, {κ, -1, 0}]
```

{κ → -0.860334}

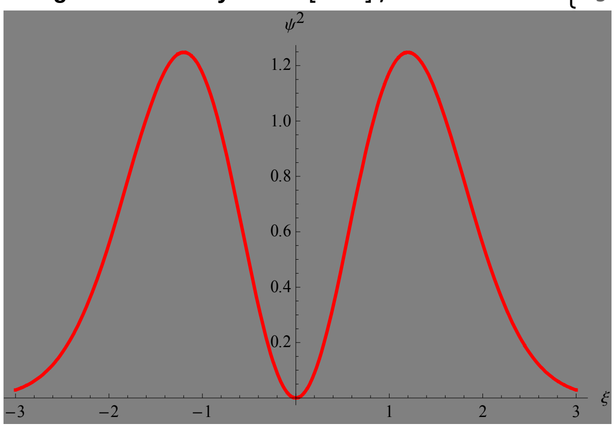
$$g2 = \int_{-\infty}^{\infty} \text{Exp}\left[-\frac{a^2 k^2}{2}\right] (i \,\text{Sin}[a\, k])\, \text{Exp}[i\, k\, x]\, dk \;//\; \text{Simplify}[\#, a > 0]\, \&$$

$$-\frac{e^{-\frac{(a+x)^2}{2 a^2}} \left(-1 + e^{\frac{2 x}{a}}\right) \sqrt{\frac{\pi}{2}}}{a}$$

```
g21 = g2 /. x → a ξ // Simplify
```

$$-\frac{e^{-\frac{1}{2}(1+\xi)^2} \left(-1 + e^{2 \xi}\right) \sqrt{\frac{\pi}{2}}}{a}$$

```
Plot[Abs[g21]^2 /. a → 1, {ξ, -3, 3}, PlotStyle → {Hue[0], Thick},
 Background → GrayLevel[0.5], AxesLabel → {"ξ", "ψ^2"}]
```



Physics constant

$$\text{phycon} = \{\mu B \to 9.274009 \times 10^{-21},\ \hbar \to 1.054571 \times 10^{-27},\ m \to 9.109382 \times 10^{-28},\ e \to 4.803242 \times 10^{-10},\ eV \to 1.60217642 \times 10^{-12}\};$$

$$\text{Energy} = \frac{\hbar^2}{2\, m} \left(\frac{0.86033}{a}\right)^2 \Big/ eV \;/.\; a \to 2.1 \times 10^{-8} \;/.\; \text{phycon}$$

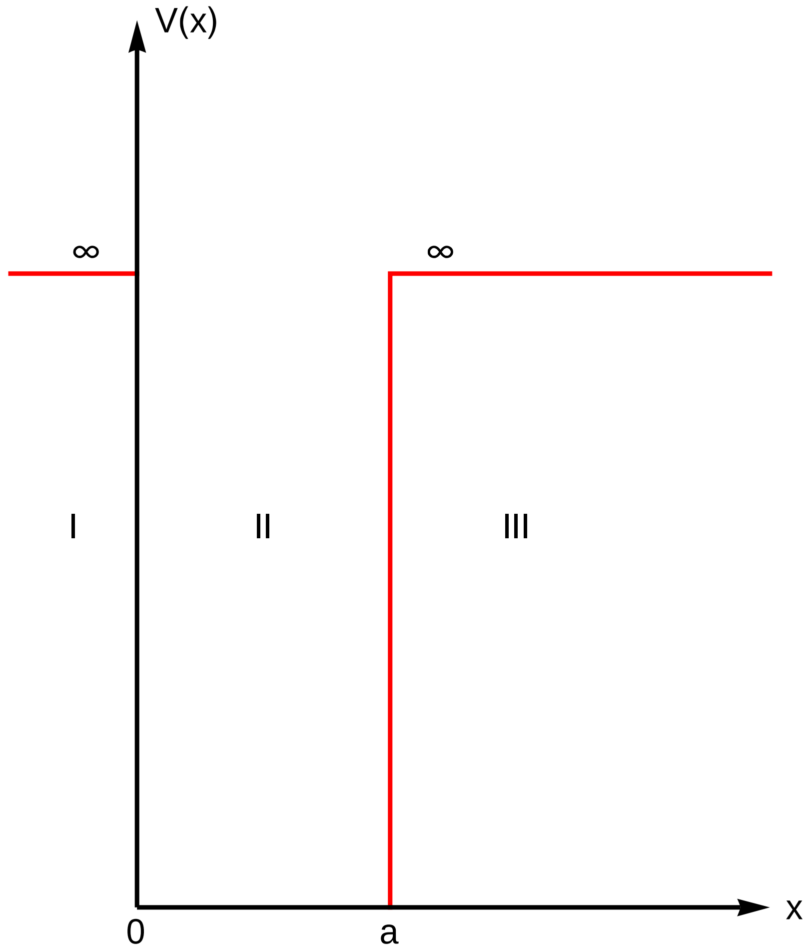
0.639461

16. ((Sakurai 1-21))

Evaluate the *x*-*p* uncertainty $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle$ for a one-dimensional particle confined between two rigid walls

$V = 0$ for $0<x<a$, $\quad\infty\quad$ otherwise.

Do this for both the ground and excited states?



The Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m},$$

$$H\varphi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x) = \frac{\hbar^2 k^2}{2m}\varphi(x).$$

The solution of this equation is

$$\varphi(x) = A\sin(kx) + B\cos(kx),$$

where

$$E = \frac{\hbar^2 k^2}{2m}.$$

Using the boundary condition:

$$\varphi(x=0)=\varphi(x=a)=0\,,$$

we have

$B = 0$ and $A \neq 0$,

$$\sin(ka)=0\,,$$

$$ka = n\pi \quad (n = 1, 2, \ldots)$$

Note that $n = 0$ is not included in our solution because the corresponding wave function becomes zero. The wave function is given by

$$\varphi_n(x)=\langle x|\varphi_n\rangle = A_n\sin(\frac{n\pi x}{a})=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\,,$$

with

$$E_n=\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2.$$

The calculation of $\langle x\rangle$ and $\langle(\Delta x)^2\rangle$

$$\langle x\rangle=\langle\varphi_n|\hat{x}|\varphi_n\rangle=\int_0^a dx\varphi_n^*(x)x\varphi_n(x)=\frac{a}{2}\,,$$

$$\langle x^2\rangle=\langle\varphi_n|\hat{x}^2|\varphi_n\rangle=\int_0^a dx\varphi_n^*(x)x^2\varphi_n(x)=\frac{a^2}{6}(2-\frac{3}{n^2\pi^2})\,,$$

$$(\Delta x)^2=\langle x^2\rangle-\langle x\rangle^2=\frac{a^2}{6}(2-\frac{3}{n^2\pi^2})-\frac{a^2}{4}=\frac{a^2}{n^2\pi^2}\left(\frac{n^2\pi^2}{12}-\frac{1}{2}\right).$$

The calculation of $\langle p\rangle$ and $\langle(\Delta p)^2\rangle$

$$\langle p \rangle = \langle \varphi_n | \hat{p} | \varphi_n \rangle = \int_0^a dx \varphi_n^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \varphi_n(x) = 0,$$

$$\langle p^2 \rangle = \langle \varphi_n | \hat{p}^2 | \varphi_n \rangle = \int_0^a dx \varphi_n^*(x) \left(\frac{\hbar}{i} \right)^2 \frac{\partial^2}{\partial x^2} \varphi_n(x) = \left(\frac{n\pi\hbar}{a} \right)^2,$$

$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \left(\frac{n\pi\hbar}{a} \right)^2.$$

Then we have

$$(\Delta x)^2 (\Delta p)^2 = \frac{a^2}{n^2\pi^2} \left(\frac{n^2\pi^2}{12} - \frac{1}{2} \right) \frac{n^2\pi^2\hbar^2}{a^2} = \hbar^2 \left(\frac{n^2\pi^2}{12} - \frac{1}{2} \right) > \frac{\hbar^2}{4}.$$

((**Mathematica**))

```
Clear["Global`*"]; Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

ψ[x_] := Sqrt[2/a] Sin[n π x/a];

avx = ∫_0^a x ψ[x]^2 dx // Simplify[#, n ∈ Integers] &
```

$$\frac{a}{2}$$

```
avsqx = ∫_0^a x^2 ψ[x]^2 dx // Simplify[#, n ∈ Integers] &
```

$$\frac{1}{6} a^2 \left(2 - \frac{3}{n^2 \pi^2}\right)$$

```
avp = ħ/i ∫_0^a ψ[x] D[ψ[x], x] dx // Simplify[#, n ∈ Integers] &
```

0

```
avsqp = (ħ/i)^2 ∫_0^a ψ[x] D[ψ[x], {x, 2}] dx // Simplify[#, n ∈ Integers] &
```

$$\frac{n^2 \pi^2 \hbar^2}{a^2}$$

```
X1 = (avsqx - avx^2) // Simplify; P1 = (avsqp - avp^2) // Simplify;

h1 = X1 P1
```

$$\frac{1}{12} n^2 \left(1 - \frac{6}{n^2 \pi^2}\right) \pi^2 \hbar^2$$

```
Sqrt[h1] /. n → 1 // Simplify[#, ħ > 0] & // N
```

$0.567862\,\hbar$

---

17. ((Sakurai 1-27))

(a) Suppose that $f(\hat{A})$ is a function of a Hermitian operator $\hat{A}$ with the property,

$$\hat{A}|a'\rangle = a'|a'\rangle$$

Evaluate $\langle b''|f(\hat{A})|b'\rangle$ when the transformation matrix from the a' basis to the b' basis is known.

$$|a'\rangle = \hat{U}|b'\rangle, \qquad |a''\rangle = \hat{U}|b''\rangle$$

where $\hat{U}$ is the unitary operator.

(b) Using the continum analogue of the result obtained in (a), evaluate

$$\langle \boldsymbol{p}''|F(\hat{\boldsymbol{r}})|\boldsymbol{p}'\rangle$$

Simplify your expression as far as you can. Note that $\hat{\boldsymbol{r}} = (\hat{x}, \hat{y}, \hat{z})$. We assume that $F(\boldsymbol{r})$ depends only on *r*;

$$F(\boldsymbol{r}) = F(r)$$

with

$$r = \sqrt{x^2 + y^2 + z^2} .$$

((**Solution**))

(a)

$$|b'\rangle = \hat{U}|a'\rangle , \qquad |b''\rangle = \hat{U}|a''\rangle$$

or

$$\langle b'| = \langle a'|\hat{U}^+ , \qquad \langle b''| = \langle a''|\hat{U}^+$$

$$\begin{aligned}
\langle b''|f(\hat{A})|b'\rangle &= \langle a''|\hat{U}^+ f(\hat{A})\hat{U}|a'\rangle \\
&= \sum_{a'''}\langle a''|\hat{U}^+ f(\hat{A})|a'''\rangle\langle a'''|\hat{U}|a'\rangle \\
&= \sum_{a'''}\langle a''|\hat{U}^+|a'''\rangle f(a''')\langle a'''|\hat{U}|a'\rangle \\
&= \sum_{a'''}\langle a'''|\hat{U}|a''\rangle^* f(a''')\langle a'''|\hat{U}|a'\rangle
\end{aligned}$$

where

$$\langle a''|\hat{U}^+|a'''\rangle = \langle a'''|\hat{U}|a''\rangle^*$$

(b)

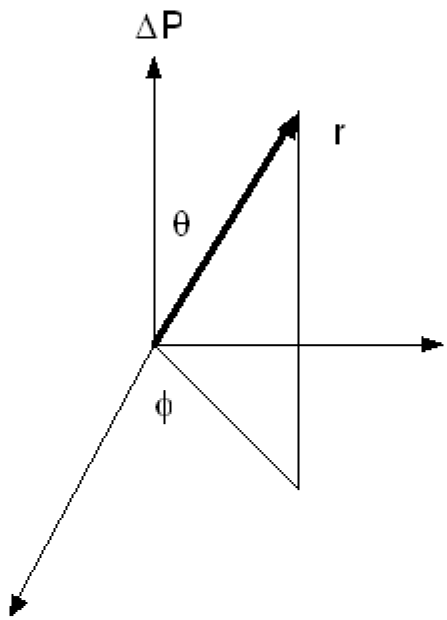
$$\begin{aligned}\langle \boldsymbol{p}''|F(\hat{\boldsymbol{r}})|\boldsymbol{p}'\rangle &= \int d\boldsymbol{r}'\int d\boldsymbol{r}''\langle \boldsymbol{p}''|\boldsymbol{r}''\rangle\langle \boldsymbol{r}''|F(\hat{\boldsymbol{r}})|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle \\ &= \int d\boldsymbol{r}'\int d\boldsymbol{r}''\langle \boldsymbol{p}''|\boldsymbol{r}''\rangle F(\boldsymbol{r}')\langle \boldsymbol{r}'|\boldsymbol{r}''\rangle\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle \\ &= \int d\boldsymbol{r}'\int d\boldsymbol{r}''\langle \boldsymbol{p}''|\boldsymbol{r}''\rangle F(\boldsymbol{r}')\delta(\boldsymbol{r}'-\boldsymbol{r}'')\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle \\ &= \int d\boldsymbol{r}'\langle \boldsymbol{p}''|\boldsymbol{r}'\rangle F(\boldsymbol{r}')\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle\end{aligned}$$

Using the transformation function

$$\langle \mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\exp(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}),$$

$$\begin{aligned}\langle \boldsymbol{p}''|F(\hat{\boldsymbol{r}})|\boldsymbol{p}'\rangle &= \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}'\exp(-\frac{i\boldsymbol{p}''\cdot\boldsymbol{r}'}{\hbar})F(\boldsymbol{r}')\exp(\frac{i\boldsymbol{p}'\cdot\boldsymbol{r}'}{\hbar}) \\ &= \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}'\exp[\frac{i(\boldsymbol{p}'-\cdot\boldsymbol{p}'')\cdot\boldsymbol{r}'}{\hbar}]F(\boldsymbol{r}')\end{aligned}$$

Here we use the spherical co-ordinate (r, θ, ϕ). The direction of $\Delta\mathbf{p} = \mathbf{p}'-\cdot\mathbf{p}''$ is the z axis.



$$d\mathbf{r}' = r'^2\sin\theta dr' d\theta d\phi$$

$$(\boldsymbol{p}'-\boldsymbol{p}'')\cdot\boldsymbol{r}' = |\boldsymbol{p}'-\boldsymbol{p}''|r'\cos\theta$$

Suppose that $F(\mathbf{r})$ is a function of the magnitude of ***r***.

$$\langle \boldsymbol{p}''|F(\hat{\boldsymbol{r}})|\,\boldsymbol{p}'\rangle = \frac{2\pi}{(2\pi\hbar)^3}\int_0^\infty F(r')r'^2\,dr'\int_0^\pi d\theta\sin\theta\exp[\frac{i|\boldsymbol{p}'-\boldsymbol{p}''|r'\cos\theta}{\hbar}]$$

Note that

$$\int_0^\pi d\theta\sin\theta\exp[\frac{i|\boldsymbol{p}'-\boldsymbol{p}''|r'\cos\theta}{\hbar}] = \frac{2\hbar}{|\boldsymbol{p}'-\boldsymbol{p}''|r'}\sin\left(\frac{|\boldsymbol{p}'-\boldsymbol{p}''|r'}{\hbar}\right)$$

Then

$$\langle \mathbf{p}''|F(\hat{\mathbf{r}})|\mathbf{p}'\rangle = \frac{4\pi}{(2\pi\hbar)^3}\int_0^\infty dr'r'^2\,F(r')\frac{\sin\left(\frac{|\mathbf{p}'-\mathbf{p}''|r'}{\hbar}\right)}{\frac{|\mathbf{p}'-\mathbf{p}''|r'}{\hbar}}$$

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Stephen Gasiorowicz, *Quantum Mechanics*, third edition (John Wiley & Sons, Inc., New York, 2003).

Richard L. Liboff, *Introductory Quantum Mechanics*, 4th edition (Addison Wesley, New York, 2003).

John S. Townsend , *A Modern Approach to Quantum Mechanics*, second edition (University Science Books, 2012).

David H. McIntyre, *Quantum Mechanics A Paradigms Approach* (Pearson Education, Inc., 2012).

APPENDIX-I Heisenberg's principle of uncertainty

Here we chose the wave function in the *x*-representation, as

$$\psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\sigma}}\exp(-\frac{x^2}{4\sigma^2})$$

So that the probability $P(x) = |\psi(x)|^2$ has a form of the Gaussian distribution function. We note that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \qquad \text{(normalization)}$$

and

$$P(x) = |\psi(x)|^2 = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{x^2}{2\sigma^2})$$

(Gaussian distribution function)

The uncertainty Δx is evaluated as

$$(\Delta x)^2 = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \sigma^2$$

Fourier transform of $\psi(x)$ can be obtained as

$$\begin{aligned}
\psi(p) &= \langle p|\psi\rangle \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp[-\frac{i}{\hbar} px] \frac{1}{\sqrt{\sqrt{2\pi}\sigma}} \exp(-\frac{x^2}{4\sigma^2}) dp \\
&= \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\frac{\sigma}{\hbar}} \exp(-\frac{p^2\sigma^2}{\hbar^2}) \\
&= \frac{1}{\sqrt{\sqrt{2\pi}\,\frac{\hbar}{2\sigma}}} \exp[-\frac{p^2}{2(\frac{\hbar}{2\sigma})^2}]
\end{aligned}$$

The probability $P(p)$ also has the form of the Gaussian distribution function.

$$\begin{aligned}
P(p) &= |\psi(p)|^2 \\
&= \sqrt{\frac{2}{\pi}} \frac{\sigma}{\hbar} \exp(-\frac{2p^2\sigma^2}{\hbar^2}) \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\hbar}{2\sigma}} \exp(-\frac{p^2}{2\frac{\hbar^2}{4\sigma^2}}) \\
&= \frac{1}{\sqrt{2\pi}\sigma_p} \exp(-\frac{p^2}{2\sigma_p{}^2})
\end{aligned}$$

where

$$\sigma_p = \frac{\hbar}{2\sigma}$$

We note that the normalization condition is satisfied,

$$\int_{-\infty}^{\infty} |\psi(p)|^2 dp = 1$$

The uncertainty Δp is evaluated as

$$(\Delta p)^2 = \int_{-\infty}^{\infty} p^2 |\psi(p)|^2 dp = \frac{\hbar^2}{4\sigma^2} = \sigma_p{}^2$$

Then we get

$$\Delta x \Delta p = \sigma \frac{\hbar}{2\sigma} = \frac{\hbar}{2}$$

((**Mathematica**))

```
Clear["Global`*"];
```

$$P[x\_] := \frac{1}{\sqrt{2\pi}\,\sigma}\,\text{Exp}\left[\frac{-1}{2\sigma^2}x^2\right];$$

$$\int_{-\infty}^{\infty} x^2\, P[x]\, dx \;//\; \text{Simplify}[\#, \sigma > 0]\ \&$$

$$\sigma^2$$

$$\int_{-\infty}^{\infty} P[x]\, dx \;//\; \text{Simplify}[\#, \sigma > 0]\ \&$$

$$1$$

$$\psi[x\_] := \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma}}\,\text{Exp}\left[\frac{-1}{4\sigma^2}x^2\right]$$

$$\chi[p\_] := \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \text{Exp}\left[\frac{-i\, p\, x}{\hbar}\right] \psi[x]\, dx$$

```
χ1 = χ[p] // Simplify[#, σ > 0] &
```

$$\frac{e^{-\frac{p^2 \sigma^2}{\hbar^2}} \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma}}{\sqrt{\hbar}}$$

```
Pp = χ1^2
```

$$\frac{e^{-\frac{2 p^2 \sigma^2}{\hbar^2}} \sqrt{\frac{2}{\pi}} \sigma}{\hbar}$$

```
∫_{-∞}^{∞} p^2 Pp ⅆp // Simplify[#, {ℏ > 0, σ > 0}] &
```

$$\frac{\hbar^2}{4 \sigma^2}$$

```
∫_{-∞}^{∞} Pp ⅆp // Simplify[#, {ℏ > 0, σ > 0}] &
```

1

APPENDIX-II

Mathematica: Fourier transform

FourierTransform

FourierTransform[*expr*, *t*, *ω*]
gives the symbolic Fourier transform of *expr*.

FourierTransform[*expr*, {t_1, t_2, …}, {ω_1, ω_2, …}]
gives the multidimensional Fourier transform of *expr*.

Details and Options

- The Fourier transform of a function $f(t)$ is by default defined to be $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i \omega t} dt$.
- Other definitions are used in some scientific and technical fields.
- Different choices of definitions can be specified using the option FourierParameters.
- With the setting FourierParameters -> {*a*, *b*} the Fourier transform computed by FourierTransform is $\sqrt{\frac{|b|}{(2\pi)^{1-a}}} \int_{-\infty}^{\infty} f(t) e^{i b \omega t} dt$.
- Some common choices for {*a*, *b*} are {0, 1} (default; modern physics), {1, -1} (pure mathematics; systems engineering), {-1, 1} (classical physics), and {0, -2 Pi} (signal processing).
- The following options can be given:

Assumptions	$Assumptions	assumptions to make about parameters
FourierParameters	{0, 1}	parameters to define the Fourier transform
GenerateConditions	False	whether to generate answers that involve conditions on parameters

- FourierTransform[*expr*, *t*, *ω*] yields an expression depending on the continuous variable *ω* that represents the symbolic Fourier transform of *expr* with respect to the continuous variable *t*. Fourier[*list*] takes a finite list of numbers as input, and yields as output a list representing the discrete Fourier transform of the input.
- In TraditionalForm, FourierTransform is output using $\mathcal{F}$. »