Quantum Mechanics I, Sheet 3, Spring 2013

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I. THE GAUSSIAN WAVE PACKET

Consider an initial gaussian wave packet

$$\varphi(t=0,p) = (\pi\sigma^2\hbar^2)^{-1/4}\exp\left(-\frac{(p-p_0)^2}{2\sigma^2\hbar^2}\right).$$

The equation of motion is given by the Schrödinger equation of a free particle

$$i\hbar\frac{\partial}{\partial t}\varphi(t,p) = \frac{p^2}{2m}\varphi(t,p)\,.$$

(a) Find the Fourier transform $\psi(0,x)$ of $\varphi(0,p)$, at $t=0$.

(b) For $t=0$, show that $\Delta x\Delta p = \hbar/2$.

(c) Show that the spatial width of the wave packet at time t is given by

$$(\Delta x(t))^2 = \frac{1}{2}\left(\frac{1}{\sigma^2} + \frac{t^2\sigma^2\hbar^2}{m^2}\right).$$

[Hint: to calculate some integrals in this exercise, it could sometimes be useful to try to manipulate the standard Gaussian integral, $\int_{-\infty}^{+\infty} e^{-ax^2}\mathrm{d}x = \sqrt{\frac{\pi}{a}}$. For example, $\int_{-\infty}^{+\infty} x^2 e^{-ax^2}\mathrm{d}x = -\frac{\partial}{\partial a}\int_{-\infty}^{+\infty} e^{-ax^2}\mathrm{d}x = -\frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}} = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$.]

(a) For $t=0$, by performing the Fourier transform of $\varphi(p)$ we get

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\frac{1}{(\pi\sigma^2\hbar^2)^{1/4}}\int_{-\infty}^{+\infty} e^{-\frac{(p-p_0)^2}{2\sigma^2\hbar^2}} e^{\frac{ipx}{\hbar}}\mathrm{d}p$$

and, if we perform the change of variable $\tilde{p} = p - p_0$, we obtain

$$\psi(x) = \frac{e^{\frac{ip_0x}{\hbar}}}{(4\pi^3\hbar^4\sigma^2)^{1/4}}\int_{-\infty}^{+\infty} e^{-\frac{\tilde{p}^2}{2\sigma^2\hbar^2}} e^{\frac{i\tilde{p}x}{\hbar}}\mathrm{d}\tilde{p}.$$

Completing the square in the exponent inside the integral in order to have the standard Gaussian integral, we get

$$\psi(x) = \frac{e^{\frac{ip_0x}{\hbar}}}{(4\pi^3\hbar^4\sigma^2)^{1/4}}\int_{-\infty}^{+\infty} e^{-\frac{1}{2\sigma^2\hbar^2}(\tilde{p}-i\sigma^2\hbar x)^2} e^{-\frac{\sigma^2x^2}{2}}\mathrm{d}\tilde{p},$$

which gives, if we perform another change of variable $p = \tilde{p} - i\sigma^2\hbar x$,

$$\psi(x) = \frac{e^{\frac{ip_0 x}{\hbar}} e^{-\frac{\sigma^2 x^2}{2}}}{(4\pi^3\hbar^4\sigma^2)^{1/4}} \int_{-\infty}^{+\infty} e^{-\frac{p^2}{2\sigma^2\hbar^2}} \mathrm{d}p,$$

and finally

$$\psi(x) = \left(\frac{\sigma^2}{\pi}\right)^{\frac{1}{4}} e^{\frac{ip_0 x}{\hbar}} e^{-\frac{\sigma^2 x^2}{2}}.$$

(b) We obtain

$$\langle x\rangle_{t=0} \equiv \langle x\rangle_0 = \int x|\psi(x)|^2 \mathrm{d}x = \left(\frac{\sigma^2}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} x e^{-\sigma^2 x^2} \mathrm{d}x = 0,$$

and then

$$\begin{aligned}(\Delta x_0)^2 = \langle x^2\rangle_0 - \langle x\rangle_0^2 = \langle x^2\rangle_0 &= \int x^2|\psi(x)|^2 \mathrm{d}x = \sqrt{\frac{\sigma^2}{\pi}} \int_{-\infty}^{+\infty} x^2 e^{-\sigma^2 x^2} \mathrm{d}x \\ &= \sqrt{\frac{\sigma^2}{\pi}} \left(-\frac{\partial}{\partial\sigma^2} \int e^{-\sigma^2 x^2} \mathrm{d}x\right) = -\sqrt{\frac{\sigma^2}{\pi}} \frac{\partial}{\partial\sigma^2} \sqrt{\frac{\pi}{\sigma^2}} = \frac{1}{2\sigma^2}.\end{aligned}$$

Analogously,

$$\langle p\rangle_0 = \int p|\varphi(p)|^2 \mathrm{d}p = \frac{1}{\sqrt{\pi\sigma^2\hbar^2}} \int p e^{-\frac{(p-p_0)^2}{\sigma^2\hbar^2}} \mathrm{d}p,$$

which, after the change of variable $\tilde{p} = p - p_0$, becomes

$$\langle p\rangle_0 = \frac{1}{\sqrt{\pi\sigma^2\hbar^2}} \int (\tilde{p} + p_0) e^{-\frac{\tilde{p}^2}{\sigma^2\hbar^2}} \mathrm{d}p = p_0,$$

and

$$\langle p^2\rangle_0 = \frac{1}{\sqrt{\pi\sigma^2\hbar^2}} \int p^2 e^{-\frac{(p-p_0)^2}{\sigma^2\hbar^2}} \mathrm{d}p.$$

By performing the change of variables $\tilde{p} = p - p_0$, the last integral becomes a sum of three integrals and, after some calculations, we get

$$\langle p^2\rangle_0 = \frac{\sigma^2\hbar^2}{2} + p_0^2.$$

Therefore,

$$(\Delta p_0)^2 = \langle p^2\rangle_0 - \langle p\rangle_0^2 = \frac{\sigma^2\hbar^2}{2}$$

and finally

$$\Delta x_0 \Delta p_0 = \hbar/2,$$

that is, the Heisenberg inequality is saturated in the case of a Gaussian wave packet.
(c) At time t, the wave function $\psi(x,t)$ is the Fourier transform of $e^{-ip^2t/(2m\hbar)}\varphi(p)$, which is still

an exponential function of a second order polynomial in the varianle p (with complex coefficients). The general results concerning the Fourier transform of Gaussian functions apply and one obtains, after a long calculation,

$$|\psi(x,t)|^2 = \frac{1}{\Delta x(t)\sqrt{2\pi}} \exp\left(-\left(x - \frac{p_0 t}{m}\right)^2 \frac{1}{2(\Delta x(t))^2}\right),$$

where

$$(\Delta x(t))^2 = \frac{1}{2}\left(\frac{1}{\sigma^2} + \frac{t^2\sigma^2\hbar^2}{m^2}\right).$$

We recover in this particular case the general results of Chapter 2 of the book: propagation of the centre of the wave packet at a velocity $\langle p\rangle_0/m$ and quadratic variation with time of the variance of the wave packet.

II. PHYSICAL MEASUREMENTS

(a) Consider the observable $\hat{A}$ of a physical quantity A, and its normalized (and orthogonal) eigenfunctions $\psi_n(\mathbf{r})$ associated to the eigenvalues a_n $(n = 1, 2)$. Calculate the variance $(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2$ when the wave function of the system is: (i) $\psi_1(\mathbf{r})$ (ii) $\psi(\mathbf{r}) = c_1\psi_1(\mathbf{r}) + c_2 e^{i\phi}\psi_2(\mathbf{r})$, where c_1, c_2 and ϕ are real constants, and $\psi(\mathbf{r})$ is normalized. [Hint: two eigenfunctions $\psi_n(\mathbf{r})$ and $\psi_m(\mathbf{r})$ are orthogonal when $\int \psi_n^*(\mathbf{r})\psi_m(\mathbf{r})\mathrm{d}^3r = \delta_{n,m}$.]

(b) Consider a particle in a one-dimensional system. At the time $t = 0$, the state of the system is described by the wave function $\psi(x, 0)$, and one measures the position x of the particle immediately after $t = 0$. This process is repeated 10 times, and one finds the following results (in nm) : 550, 478, 539, 498, 541, 497, 455, 496, 500, 479.

  (i) Calculate the expectation value $\langle x\rangle$ and the variance $(\Delta x)^2$ of the position. Since the probability law $|\psi(x, 0)|^2$ is unknown, we will use the following formulas:

$$\langle x\rangle = \frac{1}{N}\sum_{i=1}^{N} x_i \quad , \quad (\Delta x)^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \langle x\rangle)^2 \tag{1}$$

  (ii) One repeats the experiment, but immediately after every measurement of the position, one performs a new measurement of the position. What are the results for the expectation value and the variance after this series of measurements?

(a) For a system whose wave function is $\psi(\mathbf{r})$,

$$\langle A\rangle = \int \psi^*(\mathbf{r})\hat{A}\psi(\mathbf{r})\mathrm{d}^3r \quad , \quad \langle A^2\rangle = \int \psi^*(\mathbf{r})\hat{A}^2\psi(\mathbf{r})\mathrm{d}^3r$$

For (i), $\hat{A}\psi_1(\mathbf{r}) = a_1\psi_1(\mathbf{r})$, $\hat{A}^2\psi_1(\mathbf{r}) = a_1^2\psi_1(\mathbf{r})$. Therefore $\Delta A^2 = 0$. When the system is in an eigenfunction ψ_n of $\hat{A}$, a measurement of A will always yield the value a_n, then the deviation

ΔA of the results is zero. For (ii), $\hat{A}\psi(\mathbf{r}) = c_1 a_1 \psi_1(\mathbf{r}) + c_2 e^{i\phi} a_2 \psi_2(\mathbf{r})$ since $\hat{A}$ is linear, and $\hat{A}^2\psi(\mathbf{r}) = c_1 a_1^2 \psi_1(\mathbf{r}) + c_2 e^{i\phi} a_2^2 \psi_2(\mathbf{r})$. One then has:

$$\begin{aligned}
\langle A \rangle &= \int \left(c_1 \psi_1^*(\mathbf{r}) + c_2 e^{-i\phi} \psi_2^*(\mathbf{r}) \right) \left(c_1 a_1 \psi_1(\mathbf{r}) + c_2 e^{i\phi} a_2 \psi_2(\mathbf{r}) \right) \mathrm{d}^3 r \\
&= c_1^2 a_1 + c_2^2 a_2 \qquad \text{since} \qquad \int \psi_n^*(\mathbf{r}) \psi_m(\mathbf{r}) \mathrm{d}^3 r = \delta_{n,m}
\end{aligned}$$

Analogously, $\langle A^2 \rangle = c_1^2 a_1^2 + c_2^2 a_2^2$. Hence,

$$\begin{aligned}
\Delta A^2 &= c_1^2 a_1^2 + c_2^2 a_2^2 - (c_1^2 a_1 + c_2^2 a_2)^2 \\
&= c_1^2 a_1^2 (1 - c_1^2) + c_2^2 a_2^2 (1 - c_2^2) - 2 c_1^2 c_2^2 a_1 a_2 \\
&= c_1^2 c_2^2 (a_1 - a_2)^2
\end{aligned}$$

where one has used the fact that ψ is normalized: $c_1^2 + c_2^2 = 1$.

(b) For (i), one finds $\langle x \rangle \simeq 503.3$ nm and $\Delta x \simeq 30.9$ nm. For (ii), if one performs a second measurement of the position immediately after the first one (before the wave function has the time of evolving), one necessarily finds the same result of the first measurement. The mean value and the variance are unchanged.

III. PARTICLE IN A ONE-DIMENSIONAL POTENTIAL

A particle of mass m moves in one dimension under the influence of a potential $V(x)$. Suppose it is in an energy eigenstate $\psi(x) = (\gamma^2/\pi)^{1/4} e^{-\gamma^2 x^2/2}$ with energy $E = \hbar^2\gamma^2/(2m)$.

(a) Find the mean position of the particle, $\langle x \rangle$.

(b) Find the mean momentum of the particle, $\langle p \rangle$.

(c) Find V(x) by using the time-independent Schroedinger equation.

(a) The mean position of the particle is

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x) x \psi(x) \mathrm{d}x = \frac{\gamma}{\sqrt{\pi}} \int_{-\infty}^{+\infty} x e^{-\gamma^2 x^2} \mathrm{d}x = 0.$$

(b) The mean momentum is

$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x) \frac{\hbar}{i} \left(\frac{\mathrm{d}}{\mathrm{d}x} \psi(x) \right) = \frac{\gamma\hbar}{i\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-\gamma^2 x^2/2} \frac{\mathrm{d}}{\mathrm{d}x} (e^{-\gamma^2 x^2/2}) \mathrm{d}x = 0.$$

(c) The time-independent Schroedinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \right) \psi(x) = E\psi(x)$$

can be written as

$$-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \psi(x) = [E - V(x)] \psi(x).$$

As

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}e^{-\gamma^2 x^2/2} = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2)e^{-\gamma^2 x^2/2},$$

we have

$$E - V(x) = -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4 x^2),$$

or

$$V(x) = \frac{\hbar^2}{2m}(\gamma^4 x^2 - \gamma^2) + \frac{\hbar^2\gamma^2}{2m} = \frac{\hbar^2\gamma^4 x^2}{2m}.$$