QUANTUM MECHANICS
Appendix 2

The gaussian wave-packet free evolution

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Appendix2: The gaussian wave-packet

To better understand the time evolution of a free particle, in this Appendix we will consider what happens to a **gaussian free wave-packet**.

Appendix2: The gaussian wave-packet

1. Let us assume that the normalized w.f. of a free particle at $t = 0$ is the following

$$\Psi(x,0) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{i\hat{k}x}\; e^{-ax^2}$$

with $a > 0$ and $\hat{k}$ real quantities.

2. To determine the time-evolution of Ψ, we have to start by evaluating the function $\phi(k)$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-ikx}\, \Psi(x,0)$$

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2. If we define $\Delta k \equiv k - \hat{k}$, the full exponent becomes

$$-i\Delta k\; x - ax^2 = -a\left(x + i\frac{\Delta k}{2a}\right)^2 - \frac{(\Delta k)^2}{4a}$$

3. If we define the new variable $z = x + i\frac{\Delta k}{2a}$, we have

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{(\Delta k)^2}{4a}} \int dz\;\, e^{-az^2}$$

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$$\begin{aligned}\phi(k) &= \frac{1}{\sqrt{2\pi}}\left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{(\Delta k)^2}{4a}}\int dz\ e^{-az^2} = \\ &= \frac{1}{\sqrt{2\pi}}\left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{(\Delta k)^2}{4a}}\sqrt{\frac{\pi}{a}} = \\ &= \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} e^{-\frac{(k-\hat{k})^2}{4a}}\end{aligned}$$

2. The function $\phi(k)$ is another gaussian and, as it should be,

$$\int dk\,|\phi(k)|^2 = 1$$

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$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \phi(k)\, e^{ikx}\, e^{-i\frac{\hbar k^2}{2m}t} = $$
$$= \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}} \int dk\, e^{ikx}\, e^{-i\frac{\hbar k^2}{2m}t}\, e^{-\frac{(k-\hat{k})^2}{4a}}$$

2. The full exponent can be rewritten as

$$ikx - i\frac{\hbar}{2m}k^2 t - \frac{(k-\hat{k})^2}{4a} =$$
$$= -\frac{k^2}{4a} + \frac{2k\hat{k}}{4a} - \frac{\hat{k}^2}{4a} - i\frac{\hbar}{2m}k^2 t + ikx =$$
$$= -k^2\left(\frac{1}{4a} + i\frac{\hbar}{2m}t\right) + k\left(\frac{\hat{k}}{2a} + ix\right) - \frac{\hat{k}^2}{4a}$$

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Appendix2: The gaussian wave-packet

1. If we define

$$\alpha \equiv \frac{1}{4a} + i\frac{\hbar}{2m}t; \qquad \beta \equiv \frac{\hat{k}}{2a} + ix$$

the exponent of the integrand, that we have to integrate in the variable k, reads

$$-\alpha k^2 + \beta k - \frac{\hat{k}^2}{4a} = -\alpha\left(k - \frac{\beta}{2\alpha}\right)^2 + \frac{\beta^2}{4\alpha} - \frac{\hat{k}^2}{4a}$$

where the k-dependence is present only in the first term.

2. We have

$$\Psi(x,t) = \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}} e^{\frac{\beta^2}{4\alpha} - \frac{\hat{k}^2}{4a}} \int dk\, e^{-\alpha\left(k - \frac{\beta}{2\alpha}\right)^2}$$

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But, since α has a positive real part,

$$\int dk\, e^{-\alpha\left(k-\frac{\beta}{2\alpha}\right)^2} = \sqrt{\frac{\pi}{\alpha}}$$

and therefore

$$\Psi(x,t) = \sqrt{\frac{\pi}{\alpha}} \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}}\, e^{\frac{\beta^2}{4\alpha}-\frac{\hat{k}^2}{4a}} =$$

$$= \sqrt{\frac{1}{2\alpha}} \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} e^{\frac{\beta^2}{4\alpha}-\frac{\hat{k}^2}{4a}}$$

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1. Let us now consider in more detail the result that we have obtained.

2. Let us start to give a more esplicit form to the quantity α: we have

$$\begin{aligned}\alpha &\equiv \frac{1}{4a} + \frac{i\hbar}{2m}t = \frac{1}{4a}\left(1 + i\frac{2\hbar a}{m}t\right) \\ &\equiv \frac{1}{4a}\left[1 + i\gamma(t)\right]\end{aligned}$$

where we have introduced the parameter

$$\gamma = \gamma(t) \equiv \frac{2\hbar a}{m}t$$

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Therefore

$$\frac{\beta^2}{4\alpha} - \frac{\hat{k}^2}{4a} = \left(\frac{\hat{k}}{2a} + ix\right)^2 \frac{a}{1+i\gamma} - \frac{\hat{k}^2}{4a} =$$

$$= \left(\frac{\hat{k}^2}{4a^2} + \frac{2i\hat{k}x}{2a} - x^2\right) \frac{a}{1+i\gamma} - \frac{\hat{k}^2}{4a} =$$

$$= \left(\frac{\hat{k}^2}{4a} + i\hat{k}x - ax^2\right) \frac{1}{1+i\gamma} - \frac{\hat{k}^2}{4a} =$$

$$= \left(\frac{\hat{k}^2}{4a} + i\hat{k}x - ax^2\right) \frac{1-i\gamma}{1+\gamma^2} - \frac{\hat{k}^2}{4a}$$

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Let us separate the real and the imaginary parts: we have

$$\frac{\beta^2}{4\alpha} - \frac{\hat{k}^2}{4a} = \left[\frac{1}{1+\gamma^2}\left(\frac{\hat{k}^2}{4a} - ax^2 + \gamma\hat{k}x\right) - \frac{\hat{k}^2}{4a}\right] +$$

$$+ \;\; i\left[\frac{1}{1+\gamma^2}\hat{k}x - \frac{\gamma}{1+\gamma^2}\left(\frac{\hat{k}^2}{4a} - ax^2\right)\right] =$$

$$= \;\; \frac{1}{1+\gamma^2}\left[-ax^2 + \gamma\hat{k}x - \gamma^2\frac{\hat{k}^2}{4a}\right] +$$

$$+ \;\; i\,\frac{1}{1+\gamma^2}\left[\hat{k}x - \gamma\left(\frac{\hat{k}^2}{4a} - ax^2\right)\right]$$

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Therefore, in conclusion, we have

$$\Psi(x,t) = \sqrt{\frac{1}{2\alpha}}\left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} e^{\frac{\beta^2}{4\alpha}-\frac{\hat{k}^2}{4a}} =$$

$$= \left(\frac{1}{2a\pi}\right)^{\frac{1}{4}} \sqrt{\frac{2a}{1+i\gamma}}\, e^{\frac{1}{1+\gamma^2}\left[-ax^2+\gamma\hat{k}x-\gamma^2\frac{\hat{k}^2}{4a}\right]} \cdot$$

$$\cdot \quad e^{i\frac{1}{1+\gamma^2}\left[\hat{k}x-\gamma\left(\frac{\hat{k}^2}{4a}-ax^2\right)\right]} =$$

$$= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{1}{1+i\gamma}}\, e^{\frac{-a}{1+\gamma^2}\left[x-\frac{\hat{k}\gamma}{2a}\right]^2} \cdot$$

$$\cdot \quad e^{i\frac{1}{1+\gamma^2}\left[\hat{k}x-\gamma\left(\frac{\hat{k}^2}{4a}-ax^2\right)\right]}$$

where we have to remind that

$$\gamma = \gamma(t) = \frac{2\hbar a}{m} t$$

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The p.d.f. defined by $\Psi(x,t)$ is

$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}}\sqrt{\frac{1}{1+\gamma^2}}\; e^{\frac{-2a}{1+\gamma^2}\left[x-\frac{\hat{k}\gamma}{2a}\right]^2}$$

1. From what we know already about gaussians, the expectation value $<x>$ is

$$<x>=\frac{\hat{k}\gamma}{2a}=\frac{\hat{k}}{2a}\frac{2a\hbar}{m}t=\frac{\hbar\hat{k}}{m}t$$

2. and the standard deviation σ_x is

$$\sigma_x=\sqrt{\frac{1+\gamma^2}{4a}}=\sqrt{\frac{1+(\frac{2a\hbar}{m}t)^2}{4a}}$$

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1. The time behaviour of $< x >$ says that the particle described by the w.f. $\Psi(x,t)$ moves with a costant velocity

$$v = \frac{\hbar \hat{k}}{m}$$

2. Because of the Ehrenfest theorem, we have

$$< p > = m \frac{d}{dt} < x > = m\, v = \hbar \hat{k}$$

which says that the expectation value of the particle momentum is **time independent** (as it should be !) and it is simply given by $m\, v$.

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1. The standard deviation σ_x of the p.d.f. distribution $|\Psi(x,t)|^2$ is not constant but grows in time:

$$\sigma_x = \sqrt{\frac{1}{4a}}\sqrt{1+\left(\frac{2\hbar a}{m}t\right)^2}$$

   This occours because the different wave components, weighted through $\phi(k)$, tend to separate since they have different phase velocity and, therefore, the wave-packet tends to spread out.

2. In the limit $t \to \infty$, σ_x grows linearly in time, in fact

$$\frac{2\hbar a}{m}t >> 1 \quad \Rightarrow \quad \sigma_x \approx \sqrt{\frac{1}{4a}}\frac{2\hbar a}{m}t = \sqrt{a}\,\frac{\hbar}{m}\,t$$

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Concerning the expectation value p^2, we notice that, since for the free particle $2m\,\hat{p}^2 = \hat{H}$, we have $< p^2 >= 2m < E >$ and, from what we have already seen

$$< E > \; = \; \int dk \; |\phi(k)|^2 \, E_k \equiv \int \; dk|\phi(k)|^2 \, \frac{\hbar^2 k^2}{2m} =$$
$$= \int dk \; \sqrt{\frac{1}{2a\pi}} \, e^{-\frac{(k-\hat{k})^2}{2a}} \; \frac{\hbar^2 k^2}{2m}$$

therefore

$$< p^2 >= \hbar^2 \sqrt{\frac{1}{2a\pi}} \int dk \; e^{-\frac{(k-\hat{k})^2}{2a}} \; k^2$$

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If we define the variable $\xi = k - \hat{k}$, the integral becomes

$$\int dk\, e^{-\frac{(k-\hat{k})^2}{2a}}\, k^2 = \int d\xi\, e^{-\frac{\xi^2}{2a}}\, (\xi + \hat{k})^2 =$$

$$= \int d\xi\, e^{-\frac{\xi^2}{2a}}\, (\xi^2 + 2\xi\hat{k} + \hat{k}^2) =$$

and

$$\begin{aligned} \int d\xi\ e^{-\frac{\xi^2}{2a}}\ \xi^2 &= a\sqrt{2\pi\, a} \\ 2\hat{k} \int d\xi\, e^{-\frac{\xi^2}{2a}}\ \xi &= 0 \\ \hat{k}^2 \int d\xi\ e^{-\frac{\xi^2}{2a}} &= \hat{k}^2 \sqrt{2\pi\, a} \end{aligned}$$

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1. Therefore

$$< p^2 >= \hbar^2 \frac{1}{\sqrt{2\pi\, a}} \sqrt{2\pi\, a} \left(a + \hat{k}^2\right) = \hbar^2 \left(a + \hat{k}^2\right)$$

$$\Rightarrow \sigma_p^2 =< p^2 > - < p >^2 = \hbar^2\, a$$

$$\Rightarrow \sigma_p = \hbar\sqrt{a}$$

which shows that, unlike σ_x, σ_p is constant.

2. From the result of $< p^2 >$, we obtain

$$< E >= \frac{\hbar^2}{2m}\left(\hat{k}^2 + a\right)$$

It is obviously constant, but it does not coincide with $\frac{\hbar^2}{2m}\hat{k}^2$ because of the momentum spread ...

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Concerning the uncertainty relationship, since we have found that

$$\sigma_x = \sqrt{\frac{1}{4a}} \sqrt{1 + \left(\frac{2\hbar a}{m} t\right)^2}$$

their product is equal to

$$\sigma_x \, \sigma_p = \frac{\hbar}{2} \sqrt{1 + \left(\frac{2\hbar a}{m} t\right)^2}$$

which shows that the uncertainty starts at its minimum for $t = 0$, then grows up and, for $t \to \infty$ becomes linear in time ...

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