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# Some integrals with Gaussian wavepackets

## 1. Definition

The normalized Gaussian wavepacket is defined as:

$$G = \left(\frac{a}{\pi}\right)^{1/4} \exp\left(-\frac{a}{2}(x-x_0)^2 + ip_0(x-x_0)\right). \tag{1}$$

Here, $a$ is the width parameter, $x_0$ is the center of wavepacket, $p_0$ is the momentum of wavepacket.

## 2. Overlap integral

$$\begin{aligned} S_{12} &= \int G_1^* G_2 dx = \left(\frac{a}{\pi}\right)^{1/2} \int \exp\left(-\frac{a}{2}(x-x_{0,1})^2 - \frac{a}{2}(x-x_{0,2})^2 - ip_{0,1}(x-x_{0,1}) + ip_{0,2}(x-x_{0,2})\right) dx = \\ &= \left(\frac{a}{\pi}\right)^{1/2} \int \exp\left(\left[-ax^2 + a(x_{0,1}+x_{0,2})x - \frac{a}{2}(x_{0,1}^2 + x_{0,2}^2) + i(p_{0,1}x_{0,1} - p_{0,2}x_{0,2})\right] + ix(p_{0,2} - p_{0,1})\right) dx = \\ &= \left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}(x_{0,1}^2 + x_{0,2}^2) + i(p_{0,1}x_{0,1} - p_{0,2}x_{0,2})\right) \int \exp\left(-ax^2 + [a(x_{0,1}+x_{0,2}) + i(p_{0,2}-p_{0,1})]x\right) dx = \\ &= \exp\left(-\frac{a}{2}(x_{0,1}^2 + x_{0,2}^2) + i(p_{0,1}x_{0,1} - p_{0,2}x_{0,2})\right) \exp\left(\frac{[a(x_{0,1}+x_{0,2}) + i(p_{0,2}-p_{0,1})]^2}{4a}\right) = \\ &= \exp\left(-\frac{a}{4}(x_{0,1}-x_{0,2})^2 - \frac{1}{4a}(p_{0,2}-p_{0,1})^2\right) \exp\left(i\left((x_{0,1}-x_{0,2})\frac{(p_{0,1}+p_{0,2})}{2}\right)\right) \end{aligned} \tag{2}$$

Here, we have used the integral

$$\int \exp(-ax^2 + bx + c) dx = \left(\frac{\pi}{a}\right)^{1/2} \exp\left(\frac{b^2}{4a} + c\right) \tag{3}$$

## 3. Derivative coupling integral

$$\begin{aligned} D_{12} &= \int G_1^* \nabla G_2 dx = \left(\frac{a}{\pi}\right)^{1/2} \int [-a(x-x_{0,2}) + ip_{0,2}] \exp\left(-\frac{a}{2}(x-x_{0,1})^2 - \frac{a}{2}(x-x_{0,2})^2 - ip_{0,1}(x-x_{0,1}) + ip_{0,2}(x-x_{0,2})\right) dx = \\ &= (ax_{0,2} + ip_{0,2})S - a\left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}(x_{0,1}^2 + x_{0,2}^2) + i(p_{0,1}x_{0,1} - p_{0,2}x_{0,2})\right) \int x \exp\left(-ax^2 + [a(x_{0,1}+x_{0,2}) + i(p_{0,2}-p_{0,1})]x\right) dx = \\ &= (ax_{0,2} + ip_{0,2})S - a\left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}(x_{0,1}^2 + x_{0,2}^2) + i(p_{0,1}x_{0,1} - p_{0,2}x_{0,2})\right) \frac{b}{2a} \exp\left(\frac{b^2}{4a}\right)\left(\frac{\pi}{a}\right)^{1/2} = \\ &= (ax_{0,2} + ip_{0,2})S - \frac{b}{2}S = \left\{(ax_{0,2} + ip_{0,2}) - \frac{[a(x_{0,1}+x_{0,2}) + i(p_{0,2}-p_{0,1})]}{2}\right\} S = \frac{[-a(x_{0,1}-x_{0,2}) + i(p_{0,2}+p_{0,1})]}{2} S \end{aligned} \tag{4}$$

Check:

$$\int (\nabla G_1^*) G_2 dx = \int (G_2^* \nabla G_1)^* dx = \frac{[-a(x_{0,2}-x_{0,1}) - i(p_{0,1}+p_{0,2})]}{2} S \tag{5}$$

So:

$$D_{12}^* = -D_{21}. \tag{6}$$

## 4. Kinetic energy integral

$$g = \exp\left(-\frac{a}{2}(x-x_0)^2 + ip_0(x-x_0)\right) \tag{7}$$

$$g_x^{'} = (-a(x-x_0) + ip_0)G \tag{8}$$

$$\begin{aligned} g_x^{''} &= -ag + (-a(x-x_0)+ip_0)g' = -ag + (-a(x-x_0)+ip_0)^2 g = \\ &= \left(a^2(x-x_0)^2 - 2iap_0(x-x_0) - a - p_0^2\right)g \end{aligned} \tag{9}$$

$$\begin{aligned} \int G_1^* \nabla^2 G_2 dx &= \left(\frac{a}{\pi}\right)^{1/2} \int \left(a^2(x-x_{0,2})^2 - 2iap_{0,2}(x-x_{0,2}) - a - p_{0,2}^2\right) g_1^* g_2 dx = \\ &= \left(-a - p_{0,2}^2\right) S_{12} + I_2 - I_1 \end{aligned} \tag{10}$$

$$\begin{aligned} I_2 &= \left(\frac{a}{\pi}\right)^{1/2} \int a^2 (x-x_{0,2})^2 g_1^* g_2 dx = \\ &= a^2\left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right) \\ &\int (x-x_{0,2})^2 \exp\left(-ax^2 + \left[a(x_{0,1}+x_{0,2}) + i(p_{0,2}-p_{0,1})\right]x\right)dx = \\ &= C\int (x-x_{0,2})^2 \exp\left(-ax^2 + bx\right)dx = C\int (x-x_{0,2})^2 \exp\left(-a\left(x - \frac{b}{2a}\right)^2 + \frac{b^2}{4a}\right)dx = \left| x' = x - \frac{b}{2a} \right| = \\ &= C'\int \left(x' + \frac{b}{2a} - x_{0,2}\right)^2 \exp\left(-ax'^2\right)dx' = C'\left[\frac{3}{2}\left(\frac{\pi}{a^3}\right)^{1/2} + \left(\frac{b}{2a} - x_{0,2}\right)^2\left(\frac{\pi}{a}\right)^{1/2}\right] = \\ &= a^2\left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right)\exp\left(\frac{b^2}{4a}\right)\left[\frac{3}{2}\left(\frac{\pi}{a^3}\right)^{1/2} + \left(\frac{b}{2a} - x_{0,2}\right)^2\left(\frac{\pi}{a}\right)^{1/2}\right] = \\ &= a^2 \exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right) + \frac{b^2}{4a}\right)\left[\frac{3}{2a} + \left(\frac{b}{2a} - x_{0,2}\right)^2\right] = \\ &= S_{12}a^2\left[\frac{3}{2a} + \left(\frac{b}{2a} - x_{0,2}\right)^2\right] = S_{12}\left[\frac{3a}{2} + \left(\frac{b - 2ax_{0,2}}{2}\right)^2\right] \end{aligned} \tag{11}$$

$$C = a^2\left(\frac{a}{\pi}\right)^{1/2} \exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right) \tag{12}$$

$$C' = C\exp\left(\frac{b^2}{4a}\right) \tag{13}$$

$$b = \left[a(x_{0,1} + x_{0,2}) + i(p_{0,2} - p_{0,1})\right] \tag{14}$$

$$I_1 = 2iap_{0,2}\left(\frac{a}{\pi}\right)^{1/2}\exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right)$$
$$\int\left(x - x_{0,2}\right)\exp\left(-ax^2 + \left[a\left(x_{0,1} + x_{0,2}\right) + i\left(p_{0,2} - p_{0,1}\right)\right]x\right)dx =$$
$$= C\int\left(x - x_{0,2}\right)\exp\left(-ax^2 + bx\right)dx = C\int\left(x - x_{0,2}\right)\exp\left(-a\left(x - \frac{b}{2a}\right)^2 + \frac{b^2}{4a}\right)dx = \tag{15}$$
$$= C'\int\left(x - x_{0,2}\right)\exp\left(-a\left(x - \frac{b}{2a}\right)^2\right)dx = \left| x' = x - \frac{b}{2a}\right| = C'\int\left(x' + \frac{b}{2a} - x_{0,2}\right)\exp\left(-ax'^2\right)dx' =$$
$$= C'\left(\frac{b}{2a} - x_{0,2}\right)\left(\frac{\pi}{a}\right)^{1/2} = 2iap_{0,2}\left(\frac{a}{\pi}\right)^{1/2}\exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right)\exp\left(\frac{b^2}{4a}\right)\left(\frac{b}{2a} - x_{0,2}\right)\left(\frac{\pi}{a}\right)^{1/2} =$$
$$= 2iap_{0,2}\exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right) + \frac{b^2}{4a}\right)\left(\frac{b}{2a} - x_{0,2}\right) =$$
$$= S_{12}ip_{0,2}\left(b - 2ax_{0,2}\right)$$

$$C = 2iap_{0,2}\left(\frac{a}{\pi}\right)^{1/2}\exp\left(-\frac{a}{2}\left(x_{0,1}^2 + x_{0,2}^2\right) + i\left(p_{0,1}x_{0,1} - p_{0,2}x_{0,2}\right)\right) \tag{16}$$

$$C' = C\exp\left(\frac{b^2}{4a}\right) \tag{17}$$

$$b = \left[a\left(x_{0,1} + x_{0,2}\right) + i\left(p_{0,2} - p_{0,1}\right)\right] \tag{18}$$

So:

$$\int G_1^*\nabla^2 G_2 dx = \left(-a - p_{0,2}^2\right)S_{12} + I_2 - I_1 =$$
$$= \left(-a - p_{0,2}^2\right)S_{12} + S_{12}\left[\frac{3a}{2} + \left(\frac{b - 2ax_{0,2}}{2}\right)^2\right] - S_{12}ip_{0,2}\left(b - 2ax_{0,2}\right) =$$
$$= S_{12}\left\{-a - p_{0,2}^2 + \frac{3a}{2} + \frac{\left[a\left(x_{0,1} - x_{0,2}\right) + i\left(p_{0,2} - p_{0,1}\right)\right]^2}{4} - ip_{0,2}\left[a\left(x_{0,1} - x_{0,2}\right) + i\left(p_{0,2} - p_{0,1}\right)\right]\right\} = \tag{19}$$
$$= S_{12}\left\{\begin{array}{l}\frac{a}{2} - p_{0,2}^2 + \frac{1}{4}a^2\left(x_{0,1} - x_{0,2}\right)^2 + \frac{1}{2}ai\left(x_{0,1} - x_{0,2}\right)\left(p_{0,2} - p_{0,1}\right) - \frac{1}{4}\left(p_{0,2}^2 - 2p_{0,2}p_{0,1} + p_{0,1}^2\right) \\ -ai\left(x_{0,1} - x_{0,2}\right)p_{0,2} + p_{0,2}^2 - p_{0,2}p_{0,1}\end{array}\right\} =$$
$$= S_{12}\left\{\frac{a}{2} + a^2\left(\frac{x_{0,1} - x_{0,2}}{2}\right)^2 - \left(\frac{p_{0,2} + p_{0,1}}{2}\right)^2 - \frac{1}{2}ai\left(x_{0,1} - x_{0,2}\right)\left(p_{0,2} + p_{0,1}\right)\right\}$$

## 5. Summary

$$G = \left(\frac{a}{\pi}\right)^{1/4}\exp\left(-\frac{a}{2}\left(x - x_0\right)^2 + ip_0\left(x - x_0\right)\right), \tag{20}$$

$$S_{G,12} = \int G_1^* G_2 dx = \exp\left(-\frac{a}{4}\left(x_{0,1} - x_{0,2}\right)^2 - \frac{1}{4a}\left(p_{0,2} - p_{0,1}\right)^2\right)\exp\left(i\left(\left(x_{0,1} - x_{0,2}\right)\frac{\left(p_{0,1} + p_{0,2}\right)}{2}\right)\right) \tag{21}$$

$$D_{G,12} = \int G_1^*\nabla G_2 dx = \frac{\left[-a\left(x_{0,1} - x_{0,2}\right) + i\left(p_{0,2} + p_{0,1}\right)\right]}{2}S_{G,12} \tag{22}$$

$$T_{G,12} = \int G_1^*\nabla^2 G_2 dx = S_{G,12}\left\{\frac{a}{2} + a^2\left(\frac{x_{0,1} - x_{0,2}}{2}\right)^2 - \left(\frac{p_{0,2} + p_{0,1}}{2}\right)^2 - \frac{1}{2}ai\left(x_{0,1} - x_{0,2}\right)\left(p_{0,2} + p_{0,1}\right)\right\} \tag{23}$$