Some integrals with Gaussian wavepackets

1. Definition

The normalized Gaussian wavepacket is defined as:

$$G(x; x_0, p_0, \alpha, \gamma) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \exp\left(-\alpha(x - x_0)^2 + \frac{ip_0}{\hbar}(x - x_0) + \frac{i\gamma}{\hbar}\right). \qquad (1)$$

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

2. Overlap integral

$$S_{12} = \langle G_1 | G_2 \rangle = \left(\frac{2\alpha_1}{\pi}\right)^{1/4} \left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(\frac{\gamma_2 - \gamma_1}{\hbar} i\right) \int \exp\left(-\alpha_1(x - x_1)^2 - \frac{ip_1}{\hbar}(x - x_1)\right) \exp\left(-\alpha_2(x - x_2)^2 + \frac{ip_2}{\hbar}(x - x_2)\right) dx.$$

Lets simplify:

$$-\alpha_2(x - x_2)^2 - \alpha_1(x - x_1)^2 + \frac{ip_2}{\hbar}(x - x_2) - \frac{ip_1}{\hbar}(x - x_1) = \boldsymbol{-(\alpha_1 + \alpha_2)x^2} + \boldsymbol{2(\alpha_2 x_2 + \alpha_1 x_1)x} - (\alpha_2 x_2^2 + \alpha_1 x_1^2) + \boldsymbol{\frac{i(p_2 - p_1)}{\hbar} x} - \frac{i(p_2 x_2 - p_1 x_1)}{\hbar}.$$

$$\boldsymbol{-(\alpha_1 + \alpha_2)x^2 + 2\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)x} = -(\alpha_1 + \alpha_2)\left[x^2 - 2\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)}{(\alpha_1 + \alpha_2)} x + \left(\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)}{(\alpha_1 + \alpha_2)}\right)^2\right] + \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)^2}{(\alpha_1 + \alpha_2)} = -(\alpha_1 + \alpha_2)\left[x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)}{(\alpha_1 + \alpha_2)}\right]^2 + \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)^2}{(\alpha_1 + \alpha_2)}.$$

Thus,

$$S_{12} = \langle G_1 | G_2 \rangle = \left(\frac{2\alpha_1}{\pi}\right)^{1/4} \left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(\frac{\gamma_2 - \gamma_1}{\hbar} i\right) \boldsymbol{\exp\left(\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)^2}{(\alpha_1 + \alpha_2)}\right)} \exp\left(-\boldsymbol{(\alpha_2 x_2^2 + \alpha_1 x_1^2)} - \frac{i(p_2 x_2 - p_1 x_1)}{\hbar}\right) \int \exp\left(-(\alpha_1 + \alpha_2)\left[x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar}\right)}{(\alpha_1 + \alpha_2)}\right]^2\right) dx.$$

Pre-factor:

$$\frac{\left(\alpha_2 x_2+\alpha_1 x_1+\frac{i(p_2-p_1)}{2\hbar}\right)^2}{(\alpha_1+\alpha_2)}-(\alpha_2 x_2^2+\alpha_1 x_1^2)=$$
$$\frac{\alpha_2^2x_2^2+\alpha_1^2x_1^2-\frac{(p_2-p_1)^2}{4\hbar^2}+2\alpha_1\alpha_2x_1x_2+2\frac{i(p_2-p_1)}{2\hbar}(\alpha_2x_2+\alpha_1x_1)-[\alpha_1\alpha_2x_2^2+\alpha_1^2x_1^2+\alpha_2^2x_2^2+\alpha_2\alpha_1x_1^2]}{(\alpha_1+\alpha_2)},$$

$$=\frac{-\frac{(p_2-p_1)^2}{4\hbar^2}+2\alpha_1\alpha_2x_1x_2+\frac{i(p_2-p_1)}{\hbar}(\alpha_2x_2+\alpha_1x_1)-[\alpha_1\alpha_2x_2^2+\alpha_2\alpha_1x_1^2]}{(\alpha_1+\alpha_2)},$$
$$=\frac{-\frac{(p_2-p_1)^2}{4\hbar^2}+\frac{i(p_2-p_1)}{\hbar}(\alpha_2x_2+\alpha_1x_1)-[\alpha_1\alpha_2x_2^2-2\alpha_1\alpha_2x_1x_2+\alpha_2\alpha_1x_1^2]}{(\alpha_1+\alpha_2)},$$
$$=\frac{-\frac{(p_2-p_1)^2}{4\hbar^2}+\frac{i(p_2-p_1)}{\hbar}(\alpha_2x_2+\alpha_1x_1)-\alpha_1\alpha_2(x_2-x_1)^2}{(\alpha_1+\alpha_2)}.$$

The integral is:
$$\int \exp\left(-(\alpha_1+\alpha_2)\left[x-\frac{\left(\alpha_2x_2+\alpha_1x_1+\frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2\right)dx=\sqrt{\frac{\pi}{\alpha_1+\alpha_2}}.$$

$$S_{12}=\langle G_1|G_2\rangle=\left(\frac{2\alpha_1}{\pi}\right)^{1/4}\left(\frac{2\alpha_2}{\pi}\right)^{1/4}\left(\frac{\pi^2}{(\alpha_1+\alpha_2)^2}\right)^{1/4}\exp(i\phi)\exp\left(\frac{-\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_2-x_1)^2-\frac{(p_2-p_1)^2}{4\hbar^2(\alpha_1+\alpha_2)}\right),$$

$$\phi=\frac{\gamma_2-\gamma_1}{\hbar}+\frac{(\alpha_1x_1+\alpha_2x_2)}{\alpha_1+\alpha_2}\frac{(p_2-p_1)}{\hbar}-\frac{(p_2x_2-p_1x_1)}{\hbar}.$$

Simplify:
$\frac{(\alpha_1x_1+\alpha_2x_2)}{\alpha_1+\alpha_2}\frac{(p_2-p_1)}{\hbar}-\frac{(p_2x_2-p_1x_1)}{\hbar}=\frac{1}{\hbar(\alpha_1+\alpha_2)}\left[(\alpha_1x_1+\alpha_2x_2)(p_2-p_1)-(\alpha_1+\alpha_2)(p_2x_2-p_1x_1)\right]=\frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1x_1p_2+\alpha_2x_2p_2-\alpha_1x_1p_1-\alpha_2x_2p_1-(\alpha_1p_2x_2-\alpha_1p_1x_1+\alpha_2p_2x_2-\alpha_2p_1x_1)\right]=\frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1x_1p_2+\alpha_2x_2p_2-\alpha_1x_1p_1-\alpha_2x_2p_1-\alpha_1p_2x_2+\alpha_1p_1x_1-\alpha_2p_2x_2+\alpha_2p_1x_1\right]=\frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1x_1p_2-\alpha_2x_2p_1-\alpha_1p_2x_2+\alpha_2p_1x_1\right]=\frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1p_2(x_1-x_2)+\alpha_2p_1(x_1-x_2)\right]=\frac{(\alpha_2p_1+\alpha_1p_2)}{\hbar(\alpha_1+\alpha_2)}(x_1-x_2).$

So, the phase is:

$$\phi=\frac{\gamma_2-\gamma_1}{\hbar}+\frac{(\alpha_2p_1+\alpha_1p_2)}{\hbar(\alpha_1+\alpha_2)}(x_1-x_2)$$

Finally:
$$S_{12}=\langle G_1|G_2\rangle=\left(\frac{4\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}\right)^{1/4}\exp(i\phi)\exp\left(\frac{-\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_2-x_1)^2-\frac{(p_2-p_1)^2}{4\hbar^2(\alpha_1+\alpha_2)}\right).$$

$$\phi = \frac{\gamma_2 - \gamma_1}{\hbar} + \frac{(\alpha_2 p_1 + \alpha_1 p_2)}{\hbar(\alpha_1 + \alpha_2)}(x_1 - x_2)$$

When $\alpha_1 = \alpha_2 = \alpha$

$\phi = \frac{\gamma_2 - \gamma_1}{\hbar} + (x_1 - x_2)\frac{(p_2 + p_1)}{2\hbar}$.

And:
$\exp\left(\frac{-\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_2 - x_1)^2 - \frac{(p_2-p_1)^2}{4\hbar^2(\alpha_1+\alpha_2)}\right) = \exp\left(\frac{-\alpha}{2}(x_2 - x_1)^2 - \frac{(p_2-p_1)^2}{8\alpha\hbar^2}\right)$.

Also:

$\left(\frac{2\alpha_1}{\pi}\right)^{1/4}\left(\frac{2\alpha_2}{\pi}\right)^{1/4}\left(\frac{\pi^2}{(\alpha_1+\alpha_2)^2}\right)^{1/4} = \left(\frac{4\alpha^2}{\pi^2}\right)^{1/4}\left(\frac{\pi^2}{(2\alpha)^2}\right)^{1/4} = 1.$

So, that we recover the special result:

$S_{12} = \exp\left(\frac{-\alpha}{2}(x_2 - x_1)^2 - \frac{(p_2-p_1)^2}{8\alpha\hbar^2} + i\left[\frac{\gamma_2-\gamma_1}{\hbar} + (x_1 - x_2)\frac{(p_2+p_1)}{2\hbar}\right]\right)$.

3. Transition dipole moment

We will need an integral:

$\int x \exp\left(-(\alpha_1 + \alpha_2)\left[x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2\right) dx = \left| y = x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)} \right| = \int\left(y + \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right)\exp(-(\alpha_1 + \alpha_2)y^2)\,dy = \int y \exp(-(\alpha_1 + \alpha_2)y^2)\,dy + \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\int \exp(-(\alpha_1 + \alpha_2)y^2)\,dy = \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\sqrt{\frac{\pi}{\alpha_1+\alpha_2}}$.

That is:

$$\mu_{12} = \langle G_1 | x | G_2 \rangle = \left[\frac{\alpha_2 x_2 + \alpha_1 x_1}{\alpha_1 + \alpha_2} + \frac{i}{2\hbar}\frac{p_2 - p_1}{\alpha_1 + \alpha_2}\right] S_{12}$$

For $\alpha_1 = \alpha_2 = \alpha$, we recover the special result:

$$\mu_{12} = \langle G_1|x|G_2\rangle = \left[\frac{x_1+x_2}{2} + i\,\frac{p_2-p_1}{4\alpha\hbar}\right] S_{12}$$

4. Derivative coupling

Differentiation of the ket function will yield:

$$\nabla G_2 = \left[-2\alpha_2(x-x_2) + \frac{ip_2}{\hbar}\right] G_2$$

So:

$$d_{12} = \langle G_1|\nabla|G_2\rangle = -2\alpha_2\langle G_1|\mathrm{x}|G_2\rangle + \left[2\alpha_2 x_2 + \frac{ip_2}{\hbar}\right]\langle G_1|G_2\rangle = \left[-2\alpha_2\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)} + 2\alpha_2 x_2 + \frac{ip_2}{\hbar}\right] S_{12}.$$

$$-2\alpha_2\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)} + 2\alpha_2 x_2 + \frac{ip_2}{\hbar} = \frac{-2\alpha_2^2 x_2 - 2\alpha_2\,\alpha_1 x_1 - \frac{i(\alpha_2 p_2 - \alpha_2 p_1)}{\hbar}}{(\alpha_1+\alpha_2)} + \frac{2\alpha_2\alpha_1 x_2 + 2\alpha_2^2 x_2 + \frac{i\alpha_1 p_2}{\hbar} + \frac{i\alpha_2 p_2}{\hbar}}{(\alpha_1+\alpha_2)} = \frac{2\alpha_2\alpha_1(x_2-x_1) + \frac{i}{\hbar}[\alpha_1 p_2 + \alpha_2 p_2 - \alpha_2 p_2 + \alpha_2 p_1]}{(\alpha_1+\alpha_2)} = \frac{2\alpha_2\alpha_1(x_2-x_1) + \frac{i}{\hbar}[\alpha_1 p_2 + \alpha_2 p_1]}{(\alpha_1+\alpha_2)}.$$

So:

$$d_{12} = \langle G_1|\nabla|G_2\rangle = \left[\frac{2\alpha_2\alpha_1}{\alpha_1+\alpha_2}(x_2-x_1) + \frac{i}{\hbar}\frac{\alpha_1 p_2 + \alpha_2 p_1}{\alpha_1+\alpha_2}\right] S_{12}$$

For $\alpha_1 = \alpha_2 = \alpha$, we recover the special result:

$$d_{12} = \langle G_1|\nabla|G_2\rangle = \left[\alpha(x_2-x_1) + \frac{i}{\hbar}\frac{p_2+p_1}{2}\right] S_{12}$$

5. Kinetic energy matrix elements

Double differentiation of the ket function will yield:

$$\nabla G_2 = \left[-2\alpha_2(x-x_2) + \frac{ip_2}{\hbar}\right] G_2$$

$$\nabla^2 G_2 = -2\alpha_2 G_2 + \left[-2\alpha_2(x-x_2) + \frac{ip_2}{\hbar}\right]^2 G_2$$

$$= \left[4\alpha_2^2(x-x_2)^2 - \frac{4i\alpha_2 p_2}{\hbar}(x-x_2) - \frac{p_2^2}{\hbar^2} - 2\alpha_2\right] G_2$$

$$= \left[4\alpha_2^2 x^2 - 8\alpha_2^2 x_2 x + 4\alpha_2^2 x_2^2 - \frac{4i\alpha_2 p_2}{\hbar}x + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} - 2\alpha_2\right] G_2$$

So:

$$T_{12} = \langle G_1|\nabla^2|G_2\rangle$$

$$= 4\alpha_2^2\langle G_1|\mathrm{x}^2|G_2\rangle - \left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar}\right]\langle G_1|\mathrm{x}|G_2\rangle$$

$$+ \left[4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} - 2\alpha_2\right]\langle G_1|G_2\rangle =$$

$$= 4\alpha_2^2\langle G_1|\mathrm{x}^2|G_2\rangle - \left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar}\right]\left[\frac{\alpha_2 x_2 + \ \alpha_1 x_1}{\alpha_1+\alpha_2} + \frac{i}{2\hbar}\frac{p_2 - p_1}{\alpha_1+\alpha_2}\right] S_{12}$$

$$+ \left[4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} - 2\alpha_2\right] S_{12}$$

So, we need the integral:

$$\int x^2 \exp\left(-(\alpha_1+\alpha_2)\left[x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2\right) dx = \left| y = x - \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right| = \int \left(y + \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right)^2 \exp(-(\alpha_1+\alpha_2)y^2)\, dy =$$

$$\int y^2 \exp(-(\alpha_1+\alpha_2)y^2)\, dy + \left[\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2 \int \exp(-(\alpha_1+\alpha_2)y^2)\, dy =$$

$$\left(\frac{1}{2(\alpha_1+\alpha_2)}\right)\sqrt{\frac{\pi}{\alpha_1+\alpha_2}} + \left[\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2 \sqrt{\frac{\pi}{\alpha_1+\alpha_2}}.$$

That is:

$$\langle G_1|\mathrm{x}^2|G_2\rangle = \left(\frac{1}{2(\alpha_1+\alpha_2)} + \left[\frac{\left(\alpha_2 x_2 + \ \alpha_1 x_1 + \frac{i\left(p_2 - p_1\right)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2\right) S_{12}$$

Simplify:

$$T_{12} = \langle G_1|\nabla^2|G_2\rangle = \left\{4\alpha_2^2\left(\frac{1}{2(\alpha_1+\alpha_2)} + \left[\frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2\right) - \left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar}\right]\left[\frac{\alpha_2 x_2 + \alpha_1 x_1}{\alpha_1+\alpha_2} + \frac{i}{2\hbar}\frac{p_2-p_1}{\alpha_1+\alpha_2}\right] + \left[4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} - 2\alpha_2\right]\right\} S_{12}.$$

$$\begin{aligned}
\left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar}\right]\left[\frac{\alpha_2 x_2 + \ \alpha_1 x_1}{\alpha_1+\alpha_2} + \frac{i}{2\hbar}\frac{p_2 - p_1}{\alpha_1+\alpha_2}\right] \\
= \frac{1}{(\alpha_1+\alpha_2)}\left[8\alpha_2^3 x_2^2 + 8\alpha_2^2\alpha_1 x_2 x_1 - \frac{2}{\hbar^2}\left(\alpha_2 p_2^2 - \alpha_2 p_1 p_2\right)\right] \\
+ \frac{i}{\hbar(\alpha_1+\alpha_2)}\left[4\alpha_2^2 p_2 x_2 + \ 4\alpha_1\alpha_2 p_2 x_1 + 4\alpha_2^2 x_2 p_2 - 4\alpha_2^2 x_2 p_1\right]
\end{aligned}$$

$$\begin{aligned}
-\left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar}\right]\left[\frac{\alpha_2 x_2 + \ \alpha_1 x_1}{\alpha_1+\alpha_2} + \frac{i}{2\hbar}\frac{p_2 - p_1}{\alpha_1+\alpha_2}\right] + 4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} = \\
= \frac{1}{(\alpha_1+\alpha_2)}\left[-8\alpha_2^3 x_2^2 - 8\alpha_2^2\alpha_1 x_2 x_1 + \frac{2}{\hbar^2}\left(\alpha_2 p_2^2 - \alpha_2 p_1 p_2\right) + 4\alpha_2^2\alpha_1 x_2^2 + 4\alpha_2^3 x_2^2 \right. \\
\left. - \frac{\alpha_1 p_2^2}{\hbar^2} - \frac{\alpha_2 p_2^2}{\hbar^2}\right] \\
+ \frac{4i}{\hbar(\alpha_1+\alpha_2)}\left[-\alpha_2^2 p_2 x_2 - \ \alpha_1\alpha_2 p_2 x_1 - \alpha_2^2 x_2 p_2 + \alpha_2^2 x_2 p_1 \right. \\
\left. + \alpha_2\alpha_1 p_2 x_2 + \alpha_2^2 p_2 x_2\right]
\end{aligned}$$

$$= \frac{1}{(\alpha_1+\alpha_2)}\left[-4\alpha_2^3x_2^2 - 8\alpha_2^2\alpha_1x_2x_1 + \frac{2}{\hbar^2}\left(\alpha_2p_2^2 - \alpha_2p_1p_2\right) + 4\alpha_2^2\alpha_1x_2^2 - \frac{\alpha_1p_2^2}{\hbar^2} - \frac{\alpha_2p_2^2}{\hbar^2}\right] + \frac{4i}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_2^2x_2(p_1-p_2) + \alpha_2\alpha_1p_2(x_2-x_1)\right]$$

$$4\alpha_2^2\left[\frac{\left(\alpha_2x_2 + \alpha_1x_1 + \frac{i(p_2-p_1)}{2\hbar}\right)}{(\alpha_1+\alpha_2)}\right]^2 = 4\alpha_2^2\frac{\alpha_2^2x_2^2+\alpha_1^2x_1^2+2\alpha_1\alpha_2x_1x_2}{(\alpha_1+\alpha_2)^2} - \frac{\alpha_2^2}{\hbar^2}\frac{(p_2-p_1)^2}{(\alpha_1+\alpha_2)^2} + 4\alpha_2^2\frac{i}{\hbar}\frac{(p_2-p_1)(\alpha_2x_2+\alpha_1x_1)}{(\alpha_1+\alpha_2)^2}$$

Imaginary terms:

$$\frac{4i}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_2^2x_2(p_1-p_2) + \alpha_2\alpha_1p_2(x_2-x_1)\right] + 4\alpha_2^2\frac{i}{\hbar}\frac{\left(p_2-p_1\right)(\alpha_2x_2+\alpha_1x_1)}{(\alpha_1+\alpha_2)^2} = \frac{4i\alpha_2^2}{\hbar(\alpha_1+\alpha_2)^2}\left[x_2\left(p_1-p_2\right)(\alpha_1+\alpha_2) + \frac{\alpha_1}{\alpha_2}p_2(x_2-x_1)(\alpha_1+\alpha_2) + \left(p_2-p_1\right)(\alpha_2x_2+\alpha_1x_1)\right]$$

$x_2(p_1-p_2)(\alpha_1+\alpha_2) + \frac{\alpha_1}{\alpha_2}p_2(x_2-x_1)(\alpha_1+\alpha_2) + (p_2-p_1)(\alpha_2x_2+\alpha_1x_1) =$ $(p_1-p_2)(x_2\alpha_1 + x_2\alpha_2 - \alpha_2x_2 - \alpha_1x_1) + \frac{\alpha_1}{\alpha_2}p_2(x_2-x_1)(\alpha_1+\alpha_2) = \frac{\alpha_2}{\alpha_2}\alpha_1(p_1x_2 - p_2x_2 - p_1x_1 + p_2x_1) + \frac{\alpha_1}{\alpha_2}p_2(\alpha_1x_2 - \alpha_1x_1 + \alpha_2x_2 - \alpha_2x_1) =.$

$$\frac{1}{\alpha_2}(\alpha_1\alpha_2p_1x_2 - \boldsymbol{\alpha_1\alpha_2p_2x_2} - \alpha_1\alpha_2p_1x_1 + \alpha_1\alpha_2p_2x_1) + \frac{1}{\alpha_2}(\alpha_1p_2\alpha_1x_2 - \alpha_1p_2\alpha_1x_1 + \boldsymbol{\alpha_1p_2\alpha_2x_2} - \alpha_1p_2\alpha_2x_1)$$

$$\frac{1}{\alpha_2}(\alpha_1\alpha_2p_1x_2 - \alpha_1\alpha_2p_1x_1) + \frac{1}{\alpha_2}(\alpha_1p_2\alpha_1x_2 - \alpha_1p_2\alpha_1x_1)$$

$$\frac{\alpha_1}{\alpha_2}(\alpha_2p_1x_2 - \alpha_2p_1x_1 + p_2\alpha_1x_2 - p_2\alpha_1x_1)$$

$$\frac{\alpha_1}{\alpha_2}(\alpha_2p_1(x_2-x_1) + p_2\alpha_1(x_2-x_1))$$

$$\frac{\alpha_1}{\alpha_2}(\alpha_2 p_1 + p_2\alpha_1)(x_2 - x_1)$$

So, the overall imaginary term will be:

$$\frac{4i\alpha_2^2}{\hbar(\alpha_1+\alpha_2)^2}\frac{\alpha_1}{\alpha_2}\left(\alpha_2 p_1 + p_2\alpha_1\right)(x_2 - x_1) = \frac{4\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}\frac{i}{\hbar}\left(\alpha_2 p_1 + p_2\alpha_1\right)(x_2 - x_1)$$

Now, onto the real terms:

$$\frac{1}{(\alpha_1+\alpha_2)}\left[-4\alpha_2^3x_2^2 - 8\alpha_2^2\alpha_1x_2x_1 + \frac{2}{\hbar^2}\left(\alpha_2p_2^2 - \alpha_2p_1p_2\right) + 4\alpha_2^2\alpha_1x_2^2 - \frac{\alpha_1p_2^2}{\hbar^2} - \frac{\alpha_2p_2^2}{\hbar^2}\right] + 4\alpha_2^2\frac{\alpha_2^2x_2^2 + \alpha_1^2x_1^2 + 2\alpha_1\alpha_2x_1x_2}{(\alpha_1+\alpha_2)^2} - \frac{\alpha_2^2}{\hbar^2}\frac{\left(p_2 - p_1\right)^2}{(\alpha_1+\alpha_2)^2}$$

Terms with $\frac{1}{\hbar^2}$

$$\frac{1}{(\alpha_1+\alpha_2)}\left[\frac{2}{\hbar^2}\left(\alpha_2p_2^2 - \alpha_2p_1p_2\right) - \frac{\alpha_1p_2^2}{\hbar^2} - \frac{\alpha_2p_2^2}{\hbar^2}\right] - \frac{\alpha_2^2}{\hbar^2}\frac{\left(p_2 - p_1\right)^2}{(\alpha_1+\alpha_2)^2}$$

Common prefactor:

$$\frac{1}{(\alpha_1+\alpha_2)^2\hbar^2}$$

The rest:

$$(2\alpha_2p_2^2 - 2\alpha_2p_1p_2 - \alpha_1p_2^2 - \alpha_2p_2^2)(\alpha_1+\alpha_2) - \alpha_2^2(p_2 - p_1)^2$$
$$(\alpha_2p_2^2 - 2\alpha_2p_1p_2 - \alpha_1p_2^2)(\alpha_1+\alpha_2) - \alpha_2^2(p_2^2 - 2p_1p_2 + p_1^2)$$

$$(\alpha_1\alpha_2p_2^2 - 2\alpha_1\alpha_2p_1p_2 - \alpha_1^2p_2^2 + \alpha_2^2p_2^2 - 2\alpha_2^2p_1p_2 - \alpha_1\alpha_2p_2^2) + (-\alpha_2^2p_2^2 + \alpha_2^2 2p_1p_2 - \alpha_2^2p_1^2)$$

$$(-2\alpha_1\alpha_2p_1p_2 - \alpha_1^2p_2^2) + (-\alpha_2^2p_1^2)$$

$$(-2\alpha_1\alpha_2p_1p_2 - \alpha_1^2p_2^2 - \alpha_2^2p_1^2) = -(2\alpha_1\alpha_2p_1p_2 + \alpha_1^2p_2^2 + \alpha_2^2p_1^2) = -(\alpha_1p_2 + \alpha_2p_1)^2$$

So, the whole term is:

$$\frac{-(\alpha_1 p_2+\alpha_2 p_1)^2}{(\alpha_1+\alpha_2)^2\hbar^2} = -\frac{1}{\hbar^2}\left(\frac{\alpha_1 p_2+\alpha_2 p_1}{\alpha_1+\alpha_2}\right)^2$$

Terms without $\frac{1}{\hbar^2}$

$$\frac{1}{(\alpha_1+\alpha_2)}\left[-4\alpha_2^3x_2^2-8\alpha_2^2\alpha_1x_2x_1+4\alpha_2^2\alpha_1x_2^2\right]+4\alpha_2^2\frac{\alpha_2^2x_2^2+\alpha_1^2x_1^2+2\alpha_1\alpha_2x_1x_2}{(\alpha_1+\alpha_2)^2}$$

Common prefactor:

$$\frac{4\alpha_2^2}{(\alpha_1+\alpha_2)^2}$$

The rest:

$$\begin{aligned}(-\alpha_2x_2^2-2\alpha_1x_2x_1+\alpha_1x_2^2)(\alpha_1+\alpha_2)+\alpha_2^2x_2^2+\alpha_1^2x_1^2+2\alpha_1\alpha_2x_1x_2\\ = -\alpha_2\alpha_1x_2^2-2\alpha_1^2x_2x_1+\alpha_1^2x_2^2-\alpha_2^2x_2^2-2\alpha_1\alpha_2x_2x_1+\alpha_1\alpha_2x_2^2+\alpha_2^2x_2^2\\ +\alpha_1^2x_1^2+2\alpha_1\alpha_2x_1x_2\end{aligned}$$

$$-2\alpha_1^2x_2x_1+\alpha_1^2x_2^2+\alpha_1^2x_1^2=\alpha_1^2(x_1-x_2)^2$$

So, the term without $\frac{1}{\hbar^2}$ is:

$$\frac{4\alpha_2^2\alpha_1^2}{(\alpha_1+\alpha_2)^2}(x_1-x_2)^2$$

We also have the terms:

$$\frac{2\alpha_2^2}{(\alpha_1+\alpha_2)}-2\alpha_2=\frac{2\alpha_2^2}{(\alpha_1+\alpha_2)}-\frac{2\alpha_2^2+2\alpha_2\alpha_1}{(\alpha_1+\alpha_2)}=-\frac{2\alpha_1\alpha_2}{(\alpha_1+\alpha_2)}$$

So, all together we get:

$$\begin{aligned}T_{12}=\langle G_1|\nabla^2|G_2\rangle\\ =\left[-\frac{2\alpha_1\alpha_2}{(\alpha_1+\alpha_2)}+\frac{4\alpha_2^2\alpha_1^2}{(\alpha_1+\alpha_2)^2}(x_1-x_2)^2-\frac{1}{\hbar^2}\left(\frac{\alpha_1p_2+\alpha_2p_1}{\alpha_1+\alpha_2}\right)^2\right.\\ \left.+\frac{i}{\hbar}\frac{4\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}(\alpha_2p_1+p_2\alpha_1)(x_2-x_1)\right]S_{12}\end{aligned}$$

For $\alpha_1=\alpha_2=\alpha$, we recover the special result:

$$\begin{aligned}T_{12}=\langle G_1|\nabla^2|G_2\rangle\\ =\left[-\alpha+\alpha^2(x_1-x_2)^2-\frac{1}{\hbar^2}\left(\frac{p_1+p_2}{2}\right)^2\right.\\ \left.+\frac{i}{\hbar}\alpha(p_1+p_2)(x_2-x_1)\right]S_{12}\end{aligned}$$

6. Summary

$$G(x; x_0, p_0, \alpha, \gamma) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \exp\left(-\alpha(x - x_0)^2 + \frac{ip_0}{\hbar}(x - x_0) + \frac{i\gamma}{\hbar}\right).$$

Overlaps:

$$S_{12} = \langle G_1|G_2\rangle = \left(\frac{4\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}\right)^{1/4} \exp(i\phi) \exp\left(\frac{-\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_2 - x_1)^2 - \frac{(p_2-p_1)^2}{4\hbar^2(\alpha_1+\alpha_2)}\right).$$

$$\phi = \frac{\gamma_2-\gamma_1}{\hbar} + \frac{(\alpha_2 p_1+\alpha_1 p_2)}{\hbar(\alpha_1+\alpha_2)}(x_1 - x_2\ ).$$

Transition dipole moments:

$$\mu_{12} = \langle G_1|x|G_2\rangle = \left[\frac{\alpha_2 x_2+ \alpha_1 x_1}{\alpha_1+\alpha_2} + \frac{i}{2\hbar}\frac{p_2-p_1}{\alpha_1+\alpha_2}\right] S_{12}.$$

Couplings:

$$d_{12} = \langle G_1|\nabla|G_2\rangle = \left[\frac{2\alpha_2\alpha_1}{\alpha_1+\alpha_2}(x_2 - x_1) + \frac{i}{\hbar}\frac{\alpha_1 p_2+\alpha_2 p_1}{\alpha_1+\alpha_2}\right] S_{12}.$$

Kinetic energy:

$$T_{12} = \langle G_1|\nabla^2|G_2\rangle = \left[-\frac{2\alpha_1\alpha_2}{(\alpha_1+\alpha_2)} + \frac{4\alpha_2^2\alpha_1^2}{(\alpha_1+\alpha_2)^2}(x_1 - x_2)^2 - \frac{1}{\hbar^2}\left(\frac{\alpha_1 p_2+\alpha_2 p_1}{\alpha_1+\alpha_2}\right)^2 + \frac{i}{\hbar}\frac{4\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}(\alpha_2 p_1 + p_2\alpha_1)(x_2 - x_1)\right] S_{12}.$$