Some integrals with Gaussian wavepackets

1. Definition
The normalized Gaussian wavepacket is defined as:

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

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:

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

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

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

Thus,

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

Pre-factor:

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

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

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

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

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

The integral is:

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

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

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

Simplify:

$$\frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1+\alpha_2}\frac{(p_2-p_1)}{\hbar} - \frac{(p_2 x_2 - p_1 x_1)}{\hbar} = \frac{1}{\hbar(\alpha_1+\alpha_2)}\left[(\alpha_1 x_1 + \alpha_2 x_2)(p_2-p_1) - (\alpha_1+\alpha_2)(p_2 x_2 - p_1 x_1)\right] = \frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1 x_1 p_2 + \alpha_2 x_2 p_2 - \alpha_1 x_1 p_1 - \alpha_2 x_2 p_1 - (\alpha_1 p_2 x_2 - \alpha_1 p_1 x_1 + \alpha_2 p_2 x_2 - \alpha_2 p_1 x_1)\right] = \frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1 x_1 p_2 + \alpha_2 x_2 p_2 - \alpha_1 x_1 p_1 - \alpha_2 x_2 p_1 - \alpha_1 p_2 x_2 + \alpha_1 p_1 x_1 - \alpha_2 p_2 x_2 + \alpha_2 p_1 x_1\right] = \frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1 x_1 p_2 - \alpha_2 x_2 p_1 - \alpha_1 p_2 x_2 + \alpha_2 p_1 x_1\right] = \frac{1}{\hbar(\alpha_1+\alpha_2)}\left[\alpha_1 p_2(x_1 - x_2) + \alpha_2 p_1(x_1 - x_2)\right] = \frac{(\alpha_2 p_1 + \alpha_1 p_2)}{\hbar(\alpha_1+\alpha_2)}(x_1 - x_2).$$

So, the phase is:

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

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:

$$d_{12} = \langle G_1|\nabla|G_2 \rangle = -2\alpha_2\langle G_1|x|G_2 \rangle + \left[2\alpha_2 x_2 + \frac{ip_2}{\hbar} \right]\langle G_1|G_2 \rangle =$$

$$\left[-2\alpha_2 \frac{\left(\alpha_2 x_2 + \alpha_1 x_1 + \frac{i(p_2 - p_1)}{2\hbar} \right)}{(\alpha_1 + \alpha_2)} + 2\alpha_2 x_2 + \frac{ip_2}{\hbar} \right] S_{12}.$$

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

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

$$\frac{2\alpha_2\alpha_1(x_2 - x_1) + \frac{i}{\hbar}[\alpha_1 p_2 + \alpha_2 p_1]}{(\alpha_1 + \alpha_2)}.$$

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:

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

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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:

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

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

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

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

That is:

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

Simplify:

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

$$\left. \frac{4i\alpha_2 p_2}{\hbar} \right] \left[\frac{\alpha_2 x_2 + \alpha_1 x_1}{\alpha_1 + \alpha_2} + \frac{i}{2\hbar} \frac{p_2 - p_1}{\alpha_1 + \alpha_2} \right] + \left[4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} - 2\alpha_2 \right] \right\} S_{12}.$$

$$\left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar} \right] \left[\frac{\alpha_2 x_2 + \alpha_1 x_1}{\alpha_1 + \alpha_2} + \frac{i}{2\hbar} \frac{p_2 - p_1}{\alpha_1 + \alpha_2} \right]$$

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

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

$$- \left[8\alpha_2^2 x_2 + \frac{4i\alpha_2 p_2}{\hbar} \right] \left[\frac{\alpha_2 x_2 + \alpha_1 x_1}{\alpha_1 + \alpha_2} + \frac{i}{2\hbar} \frac{p_2 - p_1}{\alpha_1 + \alpha_2} \right] + 4\alpha_2^2 x_2^2 + \frac{4i\alpha_2 p_2 x_2}{\hbar} - \frac{p_2^2}{\hbar^2} =$$

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

$$\left. - \frac{\alpha_1 p_2^2}{\hbar^2} - \frac{\alpha_2 p_2^2}{\hbar^2} \right]$$

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

$$\left. + \alpha_2 \alpha_1 p_2 x_2 + \alpha_2^2 p_2 x_2 \right]$$

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

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

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

Imaginary terms:

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

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

$$\frac{1}{\alpha_2} (\alpha_1 \alpha_2 p_1 x_2 - \boldsymbol{\alpha_1 \alpha_2 p_2 x_2} - \alpha_1 \alpha_2 p_1 x_1 + \textcolor{blue}{\alpha_1 \alpha_2 p_2 x_1})$$
$$+ \frac{1}{\alpha_2} (\alpha_1 p_2 \alpha_1 x_2 - \alpha_1 p_2 \alpha_1 x_1 + \boldsymbol{\alpha_1 p_2 \alpha_2 x_2} - \textcolor{blue}{\alpha_1 p_2 \alpha_2 x_1})$$
$$\frac{1}{\alpha_2} (\alpha_1 \alpha_2 p_1 x_2 - \alpha_1 \alpha_2 p_1 x_1) + \frac{1}{\alpha_2} (\alpha_1 p_2 \alpha_1 x_2 - \alpha_1 p_2 \alpha_1 x_1)$$
$$\frac{\alpha_1}{\alpha_2} (\alpha_2 p_1 x_2 - \alpha_2 p_1 x_1 + p_2 \alpha_1 x_2 - p_2 \alpha_1 x_1)$$
$$\frac{\alpha_1}{\alpha_2} (\alpha_2 p_1 (x_2 - x_1) + p_2 \alpha_1 (x_2 - x_1))$$

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

So, the overall imaginary term will be:

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

Now, onto the real terms:

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

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

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

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

Common prefactor:

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

The rest:
$$(2\alpha_2 p_2^2 - 2\alpha_2 p_1 p_2 - \alpha_1 p_2^2 - \alpha_2 p_2^2)(\alpha_1 + \alpha_2) - \alpha_2^2(p_2 - p_1)^2$$
$$(\alpha_2 p_2^2 - 2\alpha_2 p_1 p_2 - \alpha_1 p_2^2)(\alpha_1 + \alpha_2) - \alpha_2^2(p_2^2 - 2p_1 p_2 + p_1^2)$$

$$(\textcolor{green}{\alpha_1\alpha_2 p_2^2} - 2\alpha_1\alpha_2 p_1 p_2 - \alpha_1^2 p_2^2 + \textcolor{red}{\alpha_2^2 p_2^2} - 2\alpha_2^2 p_1 p_2 - \textcolor{green}{\alpha_1\alpha_2 p_2^2})$$
$$+ (\textcolor{red}{-\alpha_2^2 p_2^2} + \textcolor{blue}{\alpha_2^2 2p_1 p_2} - \alpha_2^2 p_1^2)$$

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

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

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

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

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

The rest:

$$(-\alpha_2 x_2^2 - 2\alpha_1 x_2 x_1 + \alpha_1 x_2^2)(\alpha_1 + \alpha_2) + \alpha_2^2 x_2^2 + \alpha_1^2 x_1^2 + 2\alpha_1 \alpha_2 x_1 x_2$$
$$= -\alpha_2 \alpha_1 x_2^2 - 2\alpha_1^2 x_2 x_1 + \alpha_1^2 x_2^2 - \alpha_2^2 x_2^2 - 2\alpha_1 \alpha_2 x_2 x_1 + \alpha_1 \alpha_2 x_2^2 + \alpha_2^2 x_2^2$$
$$+ \alpha_1^2 x_1^2 + 2\alpha_1 \alpha_2 x_1 x_2$$

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

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:

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

For $\alpha_1 = \alpha_2 = \alpha$, we recover the special result:
$$T_{12} = \langle G_1 | \nabla^2 | G_2 \rangle$$
$$= \left[-\alpha + \alpha^2 (x_1 - x_2)^2 - \frac{1}{\hbar^2}\left(\frac{p_1 + p_2}{2}\right)^2\right.$$
$$\left. + \frac{i}{\hbar}\alpha(p_1 + p_2)(x_2 - x_1)\right]S_{12}$$

6. Gaussian product decomposition

$$G_1(x; x_1, p_1, \alpha_1, \gamma_1) = \left(\frac{2\alpha_1}{\pi}\right)^{1/4} \exp\left(-\alpha_1(x - x_1)^2 + \frac{ip_1}{\hbar}(x - x_1) + \frac{i\gamma_1}{\hbar}\right).$$

$$G_2(x; x_2, p_2, \alpha_2, \gamma_2) = \left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(-\alpha_2(x - x_2)^2 + \frac{ip_2}{\hbar}(x - x_2) + \frac{i\gamma_2}{\hbar}\right).$$

$$G_2(x; x_1, p_1, \alpha_1, \gamma_1)G_2(x; x_2, p_2, \alpha_2, \gamma_2)$$
$$= \left(\frac{2\alpha_1}{\pi}\right)^{1/4} \exp\left(-\alpha_1(x - x_1)^2 + \frac{ip_1}{\hbar}(x - x_1)\right.$$
$$\left. + \frac{i\gamma_1}{\hbar}\right)\left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(-\alpha_2(x - x_2)^2 + \frac{ip_2}{\hbar}(x - x_2) + \frac{i\gamma_2}{\hbar}\right)$$

$$\alpha_1(x - x_1)^2 + \alpha_2(x - x_2)^2 = (\alpha_1 + \alpha_2)x^2 - 2x(\alpha_1 x_1 + \alpha_2 x_2) + (\alpha_1 x_1^2 + \alpha_2 x_2^2)$$
$$= (\alpha_1 + \alpha_2)\left[x^2 - \frac{2(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}x + \frac{(\alpha_1 x_1^2 + \alpha_2 x_2^2)}{\alpha_1 + \alpha_2}\right] =$$

$$(\alpha_1 + \alpha_2)\left[x^2 - \frac{2(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}x + \left(\frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right)^2 - \left(\frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right)^2\right.$$
$$\left. + \frac{(\alpha_1 x_1^2 + \alpha_2 x_2^2)}{\alpha_1 + \alpha_2}\right]$$

$$(\alpha_1 + \alpha_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right]^2 + \frac{(\alpha_1 x_1^2 + \alpha_2 x_2^2)(\alpha_1 + \alpha_2)}{\alpha_1 + \alpha_2} - \frac{(\alpha_1 x_1 + \alpha_2 x_2)^2}{\alpha_1 + \alpha_2}$$

$$(\alpha_1 x_1^2 + \alpha_2 x_2^2)(\alpha_1 + \alpha_2) - (\alpha_1 x_1 + \alpha_2 x_2)^2$$
$$= \alpha_1^2 x_1^2 + \alpha_2\alpha_1 x_2^2 + \alpha_1\alpha_2 x_1^2 + \alpha_2^2 x_2^2 - (\alpha_1^2 x_1^2 + 2\alpha_1\alpha_2 x_1 x_2 + \alpha_2^2 x_2^2)$$
$$= \alpha_2\alpha_1 x_2^2 - 2\alpha_1\alpha_2 x_1 x_2 + \alpha_1\alpha_2 x_1^2 = \alpha_1\alpha_2(x_1 - x_2)^2$$

So:

$$\alpha_1(x - x_1)^2 + \alpha_2(x - x_2)^2 = (\alpha_1 + \alpha_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right]^2 + \frac{\alpha_1\alpha_2}{\alpha_1 + \alpha_2}(x_1 - x_2)^2$$

$$p_1(x - x_1) + p_2(x - x_2) = (p_1 + p_2)x - (p_1 x_1 + p_2 x_2)$$
$$= (p_1 + p_2)\left[x - \frac{(p_1 x_1 + p_2 x_2)}{p_1 + p_2}\right]$$
$$= (p_1 + p_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2} + \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2} - \frac{(p_1 x_1 + p_2 x_2)}{p_1 + p_2}\right] =$$

$$(p_1 + p_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right] + \frac{(\alpha_1 x_1 + \alpha_2 x_2)(p_1 + p_2)}{\alpha_1 + \alpha_2} - (p_1 x_1 + p_2 x_2)$$

$$(\alpha_1 x_1 + \alpha_2 x_2)(p_1 + p_2) - (\alpha_1 + \alpha_2)(p_1 x_1 + p_2 x_2)$$
$$= \textcolor{red}{\alpha_1 x_1 p_1} + \alpha_2 x_2 p_1 + \alpha_1 x_1 p_2 + \textcolor{blue}{\alpha_2 x_2 p_2}$$
$$- (\textcolor{red}{\alpha_1 p_1 x_1} + \alpha_1 p_2 x_2 + \alpha_2 p_1 x_1 + \textcolor{blue}{\alpha_2 p_2 x_2}) =$$
$$= \alpha_2 x_2 p_1 + \alpha_1 x_1 p_2 - (\alpha_1 p_2 x_2 + \alpha_2 p_1 x_1) = \alpha_1 p_2 (x_1 - x_2) + \alpha_2 p_1 (x_2 - x_1)$$
$$= (x_2 - x_1)(\alpha_2 p_1 - \alpha_1 p_2)$$

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

$$G_1(x; x_1, p_1, \alpha_1, \gamma_1) G_2(x; x_2, p_2, \alpha_2, \gamma_2)$$
$$= \left(\frac{2\alpha_1}{\pi}\right)^{1/4} \left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(-(\alpha_1 + \alpha_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right]^2\right.$$
$$- \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2}(x_1 - x_2)^2 + \frac{i}{\hbar}(p_1 + p_2)\left[x - \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}\right]$$
$$+ \frac{i}{\hbar}\frac{(x_2 - x_1)(\alpha_2 p_1 - \alpha_1 p_2)}{\alpha_1 + \alpha_2} + \frac{i}{\hbar}(\gamma_1 + \gamma_2)\Bigg)$$

$$= \left(\frac{2\alpha_1}{\pi}\right)^{1/4}\left(\frac{2\alpha_2}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_1 - x_2)^2\right)\exp\left(-(\alpha_1 + \alpha_2)[x - X]^2 +\right.$$
$$\frac{i}{\hbar}(p_1 + p_2)[x - X] + \frac{i}{\hbar}\gamma\Bigg) =$$
$$= \left(\frac{2\alpha_1}{\pi}\right)^{1/4}\left(\frac{2\alpha_2}{\pi}\right)^{1/4}\left(\frac{\pi}{2\alpha}\right)^{1/4}\exp\left(-\frac{\alpha_1\alpha_2}{\alpha_1+\alpha_2}(x_1-x_2)^2\right)\left(\frac{2\alpha}{\pi}\right)^{1/4}\exp\left(-\alpha[x-X]^2 +\right.$$
$$\frac{i}{\hbar}(p_1 + p_2)[x - X] + \frac{i}{\hbar}\gamma\Bigg)$$

$$= \left(\frac{2\alpha_1\alpha_2}{\pi\alpha}\right)^{1/4}\exp\left(-\frac{\alpha_1\alpha_2}{\alpha}(x_1 - x_2)^2\right)G(x; X, P, \alpha, \gamma)$$

$$\alpha = \alpha_1 + \alpha_2$$
$$X = \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1 + \alpha_2}$$
$$P = p_1 + p_2$$
$$\gamma = (\gamma_1 + \gamma_2) + \frac{(x_2 - x_1)(\alpha_2 p_1 - \alpha_1 p_2)}{\alpha_1 + \alpha_2}$$

7. 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:

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

Gaussian product:

$$G_1(x; x_1, p_1, \alpha_1, \gamma_1) G_2(x; x_2, p_2, \alpha_2, \gamma_2) =$$
$$= \left(\frac{2\alpha_1\alpha_2}{\pi\alpha}\right)^{1/4} \exp\left(-\frac{\alpha_1\alpha_2}{\alpha}(x_1 - x_2)^2\right) G\left(x; \frac{(\alpha_1 x_1 + \alpha_2 x_2)}{\alpha_1+\alpha_2}, p_1 + p_2, \alpha_1 + \alpha_2, (\gamma_1 + \gamma_2) + \right.$$
$$\left. \frac{(x_2-x_1)(\alpha_2 p_1 - \alpha_1 p_2)}{\alpha_1+\alpha_2}\right).$$