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Some integrals with Gaussian wavepackets

1. Definition

According to Heller's notation, the normalized Gaussian wavepacket is defined as:

$$G = \left(\frac{2a}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{a+ib}{\hbar}(x-x_0)^2 + \frac{ip_0}{\hbar}(x-x_0) + \frac{i}{\hbar}\varphi \right), \qquad (1)$$

$$\alpha = 2(a+ib)$$

Here, a is the width parameter, b is the position-momentum correlation, x_0 is the center of the wavepacket, p_0 is the momentum of the wavepacket, φ is the phase.

2. Derivatives

Now, assume all the parameters a, b, x_0, p_0, and φ depend on time explicitly. Compute the time derivative of the Gaussian:

$$\begin{aligned}
\frac{\partial}{\partial t} G &= \left(\frac{2a}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{\alpha}{2\hbar}(x-x_0)^2 + \frac{ip_0}{\hbar}(x-x_0) + \frac{i}{\hbar}\varphi \right) = \\
&= \frac{2\dot{a}}{\pi\hbar}\frac{1}{4}\left(\frac{2a}{\pi\hbar}\right)^{-3/4} \exp\left(-\frac{\alpha}{2\hbar}(x-x_0)^2 + \frac{ip_0}{\hbar}(x-x_0) + \frac{i}{\hbar}\varphi \right) + \\
&+ \left\{ -\frac{\dot{\alpha}}{2\hbar}(x-x_0)^2 + \frac{\alpha}{\hbar}(x-x_0)\dot{x}_0 + \frac{i\dot{p}_0}{\hbar}(x-x_0) - \frac{ip_0}{\hbar}\dot{x}_0 + \frac{i}{\hbar}\dot{\varphi} \right\} G = \\
&= \frac{2\dot{a}}{\pi\hbar}\frac{1}{4}\left(\frac{2a}{\pi\hbar}\right)^{-1} G + \left\{ -\frac{\dot{\alpha}}{2\hbar}(x-x_0)^2 + \frac{\alpha}{\hbar}(x-x_0)\dot{x}_0 + \frac{i\dot{p}_0}{\hbar}(x-x_0) - \frac{ip_0}{\hbar}\dot{x}_0 + \frac{i}{\hbar}\dot{\varphi} \right\} G = \\
&= \left\{ \frac{\dot{a}}{4a} - \frac{\dot{\alpha}}{2\hbar}(x-x_0)^2 + \frac{\alpha}{\hbar}(x-x_0)\dot{x}_0 + \frac{i\dot{p}_0}{\hbar}(x-x_0) - \frac{ip_0}{\hbar}\dot{x}_0 + \frac{i}{\hbar}\dot{\varphi} \right\} G
\end{aligned} \qquad (2)$$

$$\nabla G = \left(-\frac{\alpha}{\hbar}(x-x_0) + \frac{ip_0}{\hbar} \right) G, \qquad (3)$$

$$\nabla^2 G = \left\{ \left(-\frac{\alpha}{\hbar}(x-x_0) + \frac{ip_0}{\hbar} \right)^2 - \frac{\alpha}{\hbar} \right\} G, \qquad (4)$$

3. Time-dependent Schrodinger equation

$$i\hbar\frac{\partial G}{\partial t} = \left(-\frac{\hbar^2}{2M}\nabla^2 + V(x) \right) G \qquad (5)$$

Substitute derivatives and simplify

$$i\hbar\left\{\frac{\dot{a}}{4a}-\frac{\dot{\alpha}}{2\hbar}(x-x_0)^2+\frac{\alpha}{\hbar}(x-x_0)\dot{x}_0+\frac{i\dot{p}_0}{\hbar}(x-x_0)-\frac{ip_0}{\hbar}\dot{x}_0+\frac{i}{\hbar}\dot{\varphi}\right\}G=$$
$$=-\frac{\hbar^2}{2M}\left\{\left(-\frac{\alpha}{\hbar}(x-x_0)+\frac{ip_0}{\hbar}\right)^2-\frac{\alpha}{\hbar}\right\}G+V(x)G \quad (6a)$$

or

$$i\hbar\left\{\frac{\dot{a}}{4a}-\frac{\dot{\alpha}}{2\hbar}(x-x_0)^2+\frac{\alpha}{\hbar}(x-x_0)\dot{x}_0+\frac{i\dot{p}_0}{\hbar}(x-x_0)-\frac{ip_0}{\hbar}\dot{x}_0+\frac{i}{\hbar}\dot{\varphi}\right\}=$$
$$=-\frac{\hbar^2}{2M}\left\{\left(-\frac{\alpha}{\hbar}(x-x_0)+\frac{ip_0}{\hbar}\right)^2-\frac{\alpha}{\hbar}\right\}+V(x) \quad (6b)$$

This is exact propagation!!!

Simplify:

$$\left\{i\hbar\frac{\dot{a}}{4a}-\frac{i\hbar\dot{a}-\hbar\dot{b}}{\hbar}(x-x_0)^2+2(ia-b)(x-x_0)\dot{x}_0-\dot{p}_0(x-x_0)+p_0\dot{x}_0-\dot{\varphi}\right\}=$$
$$=-\frac{\hbar^2}{2M}\left\{\left(4\frac{a^2-b^2+2iab}{\hbar^2}(x-x_0)^2-\frac{p_0{}^2}{\hbar^2}-4\frac{(ia-b)}{\hbar}(x-x_0)\frac{p_0}{\hbar}\right)-\frac{\alpha}{\hbar}\right\}+V(x)= \quad (7)$$
$$=\frac{p_0{}^2}{2M}+\frac{2(ia-b)}{M}(x-x_0)p_0-2\frac{a^2-b^2+2iab}{M}(x-x_0)^2+\frac{a+ib}{M}\hbar+V(x)$$

Separate real and imaginary parts:

Real:

$$\dot{b}(x-x_0)^2-2b(x-x_0)\dot{x}_0-\dot{p}_0(x-x_0)+p_0\dot{x}_0-\dot{\varphi}=$$
$$=\frac{p_0{}^2}{2M}-2b\frac{p_0}{M}(x-x_0)-2\frac{a^2-b^2}{M}(x-x_0)^2+\frac{a}{M}\hbar+V(x) \quad (8a)$$

Imaginary:

$$\left\{\hbar\frac{\dot{a}}{4a}-\dot{a}(x-x_0)^2+2a(x-x_0)\dot{x}_0\right\}=\frac{2a}{M}(x-x_0)p_0-4\frac{ab}{M}(x-x_0)^2+\frac{b}{M}\hbar \quad (8b)$$

From Eq. 8b, comparing the powers of $(x-x_0)$, we get:

$$\dot{x}_0=\frac{p_0}{M} \quad (9a)$$

$$\dot{a}=\frac{4ab}{M} \quad (9b)$$

Eq. 8a then simplifies:

$$\dot{b}(x-x_0)^2-\dot{p}_0(x-x_0)-\dot{\varphi}=-\frac{p_0{}^2}{2M}-2\frac{a^2-b^2}{M}(x-x_0)^2+\frac{a}{M}\hbar+V(x) \quad (9c)$$

Lets use the 2-nd order expansion of $V(x)$:

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 \tag{10}$$

Then

$$\begin{aligned} &\dot{b}(x - x_0)^2 - \dot{p}_0(x - x_0) - \dot{\varphi} = -\frac{p_0^{\;2}}{2M} - 2\frac{a^2 - b^2}{M}(x - x_0)^2 + \frac{a}{M}\hbar + \\ &+ V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 \end{aligned} \tag{11}$$

Comparing the same powers of $(x - x_0)$ yields:

$$\dot{b} = -2\frac{a^2 - b^2}{M} + \frac{1}{2}V''(x_0), \tag{12a}$$

$$-\dot{p}_0 = V'(x_0), \tag{12b}$$

$$-\dot{\varphi} = -\frac{p_0^{\;2}}{2M} + \frac{a}{M}\hbar + V(x_0). \tag{12c}$$

4. Equations of motion

$$\dot{p}_0 = -V'(x_0), \tag{13a}$$

$$\dot{x}_0 = \frac{p_0}{M}, \tag{13b}$$

$$\dot{\varphi} = \frac{p_0^{\;2}}{2M} - V(x_0) - \frac{a}{2M}\hbar = L(x_0, p_0) - \frac{a}{2M}\hbar, \tag{13c}$$

$$\dot{a} = \frac{4ab}{M}, \tag{13d}$$

$$\dot{b} = \frac{1}{2}V''(x_0) - 2\frac{a^2 - b^2}{M}. \tag{13e}$$