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Quantum dynamics of semiclassical Gaussian wavepackets

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

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

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

(1)

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:

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

$$= \frac{2\dot{a}}{\pi\hbar}\frac{1}{4}\left(\frac{2a}{\pi\hbar}\right)^{-3/4}\exp\left(-\frac{\alpha}{2\hbar}(x-x_0)^2 + \frac{ip_0}{\hbar}(x-x_0) + \frac{i}{\hbar}\varphi\right) +$$

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

(2)

$$= \frac{2\dot{a}}{\pi\hbar}\frac{1}{4}\left(\frac{2a}{\pi\hbar}\right)^{-1}G + \left\{-\frac{\dot{\alpha}}{2\hbar}(x-x_0)^2 + \frac{\alpha}{\hbar}(x-x_0)\dot{x}_0 + \frac{i\dot{p}_0}{\hbar}(x-x_0) - \frac{ip_0}{\hbar}\dot{x}_0 + \frac{i}{\hbar}\dot{\varphi}\right\}G =$$

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

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

(3)

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

(4)

3. Time-dependent Schrodinger equation

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

(5)

Substitute derivatives and simplify

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

$$=-\frac{\hbar^2}{2M}\left\{\left(-\frac{\alpha}{\hbar}(x-x_0)+\frac{ip_0}{\hbar}\right)^2-\frac{\alpha}{\hbar}\right\}G+V(x)G$$ (6a)

or

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

$$=-\frac{\hbar^2}{2M}\left\{\left(-\frac{\alpha}{\hbar}(x-x_0)+\frac{ip_0}{\hbar}\right)^2-\frac{\alpha}{\hbar}\right\}+V(x)$$ (6b)

This is exact propagation!!!

Simplify:

$$\left\{i\hbar\frac{\dot{a}}{4a}-\frac{i\hbar\dot{a}-\hbar\dot{b}}{\hbar}(x-x_0)^2+2(ia-b)(x-x_0)\dot{x}_0-\dot{p}_0(x-x_0)+p_0\dot{x}_0-\dot{\varphi}\right\}=$$

$$=-\frac{\hbar^2}{2M}\left\{\left(4\frac{a^2-b^2+2iab}{\hbar^2}(x-x_0)^2-\frac{p_0^2}{\hbar^2}-4\frac{(ia-b)}{\hbar}(x-x_0)\frac{p_0}{\hbar}\right)-\frac{\alpha}{\hbar}\right\}+V(x)=$$ (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:

$$\dot{b}(x-x_0)^2-2b(x-x_0)\dot{x}_0-\dot{p}_0(x-x_0)+p_0\dot{x}_0-\dot{\varphi}=$$

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

Imaginary:

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

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

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

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

Eq. 8a then simplifies:

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

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

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

Then

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

$$+ V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 \tag{11}$$

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

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

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

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

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

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