We have developed numerical and analytics methods

Numerical Simulation of Large-Scale Nonlinear Open Quantum Mechanics

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Phys. Rev. Research **6**, 013262 (2024)

Wigner Analysis of Particle Dynamics in Wide Nonharmonic Potentials

Andreu Riera-Campeny[1,2], Marc Roda-Llordes[1,2], Piotr T. Grochowski[1,2,3], and
Oriol Romero-Isart[1,2]

Quantum **8**, 1393 (2024)

The Wigner function has all the information about the state

Definition

$$W(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy e^{-ipy/\hbar}\langle x + y/2 | \hat{\rho} | x - y/2\rangle$$

$$\hat{x}|x\rangle = x|x\rangle$$

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It's a real function, can be plotted $$W(x,p) = W^*(x,p)$$

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Some properties

$$\int_{-\infty}^{\infty} dxdpW(x,p) = 1$$

$$\int_{-\infty}^{\infty} dpW(x,p) = P(x) = \langle x\,|\,\hat{\rho}\,|\,x\rangle$$

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Can be negative and is bounded

$$-\frac{1}{\pi\hbar} \le W(x,p) \le \frac{1}{\pi\hbar}$$

Gaussian states have a positive W function

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They only depend on 5 real numbers

$$\langle \hat{x} \rangle \qquad v_x \equiv \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$$

$$\langle \hat{p} \rangle \qquad v_p \equiv \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

$$c \equiv \langle \hat{x}\hat{p} + \hat{p}\hat{x} \rangle / 2 - \langle \hat{x} \rangle \langle \hat{p} \rangle$$

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Gaussian Wigner function

$$W(x,p) = \frac{1}{2\pi\sqrt{\det s}} \exp\left[-\frac{1}{2}\mathbf{R}^T s^{-1} \mathbf{R}\right]$$

$$\mathbf{R} \equiv \begin{pmatrix} x - \langle \hat{x} \rangle \\ p - \langle \hat{p} \rangle \end{pmatrix} \qquad \mathbf{s} \equiv \begin{pmatrix} v_x & c \\ c & v_p \end{pmatrix}$$

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Coherent, thermal, squeezed states are Gaussian

Dynamics of a particle in a potential in the presence of noise

Equation of motion for open quantum dynamics of a particle in a potential

$$\partial_t \hat{\rho}(t) = -\frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m} + U(\hat{x}), \hat{\rho}(t)\right] - \frac{\Gamma}{2x_\Omega^2}[\hat{x}, [\hat{x}, \hat{\rho}(t)]]$$

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Equation of motion for the Wigner function (PDE)

$$\frac{\partial W(x,p,t)}{\partial t} = \left(\mathscr{L}_c + \mathscr{L}_q + \mathscr{L}_d\right) W(x,p,t)$$

Dynamics of a particle in a potential in the presence of noise

Eq of motion of the W function

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Conservative classical dynamics

$$\mathscr{L}_c = -\frac{p}{m}\frac{\partial}{\partial x} + \frac{\partial U(x)}{\partial x}\frac{\partial}{\partial p}$$

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Genuine quantum dynamics
(requires nonquadratic potentials!)

$$\mathscr{L}_q = \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n+1)!}\frac{\hbar^{2n}}{4^n}\frac{\partial^{2n+1}U(x)}{\partial x^{2n+1}}\frac{\partial^{2n+1}}{\partial p^{2n+1}}$$

$$= -\frac{\hbar^2}{24}\frac{\partial^3 U(x)}{\partial x^3}\frac{\partial^3}{\partial p^3} + \ldots$$

Dynamics of a particle in a potential in the presence of noise

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$$\frac{\partial W(x,p,t)}{\partial t} = \left(\mathcal{L}_c + \mathcal{L}_q + \mathcal{L}_d\right) W(x,p,t)$$

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Dissipative dynamics

$$\mathcal{L}_d = \frac{\hbar^2 \Gamma}{2x_\Omega^2}\frac{\partial^2}{\partial p^2}$$

Dynamics in the Liouville frame

W function in the Liouville frame $\tilde{W}(x,p,t) \equiv e^{-\mathcal{L}_c t} W(x,p,t)$

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$$\tilde{W}(x,p,t) = W(x_c(x,p,t), p_c(x,p,t), t)$$

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Classical solutions for a point particle

$$\frac{\partial x_c(x, p, t)}{\partial t} = \frac{p_c(x, p, t)}{m} \qquad x_c(x, p, 0) = x$$

$$\frac{\partial p_c(x, p, t)}{\partial t} = -\frac{\partial U(x)}{\partial x}\bigg|_{x = x_c(x, p, t)} \qquad p_c(x, p, 0) = p$$

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Note that if $\mathscr{L}_q = \mathscr{L}_n = 0$ then
$$\frac{\partial \tilde{W}(x,p,t)}{\partial t} = 0$$

Closed dynamics for quadratic Hamiltonians are easy!

Simply $$W(x,p,t) = W(x_c(x,p,-t), p_c(x,p,-t), 0)$$

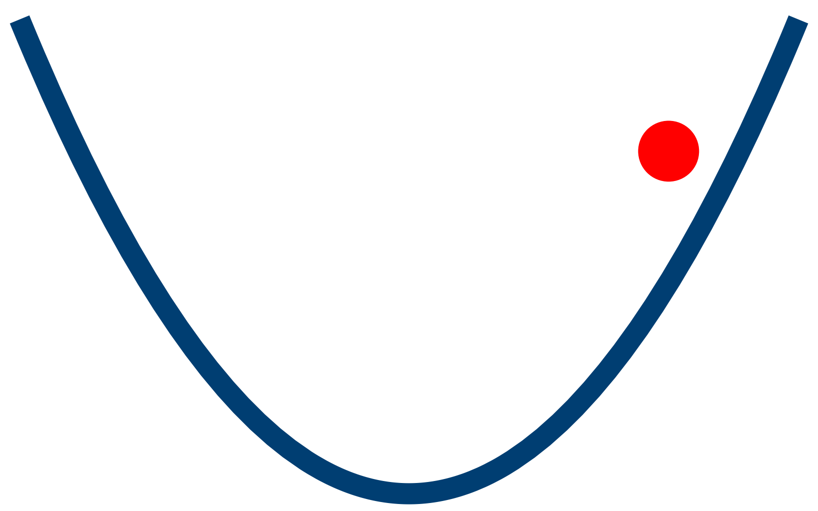
Example of free dynamics $$W(x,p,t) = W(x - pt/m, p, 0)$$

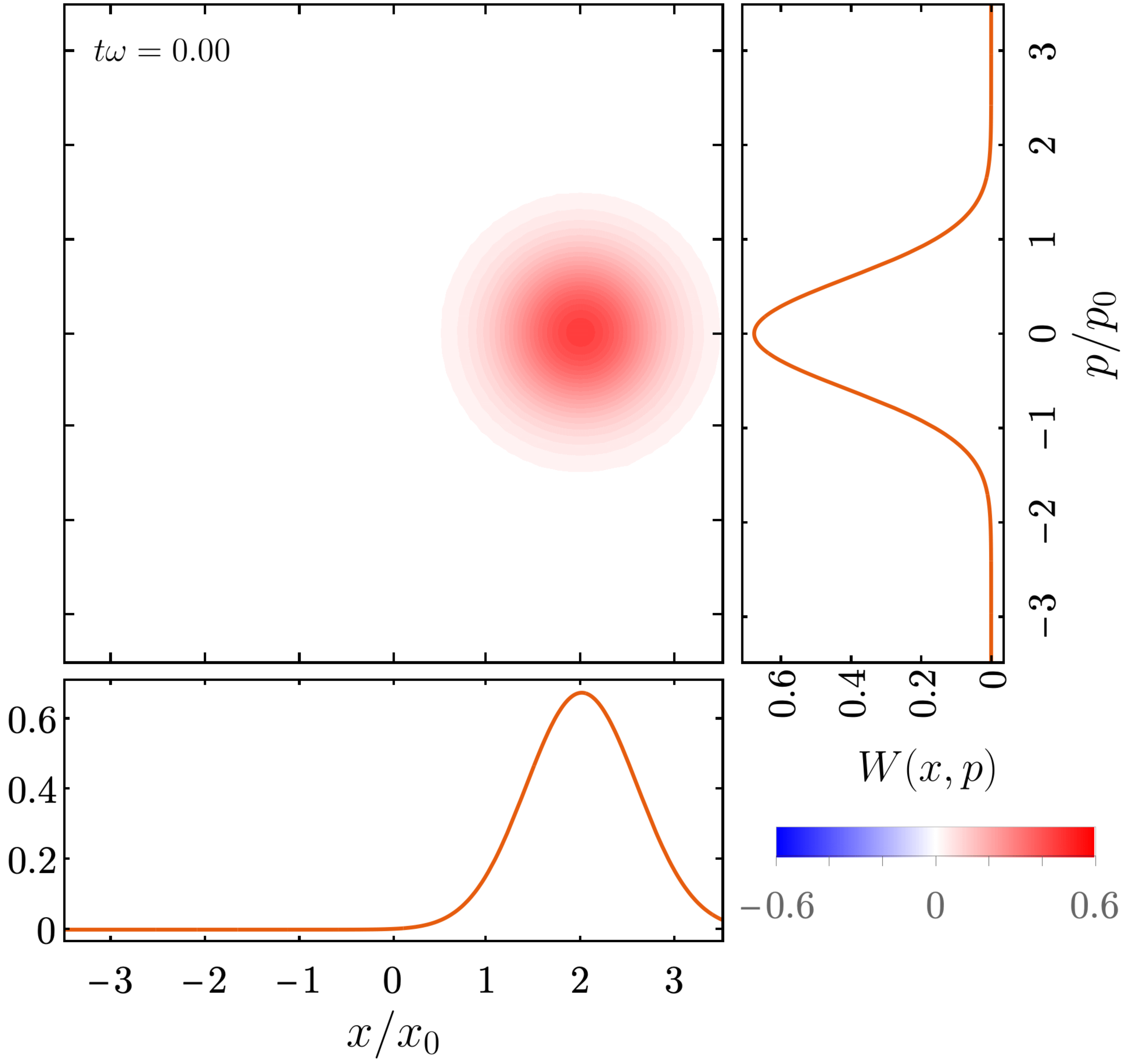
Example: Harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{4}\left(\hat{\tilde{p}}^2 + \hat{\tilde{x}}^2\right)$$

- Displaced ground state

$$|\psi_0\rangle = \hat{D}(2)\,|0\rangle$$



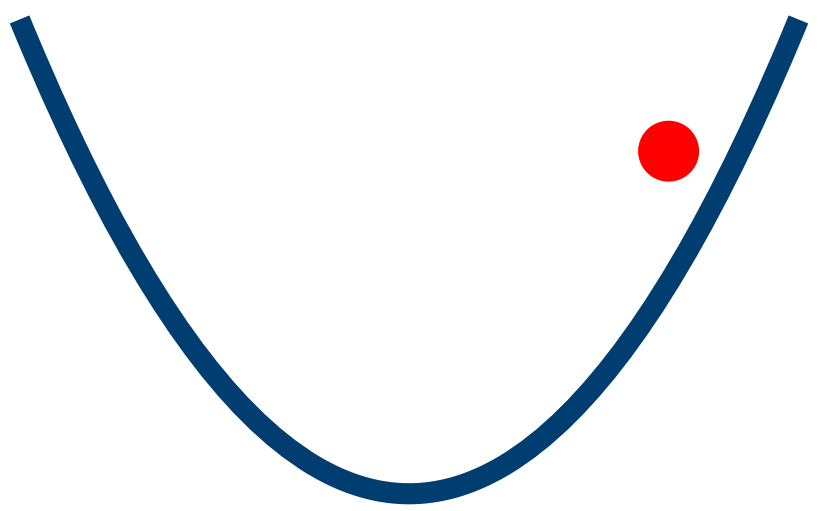


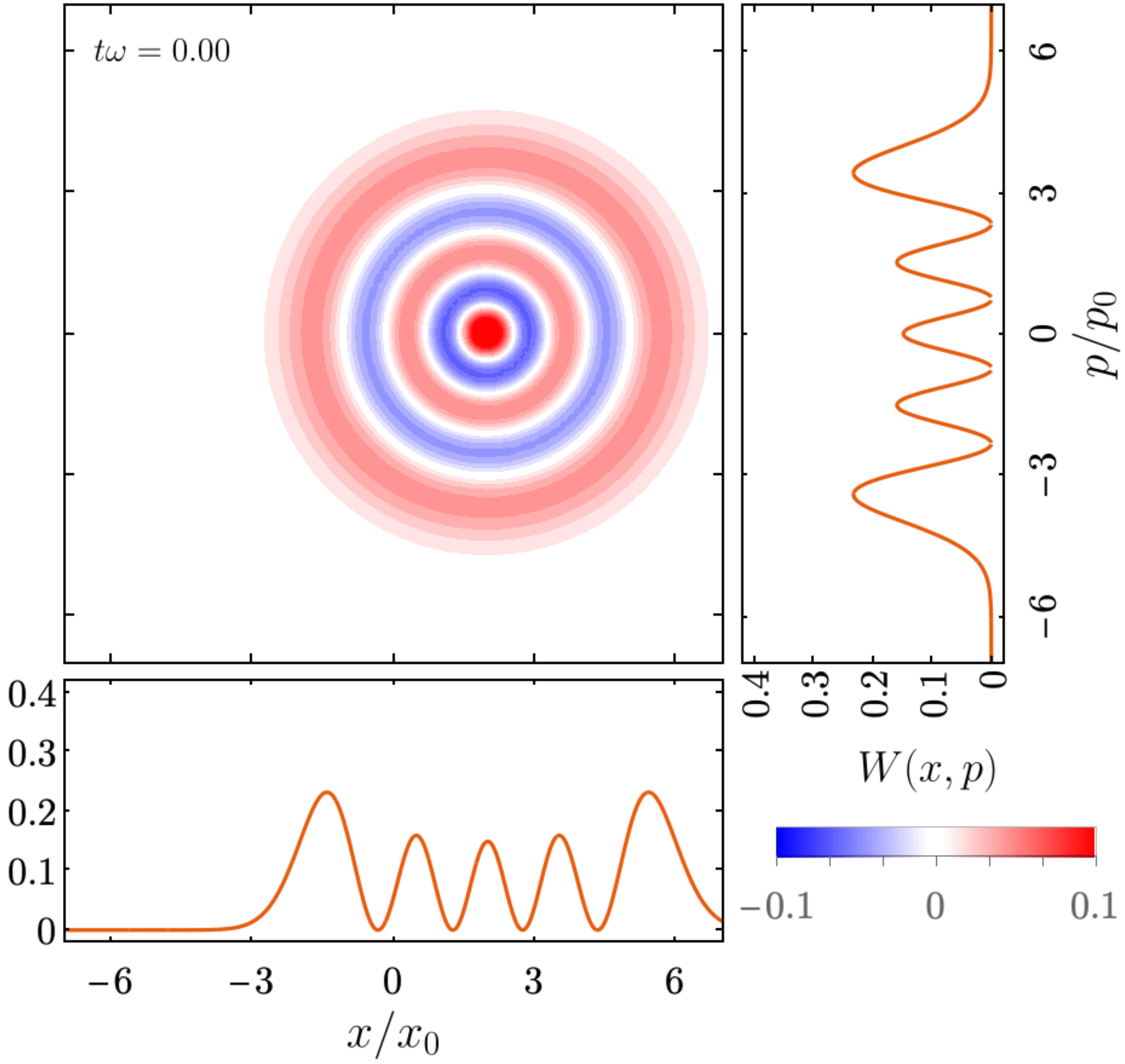
Example: Harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{4}\left(\hat{\tilde{p}}^2 + \hat{\tilde{x}}^2\right)$$

- Fock state

$$|\psi_0\rangle = \hat{D}(2)\,|4\rangle$$



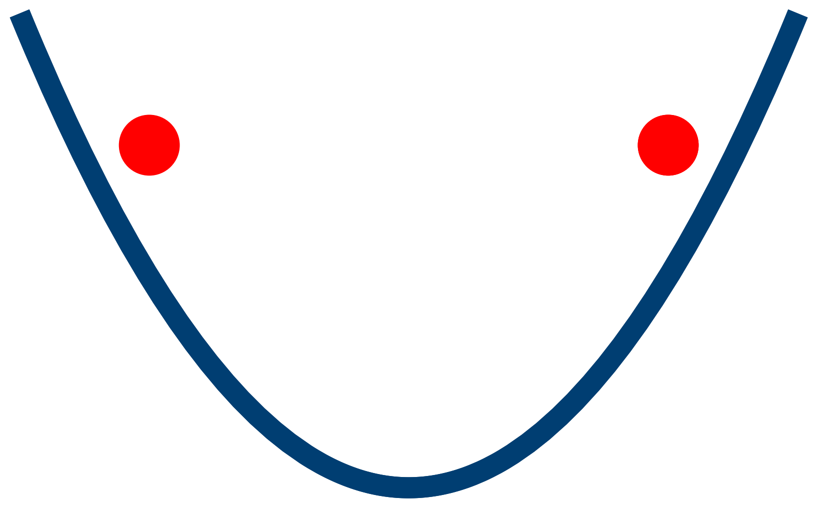


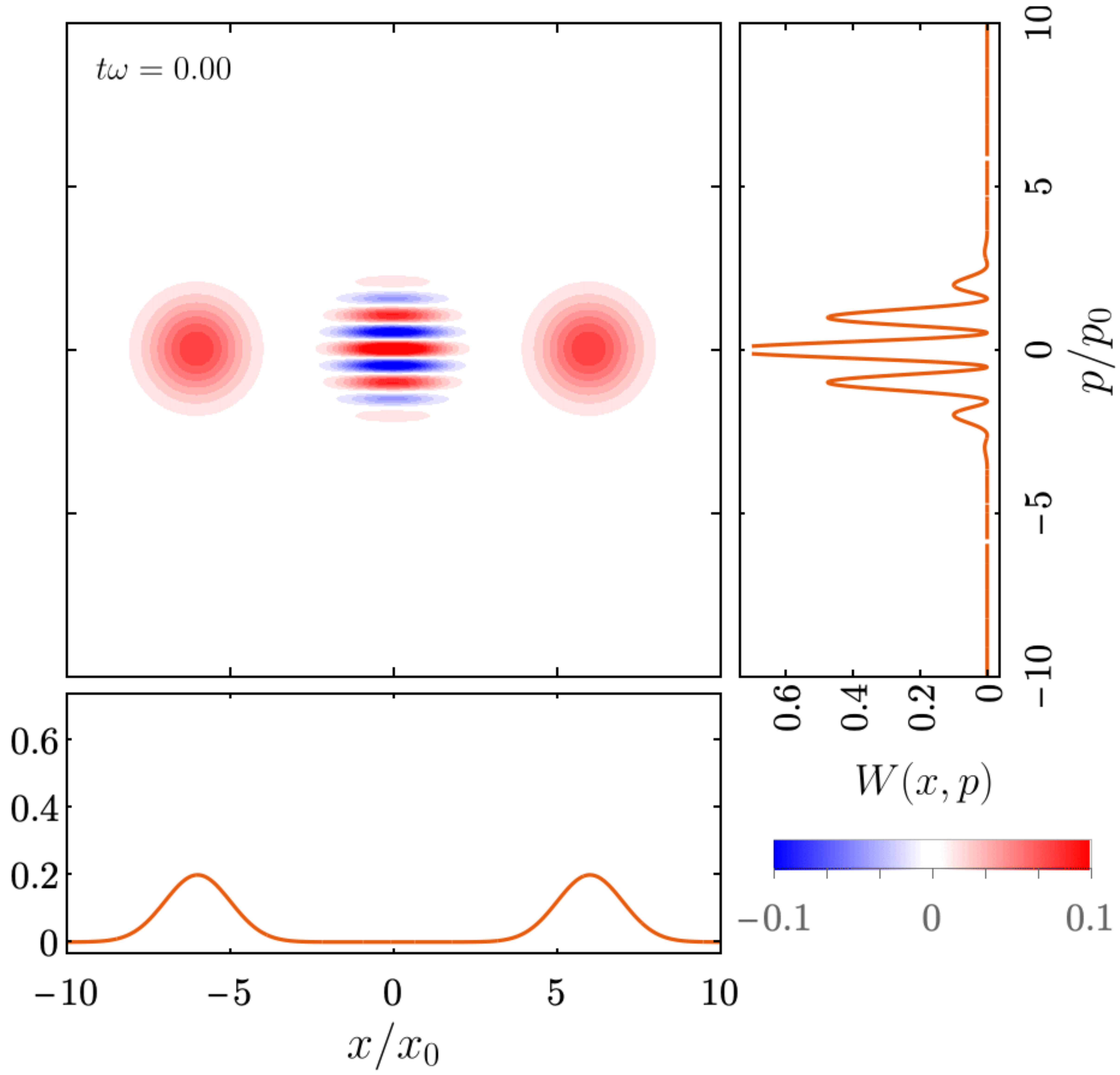
Example: Harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{4}\left(\hat{\tilde{p}}^2 + \hat{\tilde{x}}^2\right)$$

- Cat state

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left(\hat{D}(6)\,|\,0\rangle + \hat{D}(-6)\,|\,0\rangle\right)$$

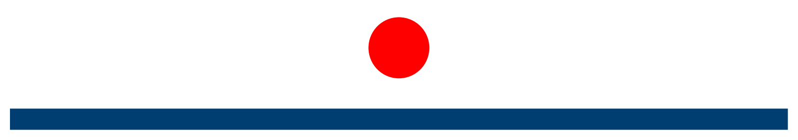


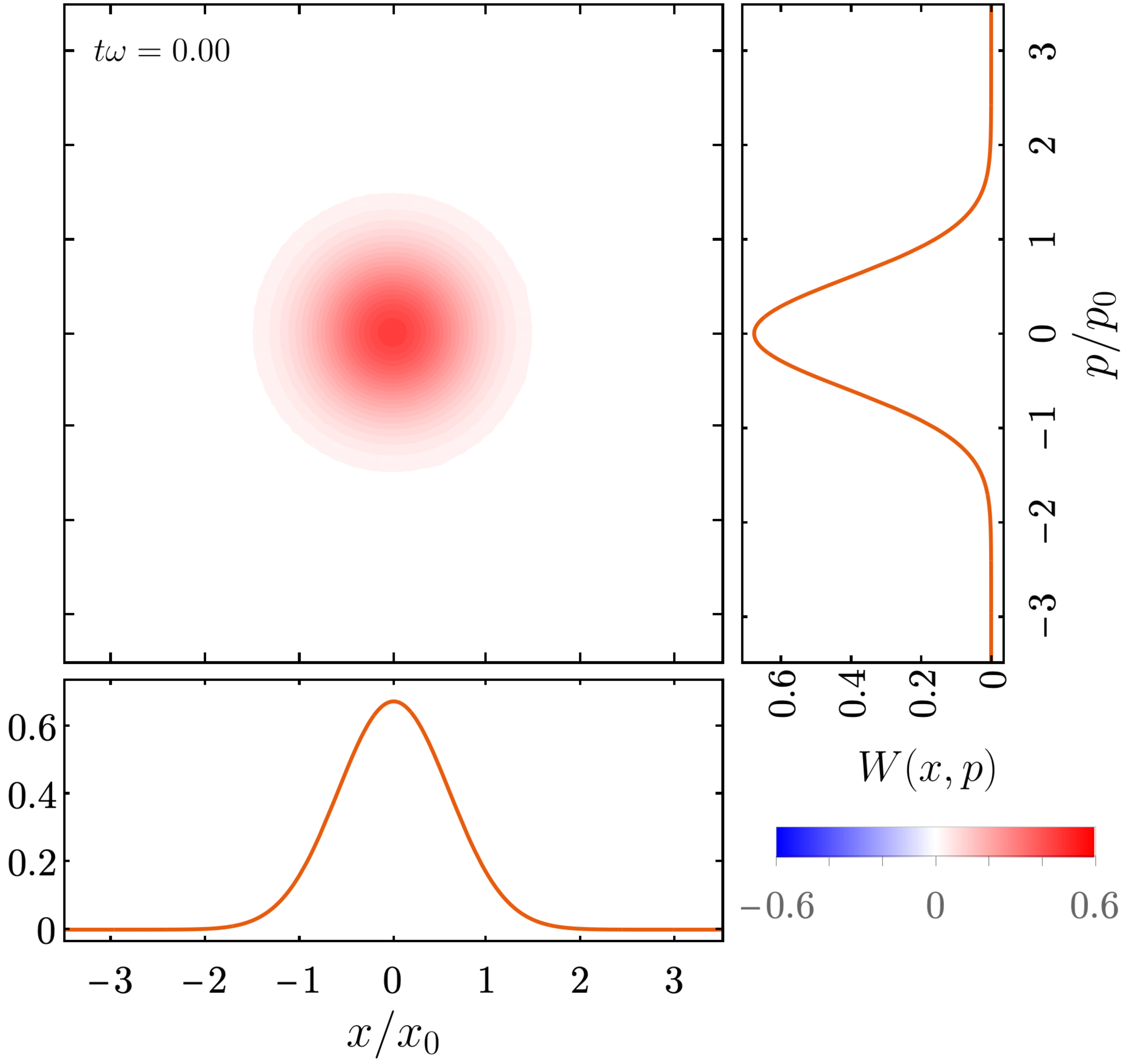


Example: Free dynamics

$$\hat{H} = \frac{\hbar\omega}{4}\hat{\tilde{p}}^2$$

$$|\psi_0\rangle = |0\rangle$$





- Spread increases quadratically

$$\begin{cases} v_x(t) = v_x(0) + v_p(0)t^2 \\ v_p(t) = v_p(0) \end{cases}$$

Example: Free dynamics

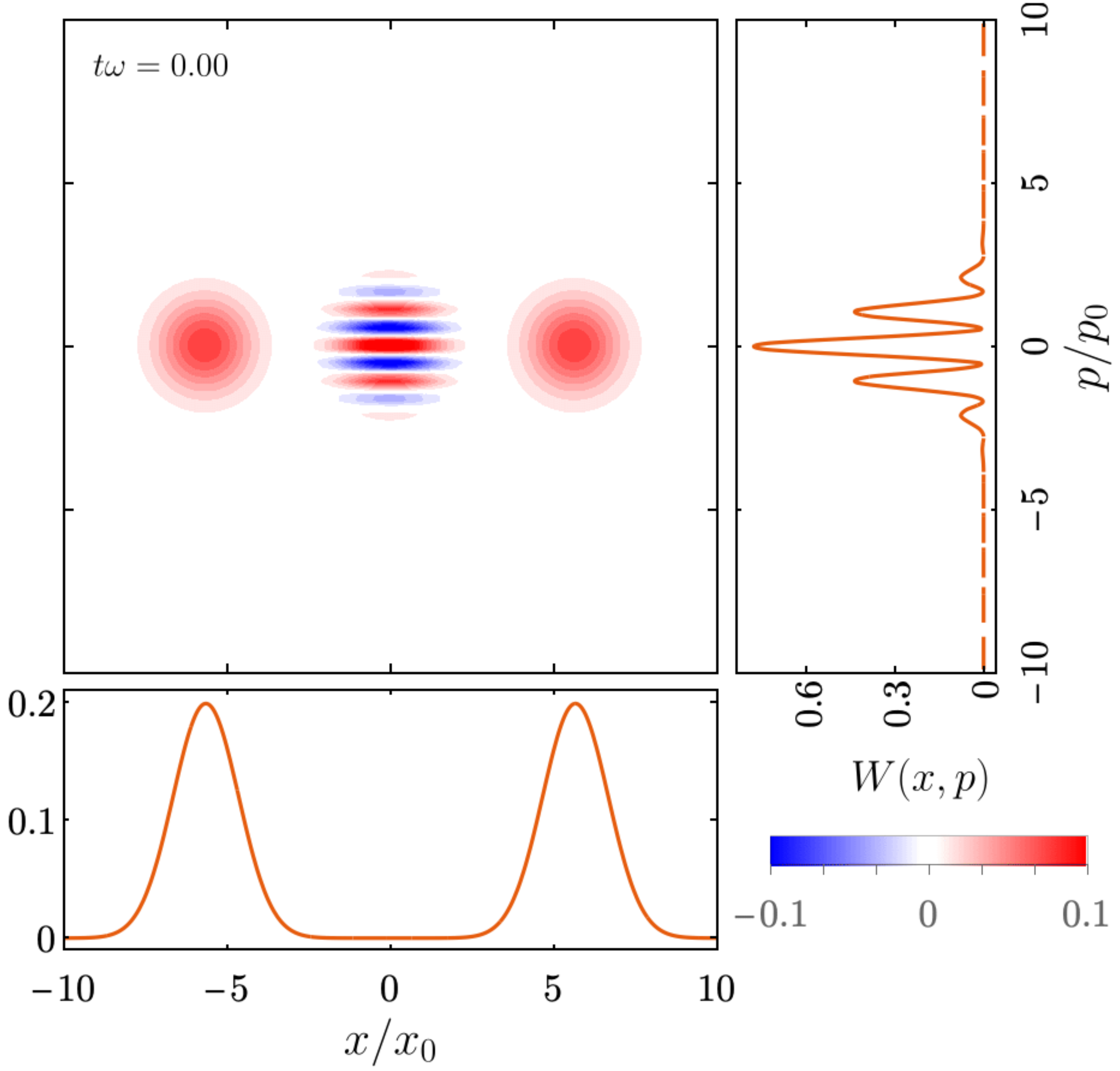
$$\hat{H} = \frac{\hbar\omega}{4}\hat{\tilde{p}}^2$$

- Cat state expanding freely

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left(\hat{D}(6)\,|\,0\rangle + \hat{D}(-6)\,|\,0\rangle\right)$$

- Fringes transferred to position!

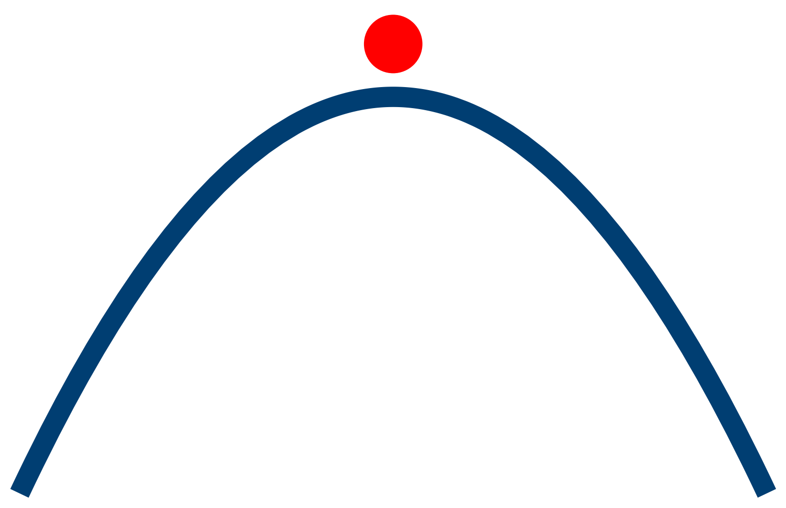
$$x(t) = x(0) + \frac{p(0)}{m}t$$

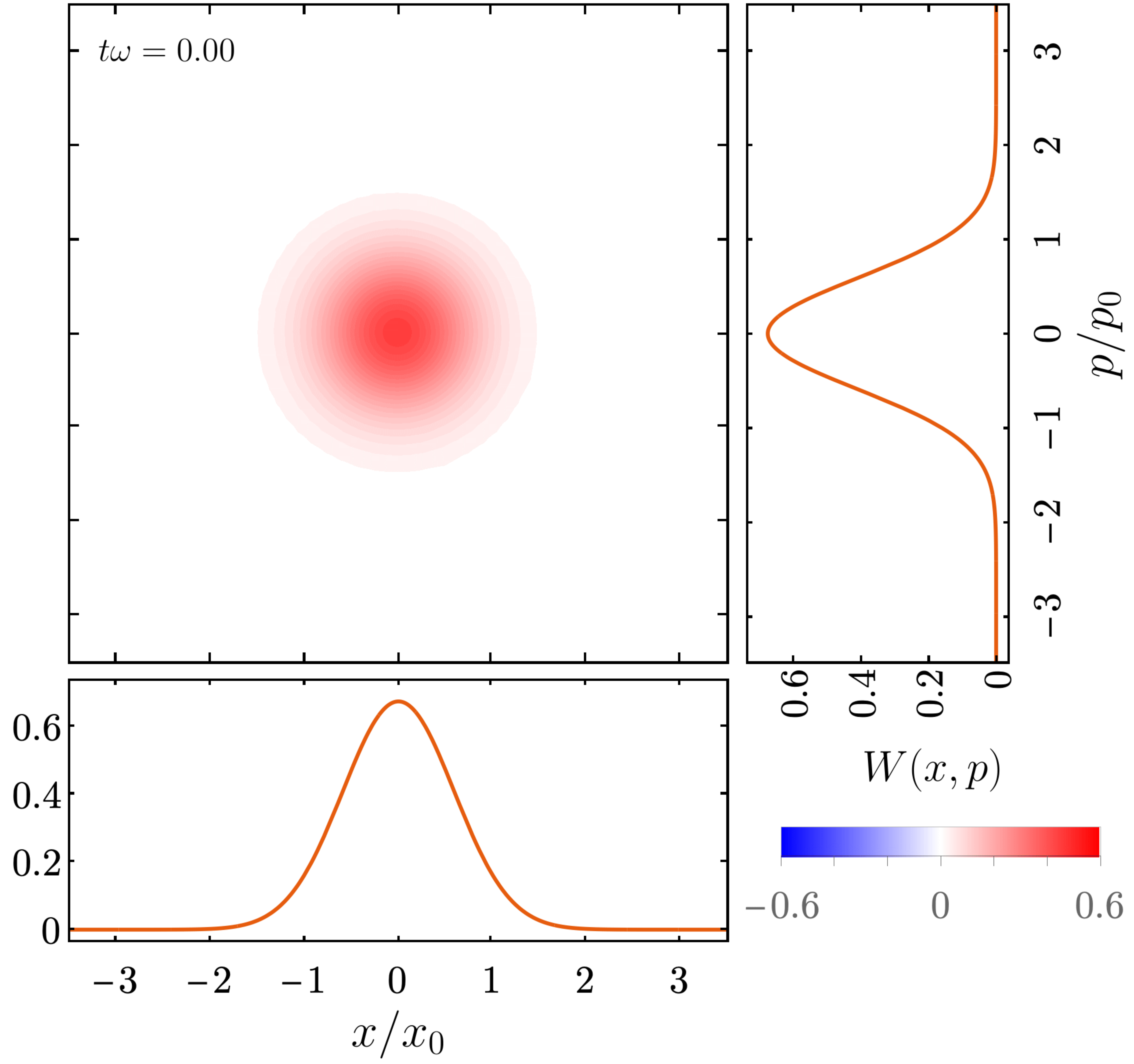


Example: Inverted harmonic oscillator

$$\hat{H} = \frac{\hbar\omega}{4}\left(\hat{\tilde{p}}^2 - \hat{\tilde{x}}^2\right)$$

$$|\psi_0\rangle = |0\rangle$$





- Spread increases exponentially!

O. Romero-Isart New J. Phys. 19, 123029 (2017)

H. Pino, …, O. Romero-Isart. Q. Sci. Technol. 3, 25001 (2018)

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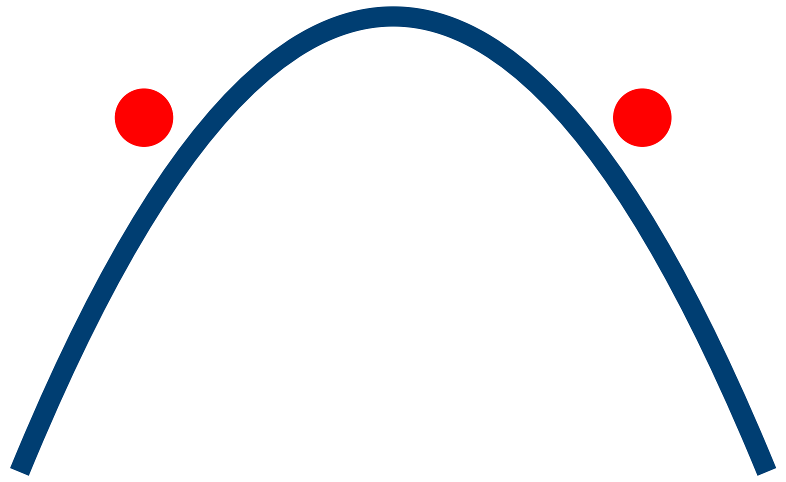

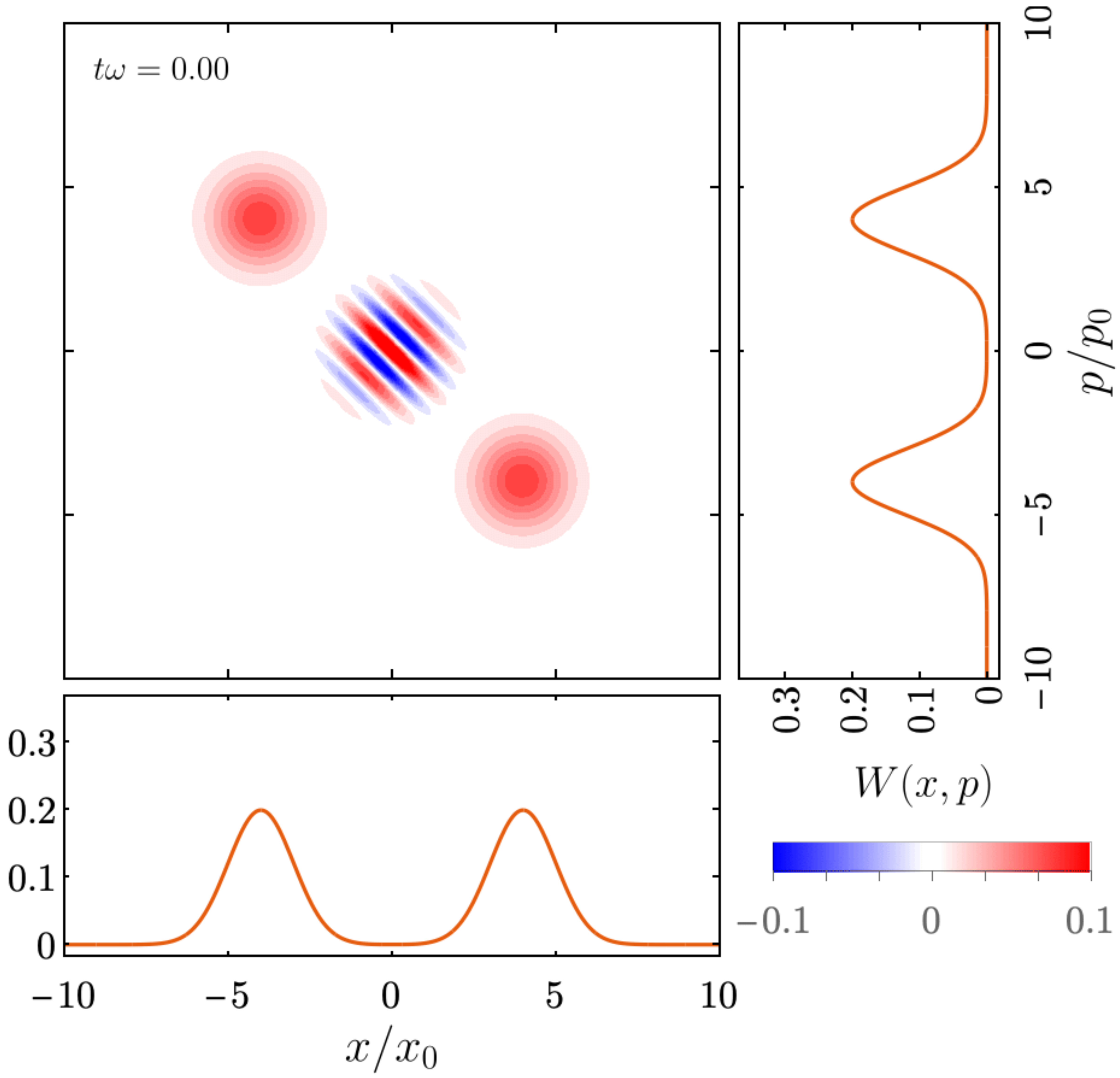

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$$\frac{\partial \tilde{W}(x,p,t)}{\partial t} = \sum_{n,m=0}^{n+m\leq N_U} g_{nm}(x,p,t)\frac{\partial^{n+m}\tilde{W}(x,p,t)}{\partial x^n \partial p^m}$$

Numerical integration of PDE in the Liouville frame can be done with a fix grid

This is equivalent to using a time-dependent "smart" grid where grid points go where they matter most

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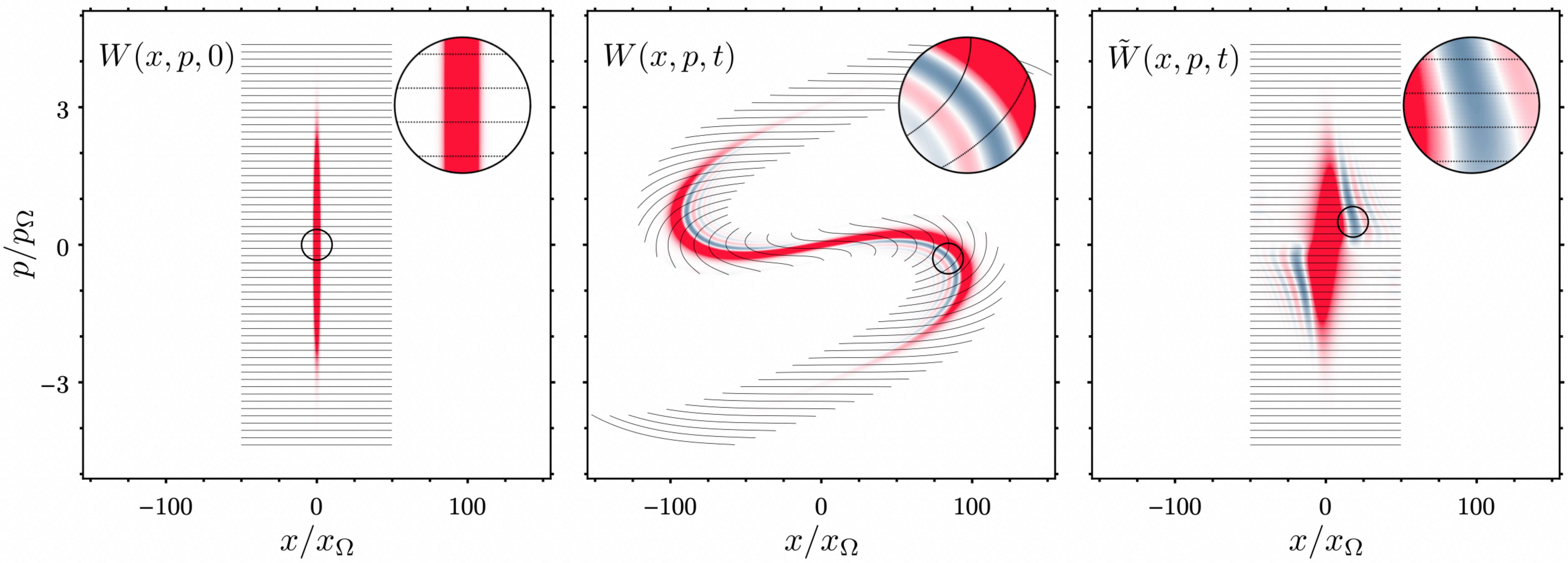

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Classical centroid frame

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$$M_c(t) = \exp\left[-x_c(t)\frac{\partial}{\partial x} - p_c(t)\frac{\partial}{\partial p}\right]$$

$$W^{(C)}(x,p,t) \equiv M_c^{-1}(t)W(x,p,t)$$

$$\frac{\partial W^{(C)}(x,p,t)}{\partial t} = \left(\mathcal{L}_c^{(C)} + \mathcal{L}_q^{(C)} + \mathcal{L}_d^{(C)}\right) W^{(C)}(x,p,t)$$

Classical centroid frame

Eq of motion of the W function

$$\frac{\partial W(x,p,t)}{\partial t} = \left(\mathscr{L}_c + \mathscr{L}_q + \mathscr{L}_d\right) W(x,p,t)$$

Move to classical centroid frame

$$M_c(t) = \exp\left[-x_c(t)\frac{\partial}{\partial x} - p_c(t)\frac{\partial}{\partial p}\right]$$

$$W^{(C)}(x,p,t) \equiv M_c^{-1}(t) W(x,p,t)$$

$$\frac{\partial W^{(C)}(x,p,t)}{\partial t} = \left(\mathscr{L}_c^{(C)} + \mathscr{L}_q^{(C)} + \mathscr{L}_d^{(C)}\right) W^{(C)}(x,p,t)$$

Effective time-dependent potential

$$U_{eff}(x,t) \equiv \sum_{n=2}^{\infty} \frac{1}{n!} \frac{\partial^n U}{\partial x^n}(x_c(t)) x^n$$

Gaussian frame

Define quadratic part of effective potential

$$U_G(x, t) \equiv \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x_c(t))x^2$$

Gaussian frame

Define quadratic part of effective potential

$$U_G(x,t) \equiv \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x_c(t))x^2$$

Gaussian dynamics given by

$$\mathscr{L}_G^{(C)}(t) \equiv -\frac{p}{m}\frac{\partial}{\partial x} + \frac{\partial U_G(x,t)}{\partial x}\frac{\partial}{\partial p}$$

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$$\mathscr{L}_G^{(C)}(t) \equiv -\frac{p}{m}\frac{\partial}{\partial x} + \frac{\partial U_G(x,t)}{\partial x}\frac{\partial}{\partial p}$$

Define propagator of Gaussian dynamics

$$M_G(t) \equiv \exp_+\left[\int_0^t dt'\mathscr{L}_G^{(C)}(t')\right]$$

Gaussian frame

Define quadratic part of effective potential

$$U_G(x,t) \equiv \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x_c(t))x^2$$

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$$M_G(t) \equiv \exp_+\left[\int_0^t dt' \mathscr{L}_G^{(C)}(t')\right]$$

Centroid+Gaussian frame

$$W^{(G)}(x,p,t) \equiv M_G^{-1}(t)M_c^{-1}(t)W(x,p,t)$$

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Define quadratic part of effective potential

$$U_G(x,t) \equiv \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x_c(t))x^2$$

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Centroid+Gaussian frame

$$W^{(G)}(x,p,t) \equiv M_G^{-1}(t)M_c^{-1}(t)W(x,p,t)$$

Non-Gaussian generator

$$\mathscr{L}_{nG}^{(C)}(t) \equiv \mathscr{L}_c^{(C)}(t) + \mathscr{L}_q^{(C)}(t) - \mathscr{L}_G^{(C)}(t)$$

Gaussian frame

Define quadratic part of effective potential

$$U_G(x,t) \equiv \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x_c(t))x^2$$

Gaussian dynamics given by

$$\mathscr{L}_G^{(C)}(t) \equiv -\frac{p}{m}\frac{\partial}{\partial x} + \frac{\partial U_G(x,t)}{\partial x}\frac{\partial}{\partial p}$$

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Non-Gaussian generator

$$\mathscr{L}_{nG}^{(C)}(t) \equiv \mathscr{L}_c^{(C)}(t) + \mathscr{L}_q^{(C)}(t) - \mathscr{L}_G^{(C)}(t)$$

Dynamical equation (exact)

$$\frac{\partial W^{(G)}(x,p,t)}{\partial t} = \left(\mathscr{L}_{nG}^{(G)}(t) + \mathscr{L}_d^{(G)}(t)\right) W^{(G)}(x,p,t)$$

Constant angle and linearized noise approximations

Exact equation to solve

$$\frac{\partial W^{(G)}(x,p,t)}{\partial t} = \left(\mathscr{L}_{nG}^{(G)}(t) + \mathscr{L}_{d}^{(G)}(t)\right) W^{(G)}(x,p,t)$$

Formal solution

$$W^{(G)}(x,p,t) = \exp_{+}\left[\int_0^t dt' \mathscr{L}_{nG}^{(G)}(t') + \mathscr{L}_{d}^{(G)}(t')\right] W^{(G)}(x,p,0)$$

After approximation

$$W^{(G)}(x,p,t) \approx \exp\left[\Delta_{nG}(t) + \Delta_{d}(t)\right] W^{(G)}(x,p,0)$$

Hence

$$W(x,p,t) \approx M_c(t) M_G(t) \exp\left[\Delta_{nG}(t) + \Delta_{d}(t)\right] W^{(G)}(x,p,0)$$

Constant angle and linearized noise approximation

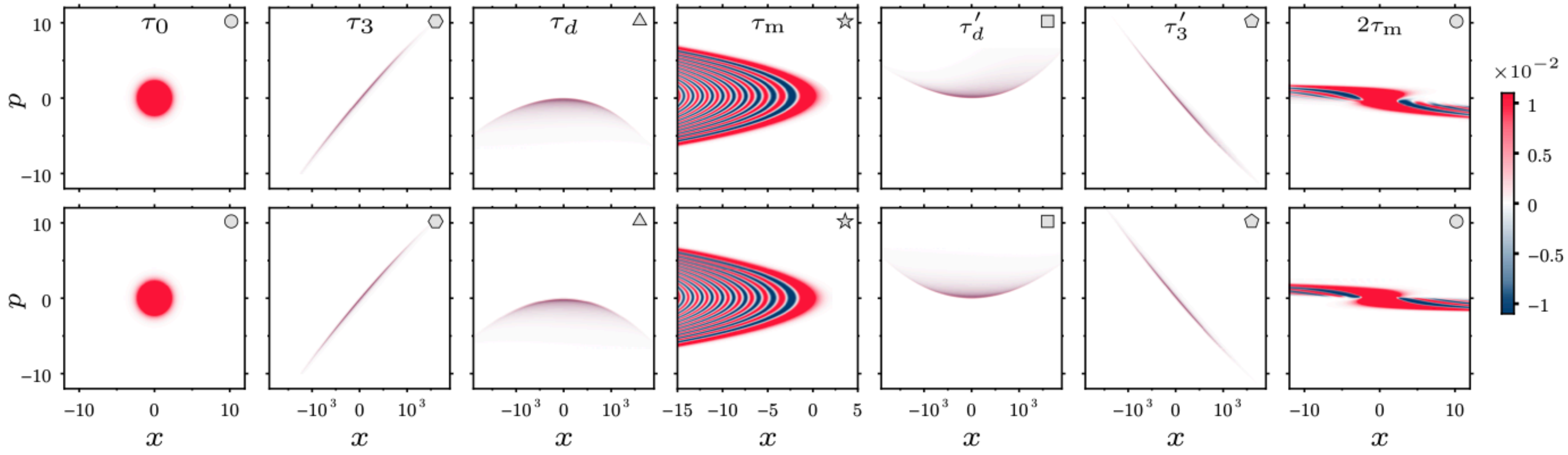

Figure 3: Wigner function of the state of a particle evolving in a double-well potential with parameters given in Table 1 at different instances of time. These instances of time are indicated by polygons and correspond to the times indicated in Fig. 1(a). The first row shows the numerically exact Wigner function $W(\boldsymbol{r} + \boldsymbol{r}_c(\tau), \tau)$ obtained using a numerically exact method whereas the second row shows the approximated Wigner function $W_{nG}(\boldsymbol{r} + \boldsymbol{r}_c(\tau), \tau)$ obtained using our analytical approach.

Constant angle and linearized noise approximation

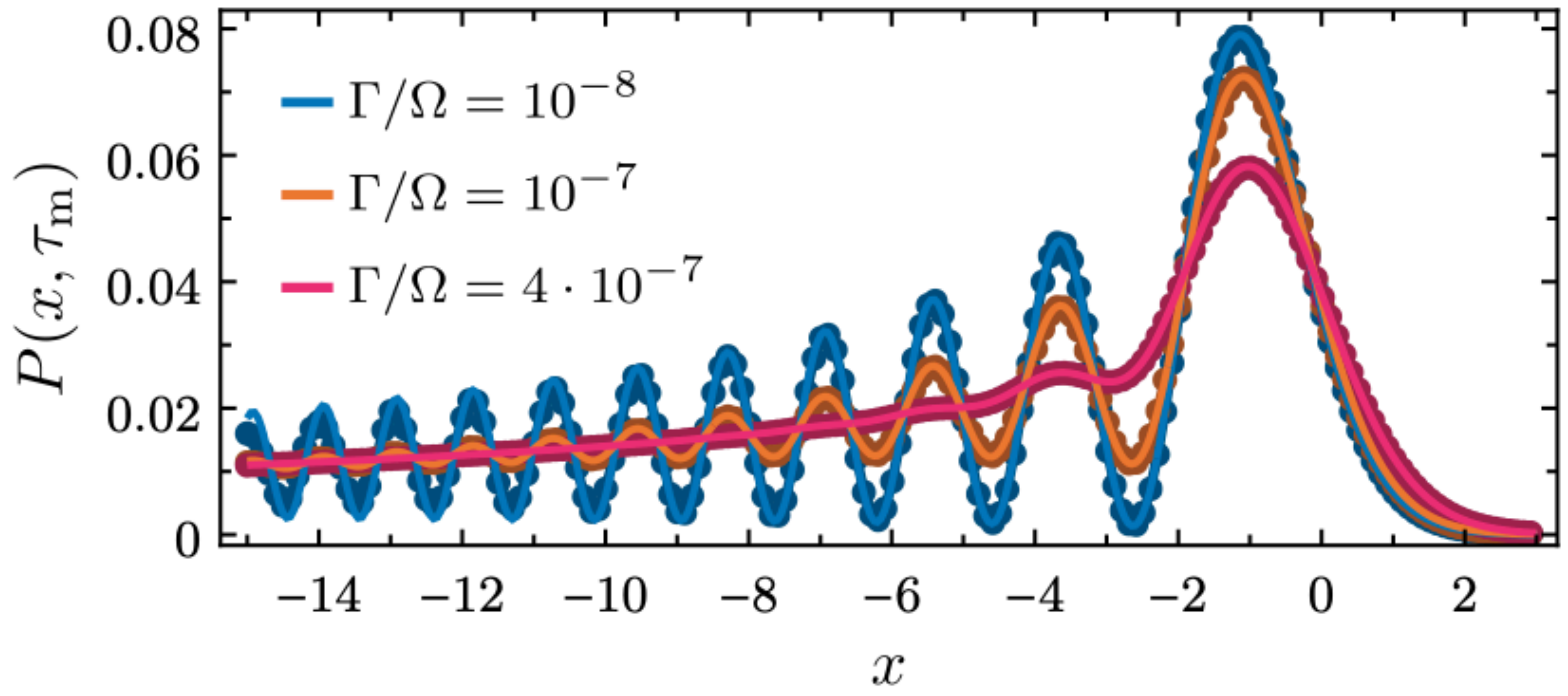

Figure 4: Position probability distribution at time τ_m for a state evolving in a double-well potential for the parameters in Table 1 and for different values of Γ. The lines are computed using the analytical method described in this paper, whereas dots correspond to a numerically exact computation using Q-Xpanse [11].

We have developed numerical and analytics methods

Numerical Simulation of Large-Scale Nonlinear Open Quantum Mechanics

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Wigner Analysis of Particle Dynamics in Wide Nonharmonic Potentials

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