# The quantum many-body non-equilibrium problem in phase space

Université de Strasbourg

cnrs

CESQ
CENTRE EUROPÉEN DE SCIENCES QUANTIQUES

www.schachenmayer.fr

www.cesq.eu

*Johannes Schachenmayer:* **schachenmayer@unistra.fr**

# The quantum many-body non-equilibrium problem in phase space

**Goal:**

A tour through numerical methods for simulating large quantum many-body dynamics (in general and) with a focus on phase space concepts

**Lecture 1:** Exact numerical methods and their limitations. How to to go beyond?

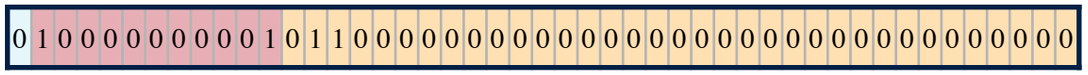
**Lecture 2:** Introduction to quantum physics on phase space. The truncated Wigner approximation (TWA).

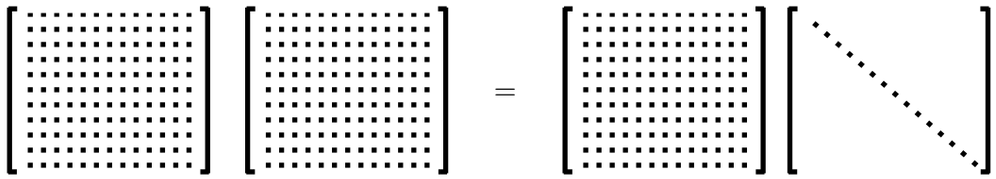
**Lecture 3:** Simulating quantum many-body dynamics with the discrete TWA (DTWA)

- Some text recommendations:
  - *For phase-space methods: Online lecture notes: A. Polkovnikov, Boulder summer school 2013: https://boulderschool.yale.edu/2013/boulder-school-2013-lecture-notes*
- Language recommendation (used for examples): Julia, **https://julialang.org/** (open source, easy, fast linear algebra)
- What these lectures are **not:**
  - *Complete: Many techniques are not discussed, many proofs are skipped: The big picture instead*
  - *Computer science class*
- Two types of lectures: Theory intro and "tutorial style" (sometimes mixed)
  Will provide code snippets, but no copy and paste!
- Philosophy: Use toolboxes only for basics (linear algebra, statistics)… let's understand things from scratch

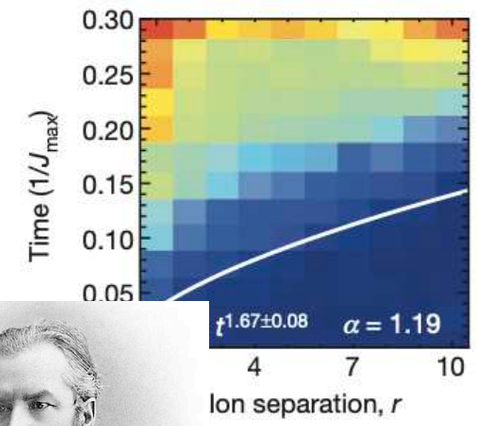
# Lecture 1 - Recap

- We discussed how to represent numbers as bits. We describe systems with state-vectors (not only in QM). If the problem is linear (QM), an exact diagonalization of the Hamiltonian solves everything, and is easily doable numerically for small systems (of order 10 spins)



- We discussed some general spin-model physics with long-range couplings, as they can e.g. be engineered in trapped ion systems. We discussed how to construct Hamiltonians using Kronecker products. It's very important to use **sparse matrices**.

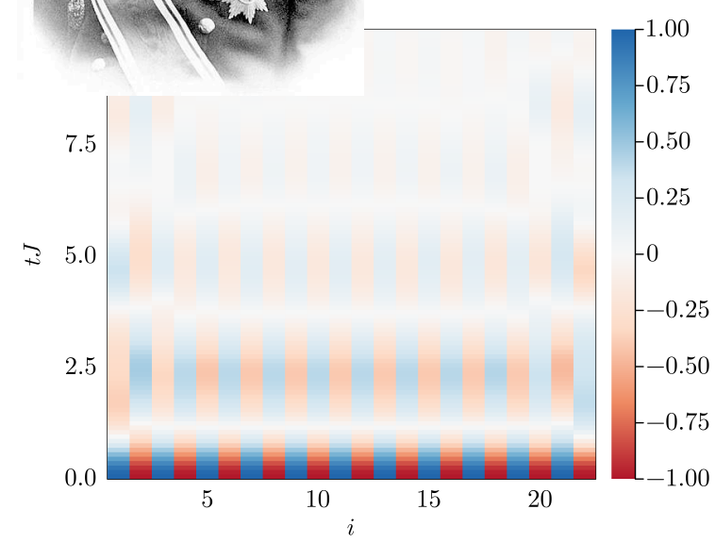



$$\hat{\sigma}_i^- = \begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{pmatrix}$$

- We introduced a time-evolution algorithm for linear systems, based on: **Krylov space**. Krylov space is a vector-space constructed from an initial state and the evolution matrix:

$$\text{span}\left(\hat{A}^0 \left|\psi_0\right\rangle, \hat{A}^1 \left|\psi_0\right\rangle, \hat{A}^2 \left|\psi_0\right\rangle, \ldots, \hat{A}^{m-1} \left|\psi_0\right\rangle\right)$$

Eigenvectors need to be made orthonormal, using **Arnoldi** or **Lanczos** iterations, then diagonalizations and matrix exponentials can be performed very efficiently on the much smaller **Krylov space.** This allows to easily simulate quantum dynamics of ~22 spins/qubits on a laptop.




- We briefly discussed how to push simulations to larger systems … next we go to **phase space!**

# Lecture 2 - Plan for today

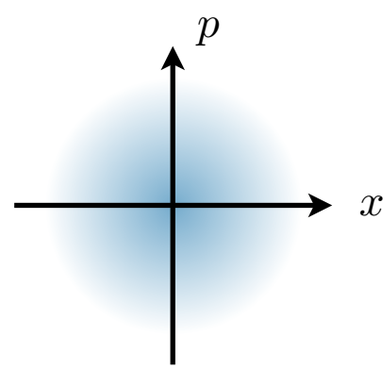
**Today mostly: Theory lecture style**

- **Part 2.1:** Describing quantum mechanics on phase space: The fundamentals

*For simplicity: Focus on particles in 1D*

$$\hat{O} = \int dx dp \, O_W(x,p) \hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}} \mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$



- **Part 2.2:** Time-evolution and the truncated Wigner approximation (TWA)

**Classical**

$$\frac{df}{dt} = \{f, H\}$$

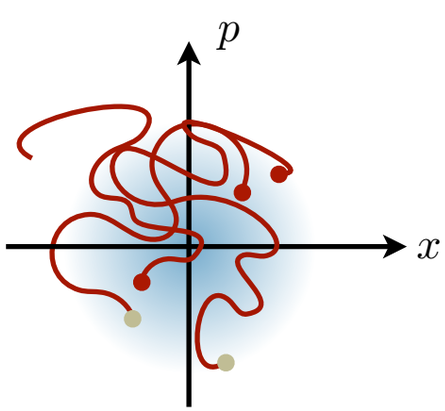
**Quantum**

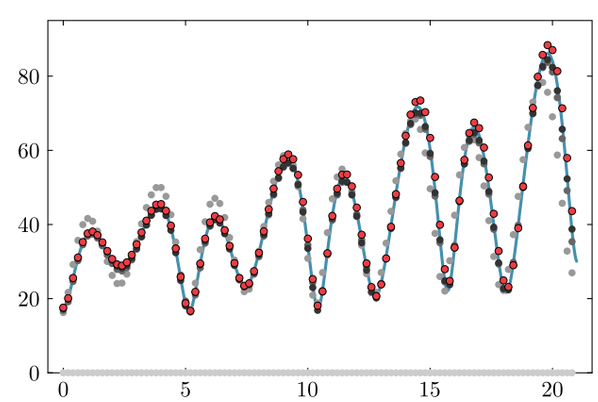
$$\frac{d}{dt} O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

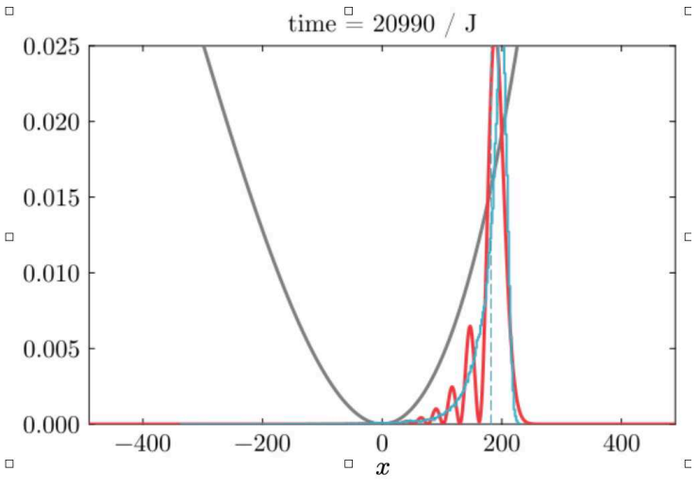
**TWA**

$$\frac{d}{dt} O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

- **Part 2.3:** The TWA as numerical method



# Lecture 2.1 - Quantum mechanics on phase space

**Hilbert space** $\Leftrightarrow$ **Phase space**

*State vector/density matrix*

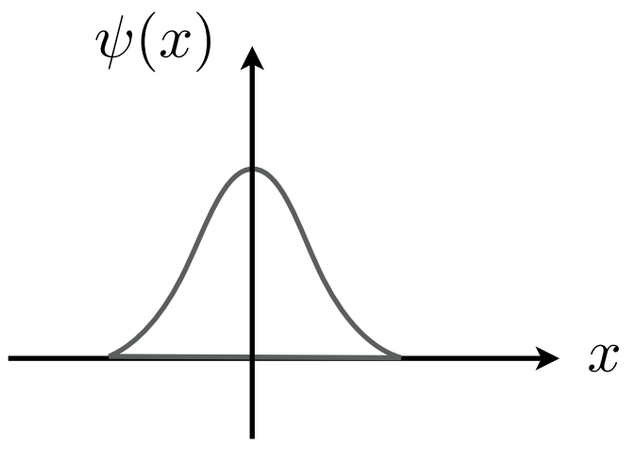
$|\psi\rangle \qquad \hat{\rho}$

*Distribution (e.g. Wigner) function*

$W(x,p)$

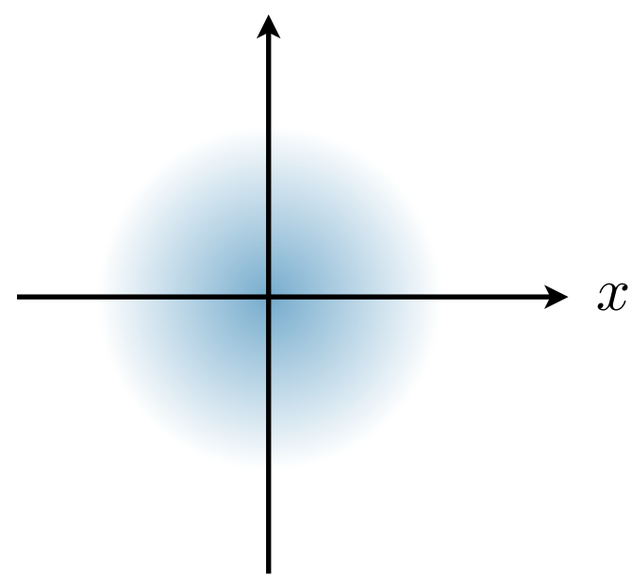
- **Example:** Single particle in 1D - Harmonic oscillator ground state:

*Position or momentum basis, complex wave-function*




$$\psi(x) = \langle x|\psi\rangle = \frac{1}{\pi^{1/4}\sqrt{a}}\mathrm{e}^{-x^2/(2a^2)}$$

*Two classical variables, description via real probability distribution*




$$W(x,p) = \frac{1}{\pi}\mathrm{e}^{-x^2/a^2 - a^2p^2}$$

**Idea:** "Describe a single quantum particle as it was an ensemble of classical ones"

# Lecture 2.1 - Quantum mechanics on phase space - History

- Historically, develop alongside the first formulations of quantum mechanics

- Foundations in ~1930s

  *Mostly questions about classical-quantum correspondence*

*Hermann Weyl (1885 - 1955)*

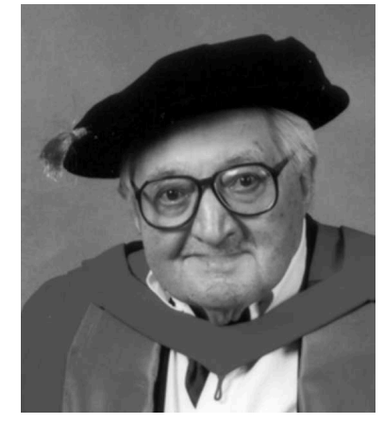
*John von Neumann (1903 - 1957)*

*Eugene Wigner (1902 - 1995)*

- Putting a full phase space description together:

  *(independently during 2nd WW time)*

*Hildebrand (Hip) Groenewold (1910 - 1996)*



*Jose Enrique (Joe) Moyal (1910 - 1998)*

- Initial heavy opposition by: Dirac and others.

*…only later more "nicely" formulated and generally accepted.*

*further reading: "A Concise Treatise on Quantum Mechanics in Phase Space", T. L. Curtright, D. B. Fairlie, C. K. Zachos, World Scientific*

# Lecture 2.1 - Reminder: Classical Physics - Hamiltonian formulation

*Ensemble of N classical particles on a phase space with positions/momenta* $x_1, x_2, \ldots, x_N$ $p_1, p_2, \ldots, p_N$

- Hamiltonian function: $H = H(x_1, x_2, \ldots, p_1, p_2, \ldots)$ *(here: time-independent)*

- Equations of motion for any phase space function: $f = f(x_1, x_2, \ldots, p_1, p_2, \ldots)$ $\boxed{\frac{df}{dt} = \{f, H\}}$

$$\{f, g\} = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i} \qquad \{f, g\} = f\mathbf{\Lambda} g \qquad \mathbf{\Lambda} = \sum_{i=1}^{N} \frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}$$

*Poisson bracket*

*skew symmetric*
*"symplectic operator"* $\mathbf{\Lambda}^T = -\mathbf{\Lambda}$

- **Example:** Free particles $H = \sum_i \frac{p_i^2}{2m}$

*Equations of motion:* $\frac{dx_i}{dt} = \{x_i, H\} = \frac{\partial x_i}{\partial x_i}\frac{\partial H}{\partial p_i} = \frac{p_i}{m}$ $\qquad \frac{dp_i}{dt} = \{p_i, H\} = 0$

- **Note:** This formulation makes it almost look like Heisenberg picture quantum mechanics

*… e.g. commutator ~ Poisson bracket* $\{x_i, x_j\} = \{p_i, p_j\} = 0 \qquad \{x_i, p_j\} = \delta_{i,j}$

*… so what's the difference to QM?*

# Lecture 2.1 - Reminder: Classical Physics - Hamiltonian formulation

- A trivial feature of classical mechanics:

The time evolution of any phase space function is determined by the evolution of only the phase space variables

*(Poisson bracket preserves chain rule)*

- **Example:** Two interacting particles $H(x_1, x_2, p_1, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1, x_2)$ $\qquad \frac{df}{dt} = \{f, H\}$

$$\{f, g\} = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i}$$

$$\dot{x}_1 = \frac{p_1}{m} \qquad \dot{p}_1 = -\frac{\partial V}{x_1} \qquad \dot{x}_2 = \frac{p_2}{m} \qquad \dot{p}_2 = -\frac{\partial V}{x_2}$$

*coupled set of equations*

*Evolution of the correlation function* $\quad f(x_1, p_2) = x_1 p_2$

$$\frac{df}{dt} = \{f, H\} = \{x_1 p_2, H\} = \frac{\partial x_1 p_2}{\partial x_1}\frac{\partial H}{\partial p_1} - \frac{\partial x_1 p_2}{\partial p_2}\frac{\partial H}{\partial x_2} = p_2 \frac{p_1}{m} - x_1 \frac{\partial V}{\partial x_2} = p_2 \dot{x}_1 + x_1 \dot{p}_2$$

*On the other hand simply:* $\frac{d}{dt}(x_1 p_2) = \dot{x}_1 p_2 + x_1 \dot{p}_2$ $\quad$ *…no need for an EOM for* $(x_1 p_2)$

*…this implies that 2N equations will always be* ***closed*** $\quad \mathbf{y} = [x_1, p_1, x_2, p_2]^T \qquad \dot{\mathbf{y}} = \ldots$

- In other words, functions of phase space variables **remain factorized!** $\quad (x_1 p_2)(t) = x_1(t) x_2(t)$

*…this is not necessarily true for quantum particles …*

# Lecture 2.1 - Wigner-Weyl phase space transformation in QM

| **Hilbert space** | $\Leftrightarrow$ | **Phase space** |
|---|---|---|
| *Operator* | | *Function of phase-space variables* |
| $\hat{O}$ | | $O_W(x,p)$ |

- **Definition:** For a **single** particle in 1D

$$\hat{O} = \int dx dp\, O_W(x,p)\hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

***"Weyl symbol"*** ***"Phase-point operator"***

- Transformation determined by the phase-point operators:
- Important properties of the phase point operators for a "good" transformation

**Normalization:** $\mathrm{tr}\left[\hat{A}(x,p)\right] = 1$

**Orthogonality:** $\mathrm{tr}\left[\hat{A}(x,p)\hat{A}(x',p')\right] = \mathcal{N}\delta(x-x')\delta(p-p')$

**Projection property:** $\frac{1}{\mathcal{N}}\int dx\, \hat{A}(x,p) = |p\rangle\langle p| \quad \frac{1}{\mathcal{N}}\int dp\, \hat{A}(x,p) = |x\rangle\langle x|$

*... simplified, for more details see e.g.: W. K. Wootters, Annals of Physics 176, 1 (1987)*

# Lecture 2.1 - Weyl quantization

| **Hilbert space** | $\Leftrightarrow$ | **Phase space** |
|---|---|---|
| *Operator* | | *Function of phase-space variables* |
| $\hat{O}$ | | $O_W(x,p)$ |

- A commonly used choice (here in the position basis):

$$\hat{A}(x,p) = \int dy\, \mathrm{e}^{\mathrm{i}py}\, |x+\frac{y}{2}\rangle\, \langle x-\frac{y}{2}| \qquad \mathcal{N} = 2\pi$$

*(other choices possible, this one is also known as Weyl quantization)*

- Check: **Normalization, Orthogonality, Projection property**

$$\mathrm{tr}\left[\hat{A}(x,p)\right] = \int dz \int dy\, \mathrm{e}^{\mathrm{i}py}\, \langle z|x+\frac{y}{2}\rangle\, \langle x-\frac{y}{2}|z\rangle = \int dz \int dy\, \mathrm{e}^{\mathrm{i}py} \delta(z-x-\frac{y}{2})\delta(z-x+\frac{y}{2}) = 1$$

$$\mathrm{tr}[\hat{A}(x,p)\hat{A}(x',p')] = \int dz \int dy_1 \int dy_2\, \mathrm{e}^{\mathrm{i}py_1}\mathrm{e}^{\mathrm{i}p'y_2}\, \langle z|x+\frac{y_1}{2}\rangle\, \langle x-\frac{y_1}{2}|x'+\frac{y_2}{2}\rangle\, \langle x'-\frac{y_2}{2}|z\rangle$$

$\frac{y_1}{2} = z - x$ $\qquad$ $\frac{y_2}{2} = x' - z$

$$= \int dz \mathrm{e}^{\mathrm{i}p2(z-x)}\mathrm{e}^{\mathrm{i}p'2(x'-z)}\, \langle 2x-z|2x'-z\rangle = 2\pi\delta(p-p')\delta(x-x')$$

*Case:* $x = x'$ $\quad$ $\mathrm{tr}[\hat{A}(x,p)\hat{A}(x',p')] = \int dz\, \mathrm{e}^{\mathrm{i}2z(p-p')} = 2\pi\delta(p-p')$

$$\hat{P}_x = \frac{1}{2\pi}\int dp \int dy\, \mathrm{e}^{\mathrm{i}py}\, |x+\frac{y}{2}\rangle\, \langle x-\frac{y}{2}| = \int dy\, \delta(y)\, |x+\frac{y}{2}\rangle\, \langle x-\frac{y}{2}| = |x\rangle\, \langle x|$$

*(exercise: other projections)*

# Lecture 2.1 - The Wigner function

**Hilbert space** $\Leftrightarrow$ **Phase space**

$$\hat{O} = \int dx dp\, O_W(x,p)\hat{A}(x,p) \qquad O_W(x,p) = \frac{1}{\mathcal{N}}\,\mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

$$\hat{A}(x,p) = \int dy\, \mathrm{e}^{\mathrm{i}py}\, |x+\frac{y}{2}\rangle\langle x-\frac{y}{2}| \qquad \mathcal{N} = 2\pi$$

- Simplified expression for Weyl-symbol in Weyl quantization:

$$O_W(x,p) = \frac{1}{\mathcal{N}}\mathrm{tr}[\hat{A}(x,p)\hat{O}] = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\mathrm{tr}(|x+\frac{y}{2}\rangle\langle x-\frac{y}{2}|\,\hat{O}) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\,\langle x-\frac{y}{2}|\,\hat{O}\,|x+\frac{y}{2}\rangle$$

- The Weyl-symbol for the density matrix is called the **Wigner function**

$$W(x,p) = \frac{1}{\mathcal{N}}\mathrm{tr}[\hat{A}(x,p)\hat{\rho}] = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\,\langle x-\frac{y}{2}|\,\hat{\rho}\,|x+\frac{y}{2}\rangle$$

*(general)* *(Weyl quantization)*

# Lecture 2.1 - The Wigner function in Weyl quantization

$$W(x,p) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\, \langle x - \frac{y}{2}|\,\hat{\rho}\,|x + \frac{y}{2}\rangle$$

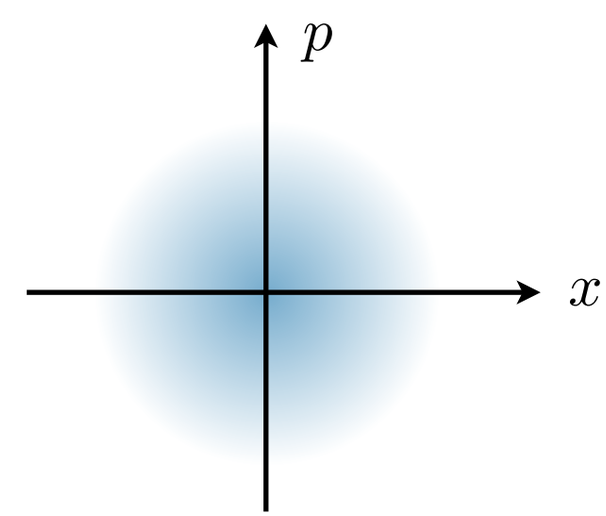
- **For example:** The harmonic oscillator ground state: $\langle x|\psi\rangle = \frac{1}{(\pi a^2)^{\frac{1}{4}}}\mathrm{e}^{-\frac{x^2}{2a^2}}$

$$\langle x - \frac{y}{2}|\,\hat{\rho}\,|x + \frac{y}{2}\rangle = \langle x - \frac{y}{2}|\psi\rangle\,\langle\psi|x + \frac{y}{2}\rangle \;=\; \frac{1}{(\pi a^2)^{\frac{1}{2}}}\mathrm{e}^{-\frac{1}{2a^2}\left(x-\frac{y}{2}\right)^2}\mathrm{e}^{-\frac{1}{2a^2}\left(x+\frac{y}{2}\right)^2} = \frac{1}{(\pi a^2)^{\frac{1}{2}}}\mathrm{e}^{-\frac{1}{2a^2}\left(2x^2+\frac{y^2}{2}\right)}$$

$$W(x,p) = \frac{1}{2\pi}\frac{1}{(\pi a^2)^{\frac{1}{2}}}\mathrm{e}^{-\frac{x^2}{a^2}}\int dy\, \mathrm{e}^{\mathrm{i}py}\mathrm{e}^{-\frac{y^2}{4a^2}} = \frac{1}{2\pi}\frac{1}{\sqrt{\pi}a}\mathrm{e}^{-\frac{x^2}{a^2}}\, 2\sqrt{\pi}a\mathrm{e}^{-p^2a^2} = \frac{1}{\pi}\mathrm{e}^{-x^2/a^2-p^2a^2}$$

*Fourier transform of Gaussian = Gaussian*

$$\int dx\, \mathrm{e}^{-\beta x^2}\mathrm{e}^{\mathrm{i}\omega x} = \sqrt{\frac{\pi}{\beta}}\mathrm{e}^{-\frac{\omega^2}{4\beta}} \qquad \beta = \frac{1}{4a^2}$$




- **Note proper normalization:**

$$\int dx \int dp\, W(x,p) = \frac{1}{\pi}\int dx\, \mathrm{e}^{-x^2/a^2}\int dp\, \mathrm{e}^{-p^2a^2} = \frac{1}{\pi}\sqrt{\pi}a\frac{\sqrt{\pi}}{a} = 1$$

- **Note also:** Heisenberg uncertainty is nicely seen by the fact that the Gaussian widths in the *x* and *p* directions are

$$\sigma_x = \frac{a}{\sqrt{2}} \quad \sigma_p = \frac{1}{a\sqrt{2}} \qquad \sigma_x\sigma_p = \frac{1}{2}$$

# Lecture 2.1 - The Wigner function - General properties

$$W(x,p) = \frac{1}{\mathcal{N}} \mathrm{tr}[\hat{A}(x,p)\hat{\rho}]$$

$$\mathrm{tr}\left[\hat{A}(x,p)\right] = 1$$

$$\mathrm{tr}\left[\hat{A}(x,p)\hat{A}(x',p')\right] = \mathcal{N}\delta(x-x')\delta(p-p')$$

$$\frac{1}{\mathcal{N}}\int dx\, \hat{A}(x,p) = |p\rangle\langle p| \qquad \frac{1}{\mathcal{N}}\int dp\, \hat{A}(x,p) = |x\rangle\langle x|$$

- **Normalization:**

$$\int dxdp\, W(x,p) = \int dxdp\, W(x,p)\mathrm{tr}[\hat{A}(x,p)] = \mathrm{tr}[\hat{\rho}] = 1$$

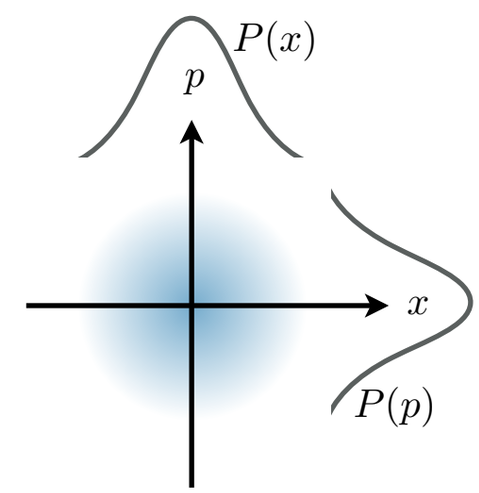
$$\hat{\rho} = \int dxdp\, W(x,p)\hat{A}(x,p)$$

The Wigner function can be considered as quasi-probability distribution … **it can be negative!**

- **Marginal probability distributions**

$$\int dp\, W(x,p) = \frac{1}{\mathcal{N}}\int dp\, \mathrm{tr}[\hat{A}(x,p)\hat{\rho}] = \mathrm{tr}[|x\rangle\langle x|\,\hat{\rho}]$$

$$\int dx\, W(x,p) = \frac{1}{\mathcal{N}}\int dx\, \mathrm{tr}[\hat{A}(x,p)\hat{\rho}] = \mathrm{tr}[|p\rangle\langle p|\,\hat{\rho}]$$




More generally it can be shown that the integral over any line gives the distribution for an observable $\propto \alpha\hat{x} + \beta p$

*[see e.g.: W. K. Wootters, Annals of Physics 176, 1 (1987)]*

*… this is a nice property to have, but we will not need it later*

# Lecture 2.1 - The Wigner function - General properties

$$W(x,p) = \frac{1}{\mathcal{N}}\mathrm{tr}[\hat{A}(x,p)\hat{\rho}]$$

$$\mathrm{tr}\left[\hat{A}(x,p)\right] = 1$$

$$\mathrm{tr}\left[\hat{A}(x,p)\hat{A}(x',p')\right] = \mathcal{N}\delta(x-x')\delta(p-p')$$

$$\frac{1}{\mathcal{N}}\int dx\, \hat{A}(x,p) = |p\rangle\langle p| \qquad \frac{1}{\mathcal{N}}\int dp\, \hat{A}(x,p) = |x\rangle\langle x|$$

- **Expectation values for an operator on phase space** $\quad O_W(x,p) = \frac{1}{\mathcal{N}}\mathrm{tr}[\hat{A}(x,p)\hat{O}]$

$$\mathcal{N}\int dxdp\, W(x,p)O_W(x,p) = \mathcal{N}\int dx_1dp_1dx_2dp_2\, W(x_1,p_1)O_W(x_2,p_2)\delta(x_1-x_2)\delta(p_1-p_2)$$

$$= \int dx_1dp_1dx_2dp_2\, W(x_1,p_1)O_W(x_2,p_2)\mathrm{tr}[\hat{A}(x_1,p_1)A(x_2,p_2)] = \mathrm{tr}[\hat{\rho}\hat{O}]$$

$$\hat{\rho} = \int dxdp\, W(x,p)\hat{A}(x,p) \qquad \hat{O} = \int dxdp\, O_W(x,p)\hat{A}(x,p)$$

- Note that this also implies the definition of a proper inner product between two Wigner functions:

$$\mathcal{N}\int dxdp\, W_1(x,p)W_2(x,p) = \mathrm{tr}[\hat{\rho}_1\hat{\rho}_2]$$

# Lecture 2.1 - The Wigner function - Many-particles

- **Generalization to many particles is straightforward:**

**Hilbert space** $\Longleftrightarrow$ **Phase space**

$$\hat{O} = \int d\mathbf{x} d\mathbf{p}\, O_W(\mathbf{x},\mathbf{p}) \hat{A}(\mathbf{x},\mathbf{p})$$

$$O_W(x,p) = \frac{1}{\mathcal{N}^N} \mathrm{tr}\left[\hat{A}(\mathbf{x},\mathbf{p})\hat{O}\right]$$

$$\hat{A}(\mathbf{x},\mathbf{p}) \equiv \bigotimes_{i=1}^{N} \hat{A}(x_i,p_i)$$

$$\mathbf{x} = [x_1, x_2, \ldots, x_N]^T$$
$$\mathbf{p} = [p_1, p_2, \ldots, p_N]^T$$

- **Normalization:** $\mathrm{tr}\left[\hat{A}(\mathbf{x},\mathbf{p})\right] = \prod_{i=1}^{N} \mathrm{tr}\left[\hat{A}(x_i,p_i)\right] = 1$

- **Orthogonality:** $\mathrm{tr}\left[\hat{A}(\mathbf{x},\mathbf{p})\hat{A}(\mathbf{x}',\mathbf{p}')\right] = \prod_{i=1}^{N} \mathrm{tr}\left[\hat{A}(x_i,p_i)\hat{A}(x_i',p_i')\right] = \mathcal{N}^N \prod_{i=1}^{N} \delta(x_i - x_i')\delta(p_i - p_i')$

**Projection properties:** $\frac{1}{\mathcal{N}} \int dx_j\, \hat{A}(\mathbf{x},\mathbf{p}) = |p_j\rangle\langle p_j| \otimes \prod_{i\neq j} \hat{A}(x_i,p_i)$

$$\int dx_j\, W(\mathbf{x},\mathbf{p}) = \frac{1}{\mathcal{N}^N} \int dx_j\, \mathrm{tr}[\hat{A}(x_j,p_j)\hat{\rho}] \prod_{i\neq j} \mathrm{tr}[\hat{A}(x_i,p_i)\hat{\rho}] = \mathrm{tr}[|p_j\rangle\langle p_j|\,\hat{\rho}]\, W(\mathbf{x}_{\neq j},\mathbf{p}_{\neq j})$$

*…also holds for individual particles*

# Lecture 2.1 - The Bopp representation

- A practical shortcut to compute the phase space transformation (only for the Weyl quantization)

**Hilbert space** $\Longleftrightarrow$ **Phase space**

$\hbar \neq 1$

**Rule:** Replace

$$\hat{x} \to x + \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial x}$$

*Friedrich Bopp*
*(1909-1987)*

- **Note:** This can also be considered as definition of the transformation, and it can also be derived from an alternative point of view of phase space dynamics using a path integral formulation.

*for more details see e.g. A. Polkovnikov, Ann. Phys., 325, 1790 (2010)*

- **Simple observations:** *Limit* $\hbar \to 0$ *... operator nature of position/momentum disappears*

- **Commutator:**

$$[\hat{x}, \hat{p}] = \left(x + \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial p}\right)\left(p - \cancel{\frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial x}}\right) - \left(p - \frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial x}\right)\left(x + \cancel{\frac{\mathrm{i}\hbar}{2}\frac{\partial}{\partial p}}\right) = \mathrm{i}\hbar$$

# Lecture 2.1 - The Bopp representation

**Hilbert space** $\Longleftrightarrow$ **Phase space**

**Rule:** Replace

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

$$\hbar \equiv 1$$

$$O_W(x,p) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\, \langle x - \frac{y}{2}|\, \hat{O}\, |x + \frac{y}{2}\rangle$$

- **Exercise:** Compute $(\hat{x}\hat{p})_W(x,p)$

$$(\hat{x}\hat{p})_W(x,p) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\, \langle x - \frac{y}{2}|\, \hat{x}\hat{p}\, |x + \frac{y}{2}\rangle = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\left(x - \frac{y}{2}\right) \langle x - \frac{y}{2}|\, \hat{p}\, |x + \frac{y}{2}\rangle$$

$$\langle x - \frac{y}{2}|\, \hat{p}\, |x + \frac{y}{2}\rangle = \frac{1}{2\pi}\int dk\, k\, \langle x - \frac{y}{2}|k\rangle\, \langle k|x + \frac{y}{2}\rangle = \frac{1}{2\pi}\int dk\, k\mathrm{e}^{-\mathrm{i}yk} \qquad \langle x - \frac{y}{2}|k\rangle = \mathrm{e}^{-\mathrm{i}(x - \frac{y}{2})}$$

$$\mathbb{1} = \frac{1}{2\pi}\int dk\, |k\rangle\, \langle k|$$

$$(\hat{x}\hat{p})_W(x,p) = \frac{1}{2\pi}\int dydk\, \mathrm{e}^{\mathrm{i}(p-k)y} k\left(x - \frac{y}{2}\right) = px - \frac{1}{4\pi}\int dydk\, \mathrm{e}^{\mathrm{i}(p-k)y} ky = px + \frac{\mathrm{i}}{2}$$

$$\frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}(p-k)y} = \delta(p-k)$$

$$\frac{1}{4\pi}\int dy\, y\mathrm{e}^{\mathrm{i}py}\int dk\, k\mathrm{e}^{-\mathrm{i}ky} = \frac{1}{2}\int dy\, y\mathrm{e}^{\mathrm{i}py}\mathrm{i}\delta'(y) = 0 - \frac{\mathrm{i}}{2}\int dy\, \left(\mathrm{e}^{\mathrm{i}py} + \mathrm{i}py\mathrm{e}^{\mathrm{i}py}\right)\delta(y) = -\frac{\mathrm{i}}{2}$$

*Fourier transform formula*

$$\frac{1}{2\pi}\int dx\, x\, \mathrm{e}^{\mathrm{i}\omega x} = \mathrm{i}\delta'(\omega)$$

*Integration by parts*

*…first derivative of delta distribution*

# Lecture 2.1 - The Bopp representation

**Hilbert space** $\Longleftrightarrow$ **Phase space**

**Rule:** Replace

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$

$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

$$\hbar \equiv 1$$

$$O_W(x,p) = \frac{1}{2\pi}\int dy\, \mathrm{e}^{\mathrm{i}py}\, \langle x - \frac{y}{2}|\, \hat{O}\, |x + \frac{y}{2}\rangle$$

- **Exercise:** Compute $(\hat{x}\hat{p})_W(x,p)$

- **Or…** with Bopp:

$$\hat{x}\hat{p} \to (\hat{x}\hat{p})_W = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)\left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right) = xp + \frac{\mathrm{i}}{2}$$

✔

# Lecture 2.1 - The Bopp representation

**Hilbert space** $\Leftrightarrow$ **Phase space**

**Rule:** Replace

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

- **Note:** It's not difficult to generally prove that the Bopp representation produces the correct Weyl symbols in the Weyl quantization *(exercise)* … *see e.g. A. Polkovnikov, Boulder summer school 2013 lecture notes*.

- **More examples:** $\hat{x} \Leftrightarrow O_W = x$ $\qquad$ $\hat{p} \Leftrightarrow O_W = p$

$$\hat{x}\hat{p} \Leftrightarrow O_W = xp + \frac{\mathrm{i}}{2} \qquad \hat{p}\hat{x} \Leftrightarrow O_W = \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) = px - \frac{\mathrm{i}}{2}$$

- **Note:** Operator non-hermitian $\Leftrightarrow$ Weyl symbol is complex

$$\hat{O}_{xp} = \frac{1}{2}\left(\hat{x}\hat{p} + \hat{p}\hat{x}\right) \Leftrightarrow O_W = xp$$

$$\hat{O}_{x^2p} = \frac{1}{2}\left(\hat{x}\hat{O}_{xp} + \hat{O}_{xp}\hat{x}\right) = \frac{1}{4}\left(\hat{x}^2\hat{p} + 2\hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2\right) \Leftrightarrow O_W = x^2p$$

$$4O_W = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)\left(xp + \frac{i}{2}\right) + 2\left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)\left(px - \frac{i}{2}\right) + \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(x + \cancel{\frac{\mathrm{i}}{2}\frac{\partial}{\partial p}}\right)\left(x + \cancel{\frac{\mathrm{i}}{2}\frac{\partial}{\partial p}}\right)$$

$$= x^2p + \cancel{\mathrm{i}x} + 2\left(x^2p + \cancel{\frac{\mathrm{i}}{2}x} - \cancel{\frac{\mathrm{i}}{2}x}\right) + px^2 - \cancel{\mathrm{i}x}$$

# Lecture 2.1 - The Bopp representation

**Hilbert space** $\Leftrightarrow$ **Phase space**

**Rule:** Replace

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

- **Note:** It's not difficult to generally prove that the Bopp representation produces the correct Weyl symbols in the Weyl quantization *(exercise)* *… see e.g. A. Polkovnikov, Boulder summer school 2013 lecture notes.*

- **General hermitian observable constructed from x and p:**

$$\hat{O}_{xp} = \frac{1}{2}\left(\hat{x}\hat{p} + \hat{p}\hat{x}\right) \Leftrightarrow O_W = xp$$

$$\hat{O}_{x^2p} = \frac{1}{2}\left(\hat{x}\hat{O}_{xp} + \hat{O}_{xp}\hat{x}\right) = \frac{1}{4}\left(\hat{x}^2\hat{p} + 2\hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2\right) \Leftrightarrow O_W = x^2p$$

$$\vdots$$

*Symmetrized polynomial*

$$\langle \hat{O}_{x^np^m} \rangle = \int dx\, dp\, W(x,p) x^n p^m$$

*… we will take this as general* ***definition*** *of a good phase-space representation!*

Any observable can be computed from the Wigner function

- General proof: *(exercise)* *… see e.g. A. Polkovnikov, Boulder summer school 2013 lecture notes.*

# Lecture 2 - Plan for today

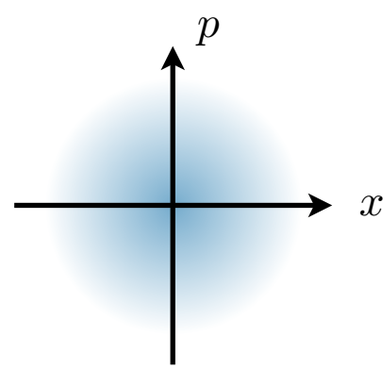
**Today mostly: Theory lecture style**

- **Part 2.1:** Describing quantum mechanics on phase space: The fundamentals

*For simplicity: Focus on particle in 1D*

$$\hat{O} = \int dx dp \, O_W(x,p) \hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}} \mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$



- **Part 2.2:** Time-evolution and the truncated Wigner approximation (TWA)

**Classical**

$$\frac{df}{dt} = \{f, H\}$$

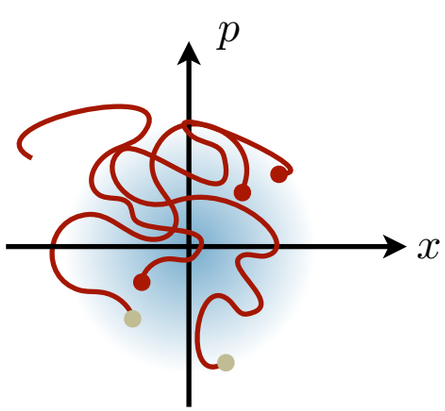
**Quantum**

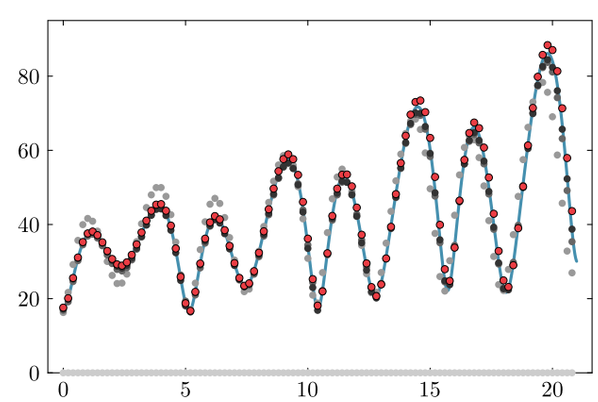
$$\frac{d}{dt} O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

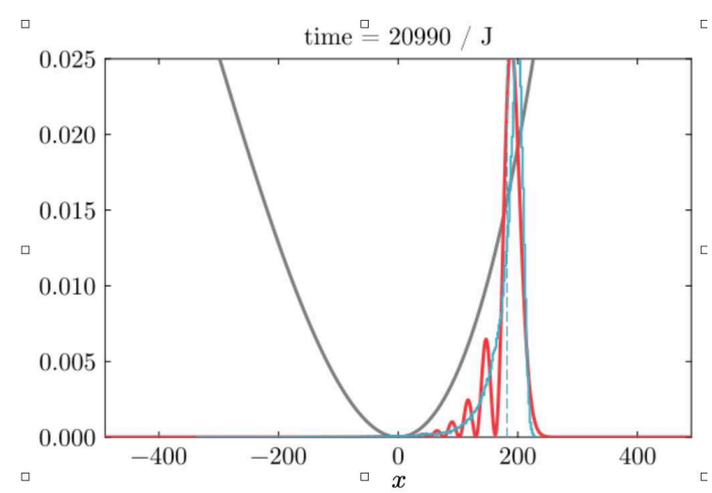
**TWA**

$$\frac{d}{dt} O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

- **Part 2.3:** The TWA as numerical method



# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Heisenberg picture** (density matrix and Wigner function do not evolve)

**Hilbert space** $\Longleftrightarrow$ **Phase space**

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

$$\frac{d}{dt}\hat{O} = \mathrm{i}[\hat{H}, \hat{O}] \qquad \frac{d}{dt}O_W = \dots$$

*Wigner-Weyl transform (both sides)*

- **Free particle:** $\hat{H} = \dfrac{\hat{p}^2}{2m}$ *Evolution of particle position*

$$\frac{d}{dt}(\hat{x})_W = \frac{\mathrm{i}}{2m}\left[(\hat{p}^2\hat{x})_W - (\hat{x}\hat{p}^2)_W\right]$$

$$\left(\hat{p}^2\hat{x}\right)_W = \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) = \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(px - \frac{\mathrm{i}}{2}\right) = p^2x - \mathrm{i}p$$

$$\left(\hat{x}\hat{p}^2\right)_W = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)\left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)\left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right) = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)p^2 = xp^2 + \mathrm{i}p$$

$$\left(\hat{p}^2\hat{x}\right)_W - \left(\hat{x}\hat{p}^2\right)_W = -2\mathrm{i}p$$

$$\frac{d}{dt}(\hat{x})_W = \frac{p}{m} \qquad \frac{d}{dt}(\hat{p})_W = 0$$

*(trivial)* $p^3 - p^3 = 0$

*Quantum equations*
*=*
*Classical equations*

**!**

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Question:** So when is an evolution "truly quantum"?

*Evolution of Observable*

$$\frac{d}{dt}(\hat{p}^3)_W = \mathrm{i}\left[(\hat{H}\hat{p}^3)_W - (\hat{p}^3\hat{H})_W\right]$$

- **Example Hamiltonian:** $\hat{H} = \frac{\hat{p}^2}{2m} + V\hat{x}^3$

- Kinetic energy part: $\frac{d}{dt}(\hat{p}^3)_W = \frac{\mathrm{i}}{2m}\left[(\hat{p}^2\hat{p}^3)_W - (\hat{p}^3\hat{p}^2)_W\right]$ *(trivial)*

- Potential energy part:

$$\begin{aligned}
(\hat{x}^3\hat{p}^3)_W &= \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)^3 \left(p - \cancel{\frac{\mathrm{i}}{2}\frac{\partial}{\partial x}}\right)^3 \\
&= \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)^2 \left(xp^3 + \frac{3\mathrm{i}}{2}p^2\right) \\
&= \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right) \left(x^2p^3 + 3\mathrm{i}p^2x - \frac{3}{2}p\right) \\
&= x^3p^3 + 3\mathrm{i}p^2x^2 - \frac{3}{2}px + \frac{3\mathrm{i}}{2}x^2p^2 - 3px - \frac{3\mathrm{i}}{4} = x^3p^3 + \frac{9\mathrm{i}}{2}x^2p^2 - \frac{9}{2}xp - \frac{3\mathrm{i}}{4}
\end{aligned}$$

$$(\hat{p}^3\hat{x}^3)_W = \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)^3 \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)^3 = x^3p^3 - \frac{9\mathrm{i}}{2}x^2p^2 - \frac{9}{2}xp + \frac{3\mathrm{i}}{4}$$

*flip x and p, real parts must be identical (observable is real), …*
*check signs of imaginary parts.*

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Question:** So when is an evolution "truly quantum"?

*Evolution of Observable*

$$\frac{d}{dt}(\hat{p}^3)_W = \mathrm{i}\left[(\hat{H}\hat{p}^3)_W - (\hat{p}^3\hat{H})_W\right]$$

- **Example Hamiltonian:** $\hat{H} = \frac{\hat{p}^2}{2m} + V\hat{x}^3$

- Kinetic energy part: $\frac{d}{dt}(\hat{p}^3)_W = \frac{\mathrm{i}}{2m}\left[(\hat{p}^2\hat{p}^3)_W - (\hat{p}^3\hat{p}^2)_W\right]$ *(trivial)*

- Potential energy part:

$$(\hat{x}^3\hat{p}^3)_W = \cancel{x^3p^3} + \frac{9\mathrm{i}}{2}x^2p^2 - \cancel{\frac{9}{2}xp} - \frac{3\mathrm{i}}{4} \qquad (\hat{p}^3\hat{x}^3)_W = \cancel{x^3p^3} - \frac{9\mathrm{i}}{2}x^2p^2 - \cancel{\frac{9}{2}xp} + \frac{3\mathrm{i}}{4}$$

$$\frac{d}{dt}(\hat{p}^3)_W = -9Vx^2p^2 + \frac{3}{2}V$$

- **Observation:** Instead, evolution of momentum $\frac{d}{dt}(\hat{p})_W = \mathrm{i}\left[(\hat{H}\hat{p})_W - (\hat{p}\hat{H})_W\right] = -3Vx^2$

*...since*

$$(\hat{x}^3\hat{p})_W = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)^3 p^3 = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)^2\left(xp + \frac{i}{2}\right) = \left(x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}\right)(x^2p + \mathrm{i}x) = x^3p + \frac{3\mathrm{i}}{2}x^2$$

$$(\hat{p}\hat{x}^3)_W = \left(p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}\right)x^3 = px^3 - \frac{3\mathrm{i}}{2}x^2$$

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Question:** So when is an evolution "truly quantum"?

*Evolution of Observable*

$$\frac{d}{dt}(\hat{p}^3)_W = \mathrm{i}\left[(\hat{H}\hat{p}^3)_W - (\hat{p}^3\hat{H})_W\right]$$

- **Example Hamiltonian:** $\hat{H} = \frac{\hat{p}^2}{2m} + V\hat{x}^3$

$$\frac{d}{dt}(\hat{p}^3)_W = -9Vx^2p^2 + \frac{3}{2}V \qquad \frac{d}{dt}p = \frac{d}{dt}(\hat{p})_W = -3Vx^2$$

- **This implies:** $\frac{dp^3}{dt} = 3p^2\frac{dp}{dt} = 3p^2(-3Vx^2) = -9Vx^2p^2$

*…thus:* $\frac{d}{dt}(\hat{p}^3)_W \neq \frac{dp^3}{dt}$

In contrast to a classical system:
The Weyl symbol of a general observable **does not necessarily factorize** into the Weyl symbols for $x$ and $p$

!

- In a classical system: $H(x,p) = \frac{p^2}{2m} + Vx^3 \qquad \{f,g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x}$

$$\dot{p} = \{p, H\} = -\frac{\partial H}{\partial x} = -3Vx^2 \qquad \frac{dp^3}{dt} = 3p^2\dot{p} = -9V^2x^2p^2$$

*…or equally* $\frac{dp^3}{dt} = \{p^3, H\} = -3p^2\frac{\partial H}{\partial x} = -9Vx^2p^2$

*(the Poisson bracket ensures the trivial factorization property)*

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Question:** So when is an evolution "truly quantum"?

*Evolution of Observable*

- **Example Hamiltonian:** $\hat{H} = \frac{\hat{p}^2}{2m} + V\hat{x}^3$

$$\frac{d}{dt}(\hat{p}^3)_W = \mathrm{i}\left[(\hat{H}\hat{p}^3)_W - (\hat{p}^3\hat{H})_W\right]$$

- **Summary:**

$$\frac{d}{dt}(\hat{p}^3)_W = \underbrace{-9Vx^2p^2}_{\textbf{Classical part}} + \underbrace{\frac{3}{2}V}_{\textbf{Quantum part}} \neq \frac{dp^3}{dt}$$

*Assuming that the Weyl symbol* $(\hat{p}^3)_W$ *would simply factorize, i.e.* $(\hat{p}^3)_W = (p)^3_W$

*would produce the* ***classical part*** *only!*

Making the approximation of neglecting the **quantum part** is the:
**Truncated Wigner approximation (TWA)**

*(…properly defined in below)*

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Moyal product** and **Moyal bracket**: *(for Weyl quantization, many particles)*

*The Weyl symbol of a product of operators can be written as "**Moyal product**"*

$\hbar \neq 1$

$$(\hat{A}\hat{B})_W = (\hat{A})_W \mathrm{e}^{-\mathrm{i}\hbar\mathbf{\Lambda}/2}(\hat{B})_W$$

$$\mathbf{\Lambda} = \sum_{i=1}^{N} \frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}$$

*(symplectic operator)*

- … meaning:

$$\exp\left[-\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)\right] = \sum_{\alpha=0}^{\infty}\frac{(-\mathrm{i}\hbar/2)^\alpha}{\alpha!}\left[\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)\right]^\alpha$$

*Proof lengthy (can use Bopp), see:* *A. Polkovnikov, Ann. Phys., 325, 1790 (2010)*

- Examples:

$$(\hat{x}_i\hat{p}_i)_W = x_i \exp\left[-\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}\right)\right]p_i$$

$$= x_i\left[1 - \frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\cancel{\frac{\overrightarrow{\partial}}{\partial x_i}} + 0\right)\right]p_i = x_i p_i - \frac{\mathrm{i}\hbar}{2}$$

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

- **Moyal product** and **Moyal bracket**: *(for Weyl quantization, many particles)*

$\hbar \neq 1$

$$(\hat{A}\hat{B})_W = (\hat{A})_W \mathrm{e}^{-\mathrm{i}\hbar\mathbf{\Lambda}/2}(\hat{B})_W \qquad \mathbf{\Lambda} = \sum_{i=1}^{N} \frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}$$

- Switching: $\hat{A} \leftrightarrow \hat{B} \quad \Leftrightarrow \quad \sum_{i=1}^{N} \frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i} \leftrightarrow \sum_{i=1}^{N} \frac{\overrightarrow{\partial}}{\partial x_i}\frac{\overleftarrow{\partial}}{\partial p_i} - \frac{\overrightarrow{\partial}}{\partial p_i}\frac{\overleftarrow{\partial}}{\partial x_i} \quad \Leftrightarrow \quad \mathbf{\Lambda} \to -\mathbf{\Lambda}$

*…therefore* $(\hat{B}\hat{A})_W = (\hat{A})_W \mathrm{e}^{\mathrm{i}\hbar\mathbf{\Lambda}/2}(\hat{B})_W$

- Commutator:

$$(\hat{A}\hat{B})_W - (\hat{B}\hat{A})_W = (\hat{A})_W \mathrm{e}^{-\mathrm{i}\hbar\mathbf{\Lambda}/2}(\hat{B})_W - (\hat{A})_W \mathrm{e}^{\mathrm{i}\hbar\mathbf{\Lambda}/2}(\hat{B})_W$$
$$= 2\mathrm{i}(\hat{A})_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right](\hat{B})_W$$

*This is motivates to define a phase space equivalent of the commutator, known as **Moyal bracket**:*

$$\{O_W, O'_W\}_{\mathrm{MB}} \equiv \frac{2}{\hbar} O_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right] O'_W = \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\{O_W, O'_W\}\right]$$

*Poisson bracket*

- Heisenberg equation of motion on phase space then simply reads:

$$\frac{d}{dt}\hat{O} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{O}] \qquad \frac{d}{dt}O_W = -\frac{2}{\hbar}O_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right] H_W = -\{H_W, O_W\}_{\mathrm{MB}} = \{O_W, H_W\}_{\mathrm{MB}}$$

# Lecture 2.2 - Time evolution - The truncated Wigner approximation (TWA)

*(for Weyl quantization, many particles)*

*This is motivates to define a phase space equivalent of the commutator, known as **Moyal bracket**:*

$$\{O_W, O'_W\}_{\mathrm{MB}} \equiv \frac{2}{\hbar} O_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right] O'_W = \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\{O_W, O'_W\}\right]$$

$$\{f, g\} = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i}$$

*Poisson bracket*

- This gives a beautiful connection between quantum and classical:

| **Classical** | **Quantum** |
|---|---|
| $\frac{df}{dt} = \{f, H\}$ | $\frac{d}{dt}O_W = \{O_W, H_W\}_{\mathrm{MB}}$ |

*In the classical limit:* $\hbar \to 0$

$$\{O_W, H_W\}_{\mathrm{MB}} = \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\{O_W, H_W\}\right] \approx \frac{2}{\hbar}\left[0 + \frac{\hbar}{2}\{O_W, H_W\} - \frac{1}{3!}\frac{\hbar^3}{2^3}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^5}{4!2^5}\right)\right]$$

$$\frac{d}{dt}O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

Keeping the leading order term is the **TWA**

# Lecture 2 - Time evolution - The truncated Wigner approximation (TWA)

- **The TWA** *(for Weyl quantization, many particles)*

**Classical**

$$\frac{df}{dt} = \{f, H\}$$

**Quantum**

$$\frac{d}{dt}O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

$$\{f, g\} = \sum_{i=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i}$$

*Poisson bracket*

$$\frac{d}{dt}O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

Keeping the leading order term is the **TWA**

- **Remark:** This is still more than classical! Because we describe the evolution not with variables, but with Weyl symbols, which are phase-space descriptions of quantum operators.

- **Remark:** The Poisson bracket evolution ensures that Weyl symbols remain factorized, enforcing this factorization is equivalent to the TWA. This is reminiscent of a mean-field product state ansatz, but TWA is still more.

- **Remark:** The next order term involves third derivatives of the Weyl symbols for the observable and for the Hamiltonian. If those vanish, then the TWA is exact! This is e.g. the case for quadratic systems! **Only e.g. with cubic terms as in our previous examples, the TWA is not exact.**

# Lecture 2 - Plan for today

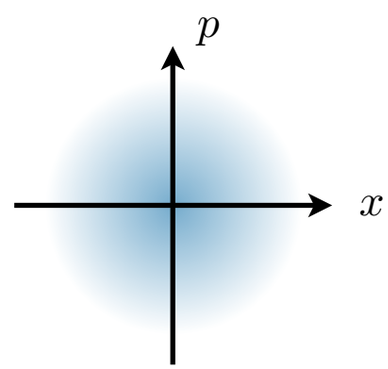
**Today mostly: Theory lecture style**

- **Part 2.1:** Describing quantum mechanics on phase space: The fundamentals

*For simplicity: Focus on particle in 1D*

$$\hat{O} = \int dx dp \, O_W(x,p) \hat{A}(x,p)$$

$$O_W(x,p) = \frac{1}{\mathcal{N}} \mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$



- **Part 2.2:** Time-evolution and the truncated Wigner approximation (TWA)

**Classical**

$$\frac{df}{dt} = \{f, H\}$$

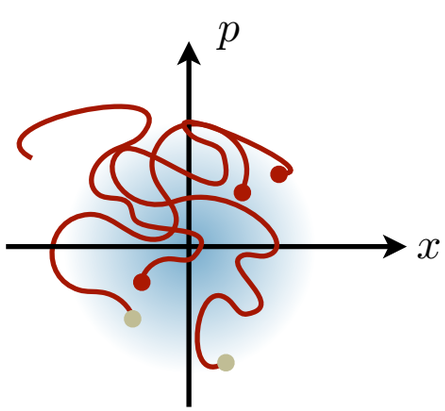
**Quantum**

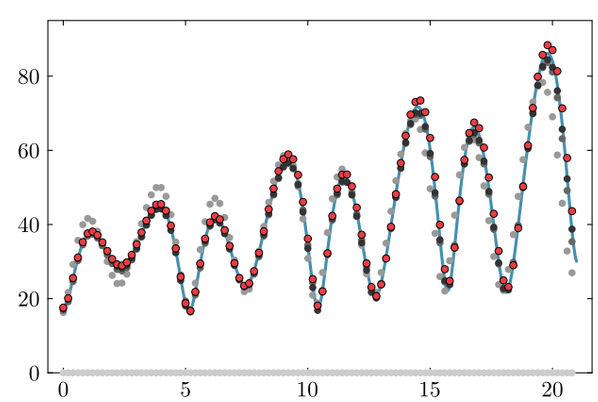
$$\frac{d}{dt} O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

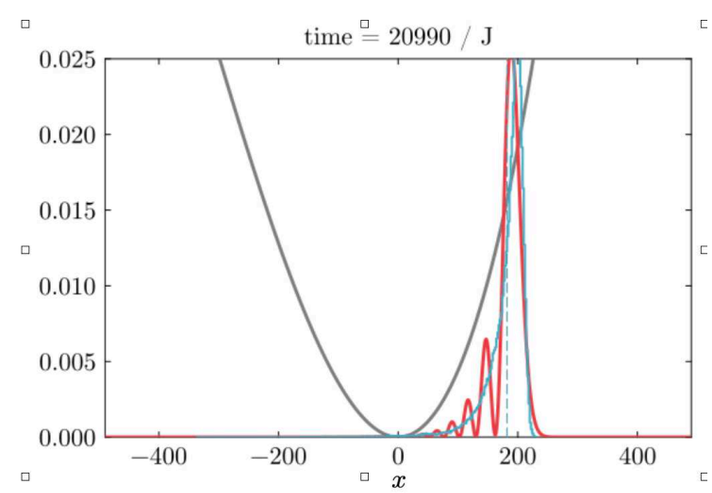
**TWA**

$$\frac{d}{dt} O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

- **Part 2.3:** The TWA as numerical method



# Lecture 2.3 - TWA as numerical method

- **Summary Phase space and TWA:**
- Good phase space space representation defined by proper phase point operators. Then any hermitian observable described by a proper Wigner function:

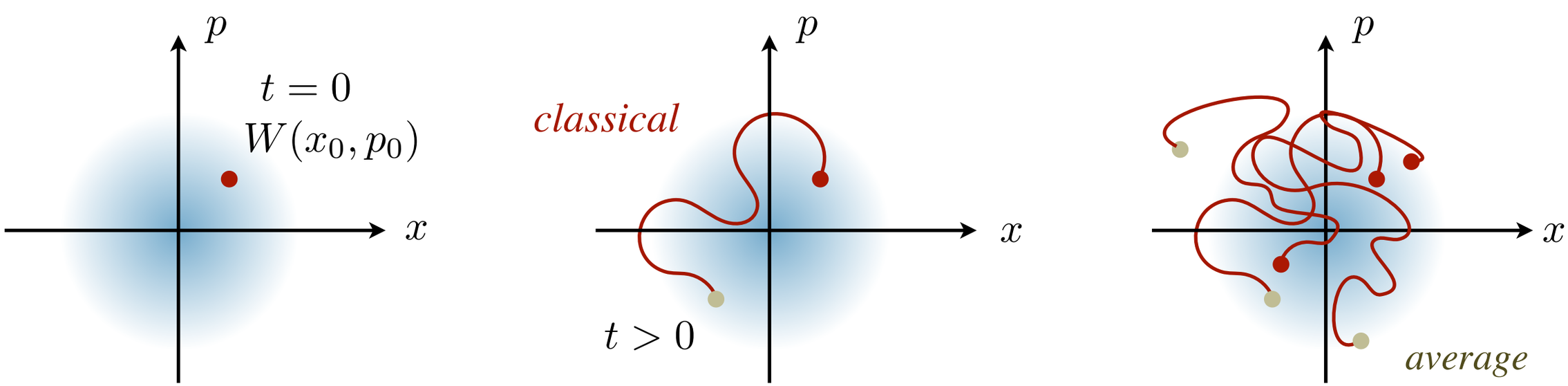
$$\langle \hat{O}_{x^n p^m} \rangle = \int dx\, dp\, W(x,p) x^n p^m$$

- In the **TWA** ensures that only the evolution of the Weyl symbols for x and p needs to be computed. More complex Weyl symbols will always factorize:

$$\frac{d}{dt} O_W \approx \{O_W, H_W\} \qquad \Leftrightarrow \qquad (\hat{O}_{x^n p^m})_W(t) = (\hat{x})^n_W(t)(\hat{p})^m_W(t)$$

- **Key idea:** Monte-Carlo sampling of the WF

$$\langle \hat{O}_{x^n p^m} \rangle(t) \approx \int dx_0\, dp_0\, W(x_0,p_0) x^n_{\mathrm{cl}}(t) p_{\mathrm{cl}}(t)^m$$



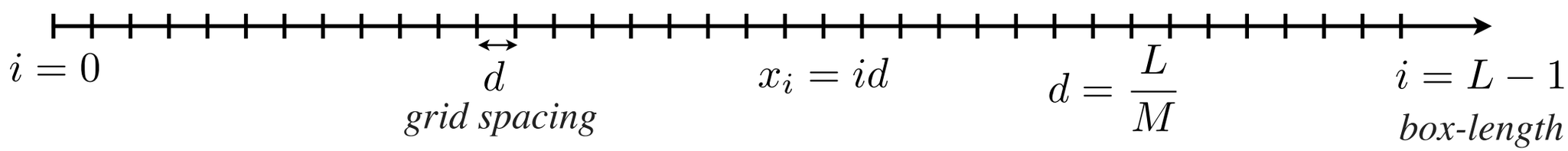

- **Remark:** This is of course only possible if the initial state Wigner function can be sampled, which means: No negative values and product state in case of a many-body system.

# Lecture 2.3 - Test case: Exact diagonalization for a 1D particle

- For a continuous space, we need to introduce a discretization: $\hat{H} = \frac{\hat{p}^2}{2m} + \int dx\, V(x)\, |x\rangle \langle x|$

$$\frac{\hat{p}^2}{2m}\psi(x) = -\frac{1}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{1}{2m}\lim_{d\to 0}\frac{\psi(x+d) - 2\psi(x) + \psi(x-d)}{d^2}$$

$M \gg 1$ *grid points*




- Matrix for kinetic energy:

*... if we want periodic boundary conditions*

$$\frac{\hat{p}^2}{2m} \approx \frac{1}{2md^2}\begin{pmatrix} 0 & -1 & & & & -1 \\ -1 & 0 & -1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -1 & 0 & -1 & \\ -1 & & & -1 & 0 & -1 \end{pmatrix} + \text{const.} \qquad \text{... acting on ...} \qquad \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{M-1} \\ \psi_M \end{pmatrix}$$

- **Note:** Kinetic energy is just nearest-neighbor hopping on a grid with amplitude $J = \frac{1}{2md^2}$
- Indeed, the physics in continuous space is identical to lattice physics $\hat{H} = -J\sum_i \left(|i\rangle\langle i+1| + |i+1\rangle\langle i|\right)$
- The external potential are diagonal elements $\int dx\, V(x)\, |x\rangle\langle x| \approx \text{diag}[V(x_1), V(x_2), \ldots, V(x_M)]$

# Lecture 2.3 - 1D particle in anharmonic potential - ED

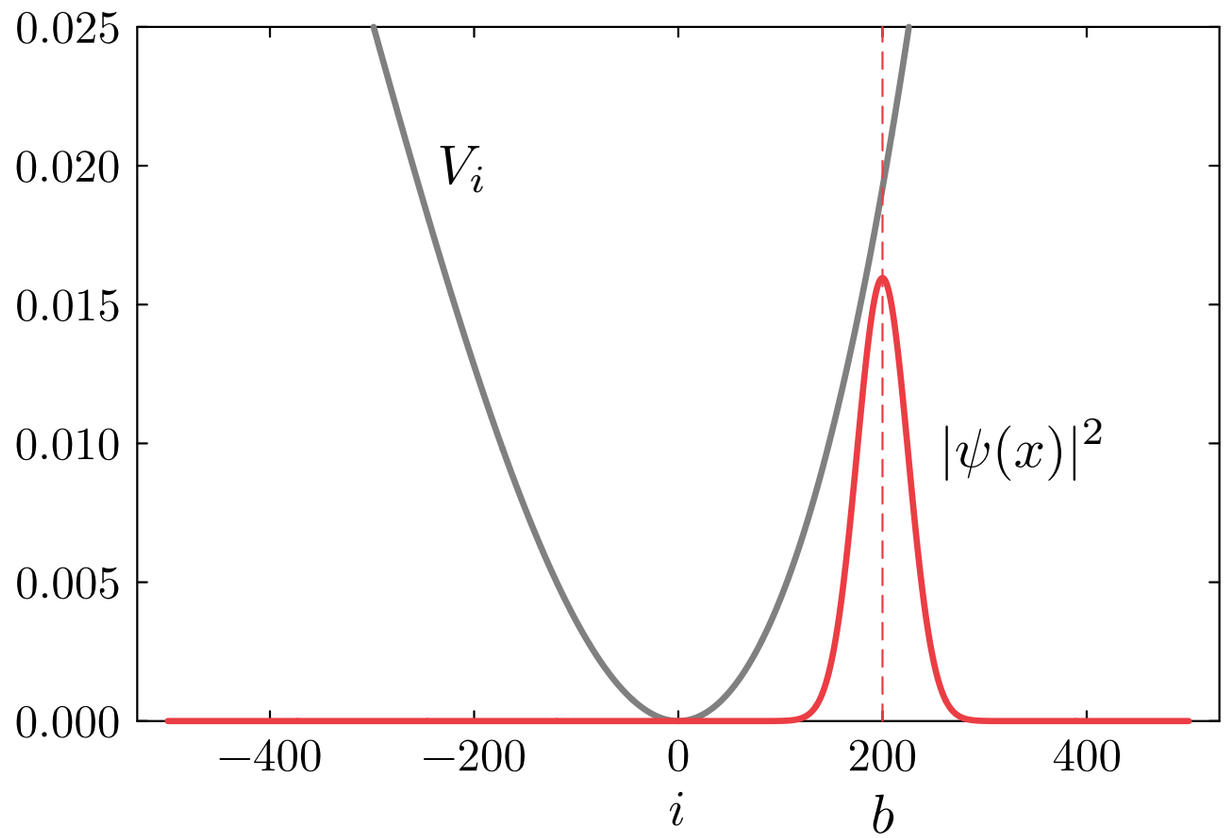
*Box:*

```
Nh = 500
N = 2 * Nh + 1
xs = -Nh:Nh
```

$d \equiv 1$

*Initial state:* $\psi(x) \propto \exp\left[-\frac{(x-b)^2}{2a^2}\right]$

```
a = 25
b = 200
psi = exp.(-((xs .- b).^2 ./ (2 * a^2)))
psi./= norm(psi)
```




*Potential:*

```
om2 =0.1/Nh^2
om3 = 0.05/Nh^3
Vx = om2 .* (xs) .^ 2 + om3 .* (xs) .^ 3
```

*Full Hamiltonian:* $J = \frac{1}{2md^2} \equiv 1$

```
H = sparse(SymTridiagonal(Vx, -J .* ones(N-1)))
```

- Time-step (here with Krylov)

```
psi, info = exponentiate(H, -1im * dt, psi)
```

*Expectation values:*

$\langle x \rangle$

```
mx = sum(xs .* abs.(psi).^2)
```

$\langle x^2 \rangle$

```
mx2 = sum(xs .^2 .* abs.(psi).^2)
```

*Momentum space:*
*Discrete Fourier transform*

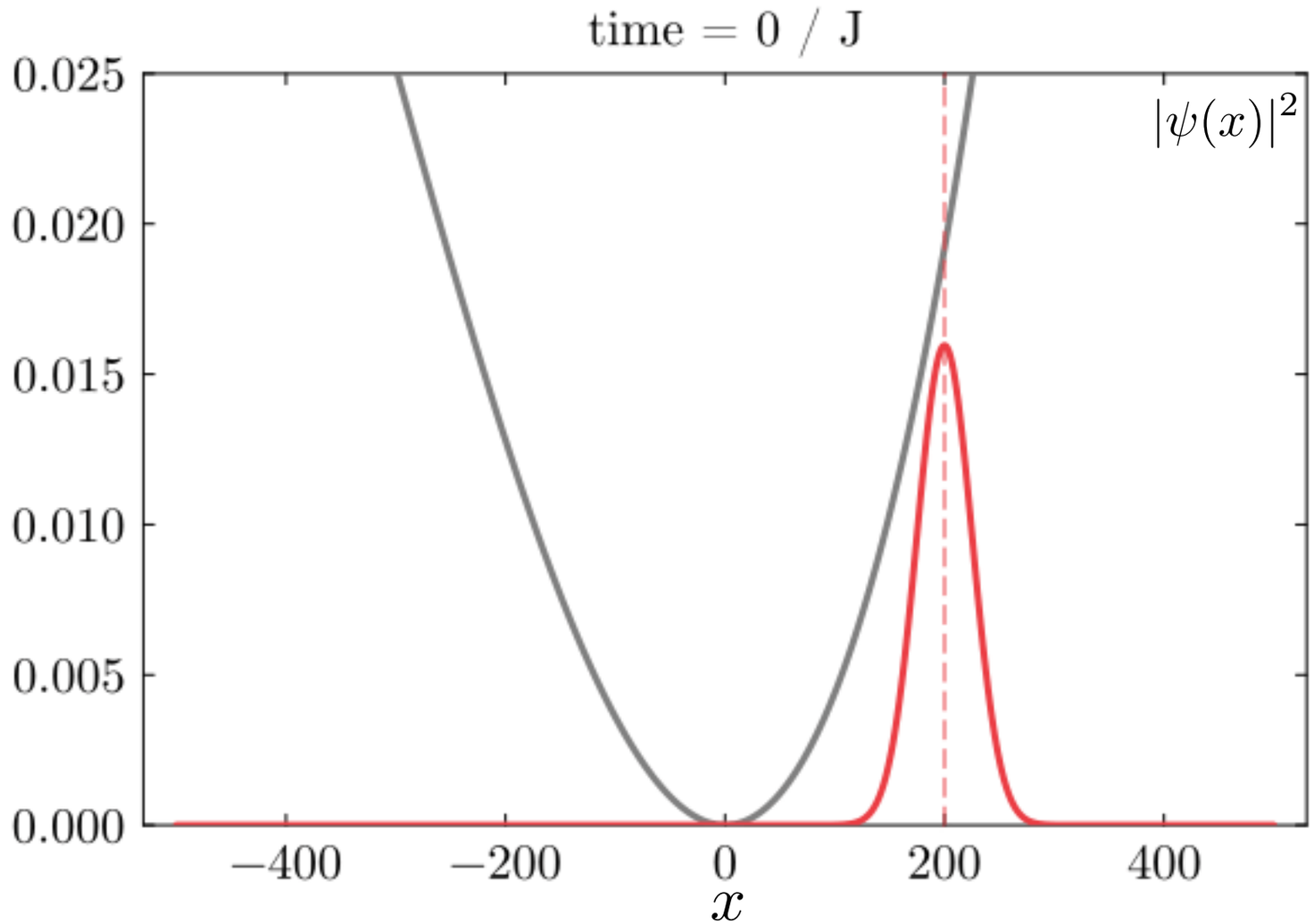
```
using FFTW
ppsi = fftshift(fft(psi))
ppsi ./= norm(ppsi)
```

# Lecture 2.3 - 1D particle in anharmonic potential - ED

- Full evolution:

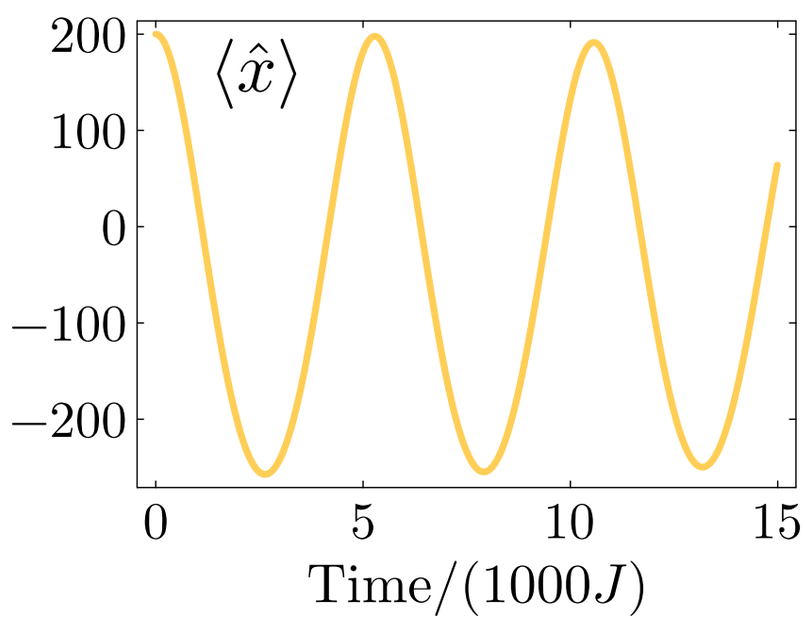
$$d \equiv 1$$

$$J = \frac{1}{2md^2} \equiv 1$$

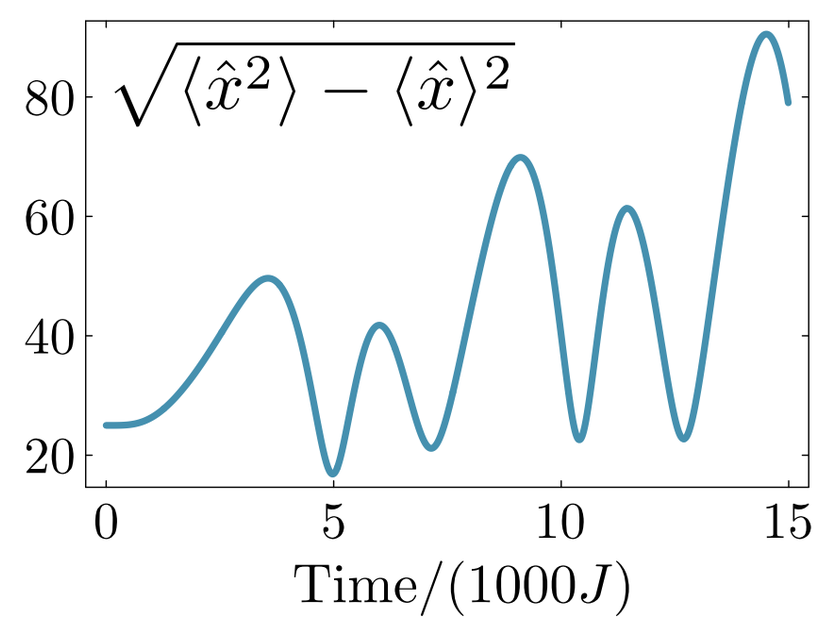



- Observables:

*Position*




*Width*



# Lecture 2.3 - 1D particle in anharmonic potential - TWA

- Classical equations of motion for each trajectory $\dot{x} = \frac{p}{m}$ $\quad \dot{p} = -V'(x)$

$$d \equiv 1 \qquad J = \frac{1}{2md^2} \equiv 1 \qquad m = \frac{1}{2}$$

$$V(x) = \omega_2 x^2 + \omega_3 x^3$$

$$V'(x) = 2\omega_2 x + 3\omega_3 x^2$$

- Ordinary differential equation (non-linear) $\dot{\mathbf{y}}(t) = f(\mathbf{y}(t))$

$$\mathbf{y} = \begin{pmatrix} x \\ p \end{pmatrix} \qquad f(\mathbf{y}(t)) = \begin{pmatrix} 2y_2 \\ -2\omega_2 y_1 - 3\omega_3 y_1^2 \end{pmatrix}$$

- Will discuss ODE solvers next time, need to numerically implement the function $f$

```
f(y) = [2 * y[2]; -2 * om2 * y[1] - 3 * om2 * y[1]^2]
```

- For each trajectory: Sample from the Wigner function $W(x,p) = \frac{1}{\pi} \mathrm{e}^{-(x-b)^2/a^2 - a^2 p^2}$

- Sample from a normal distribution $\mathcal{N}(\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}}$

*seed for pseudo random number generator*

```
rng = MersenneTwister(1907)
sample = mu + sigma * randn(rng)
```

$\mathcal{N}(0,1)$

- Samples from Wigner function

```
a = 25
b = 200
x = b + a * randn(rng) / sqrt(2)
p = randn(rng) / (a * sqrt(2))
```

# Lecture 2.3 - 1D particle in anharmonic potential - TWA

- Advantage of TWA: All trajectories independent - ideal parallelization!
- In practice: Still useful to group trajectories

```
a = 25
b = 200
nt = 1000
y = [b .+ a .* randn(rng, nt) / sqrt(2);
    randn(rng, nt) ./ (a * sqrt(2))]
```

$$\mathbf{Y} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n_T} \\ p_1 \\ p_2 \\ \vdots \\ p_{n_T} \end{pmatrix}$$

```
function f(y)
    yout =
    [2 .* y[(nt+1):end];
    -2 .* om2 .* y[1:nt] .- 3 .* om3 .* y[1:nt] .^2]
    return yout
end
```

$$f(\mathbf{y}(t)) = \begin{pmatrix} 2y_2 \\ -2\omega_2 y_1 - 3\omega_3 y_1^2 \end{pmatrix}$$

- For expectation values now

```
using Statistics
```

$\langle \hat{x} \rangle$ `mean(y[1:nt])`

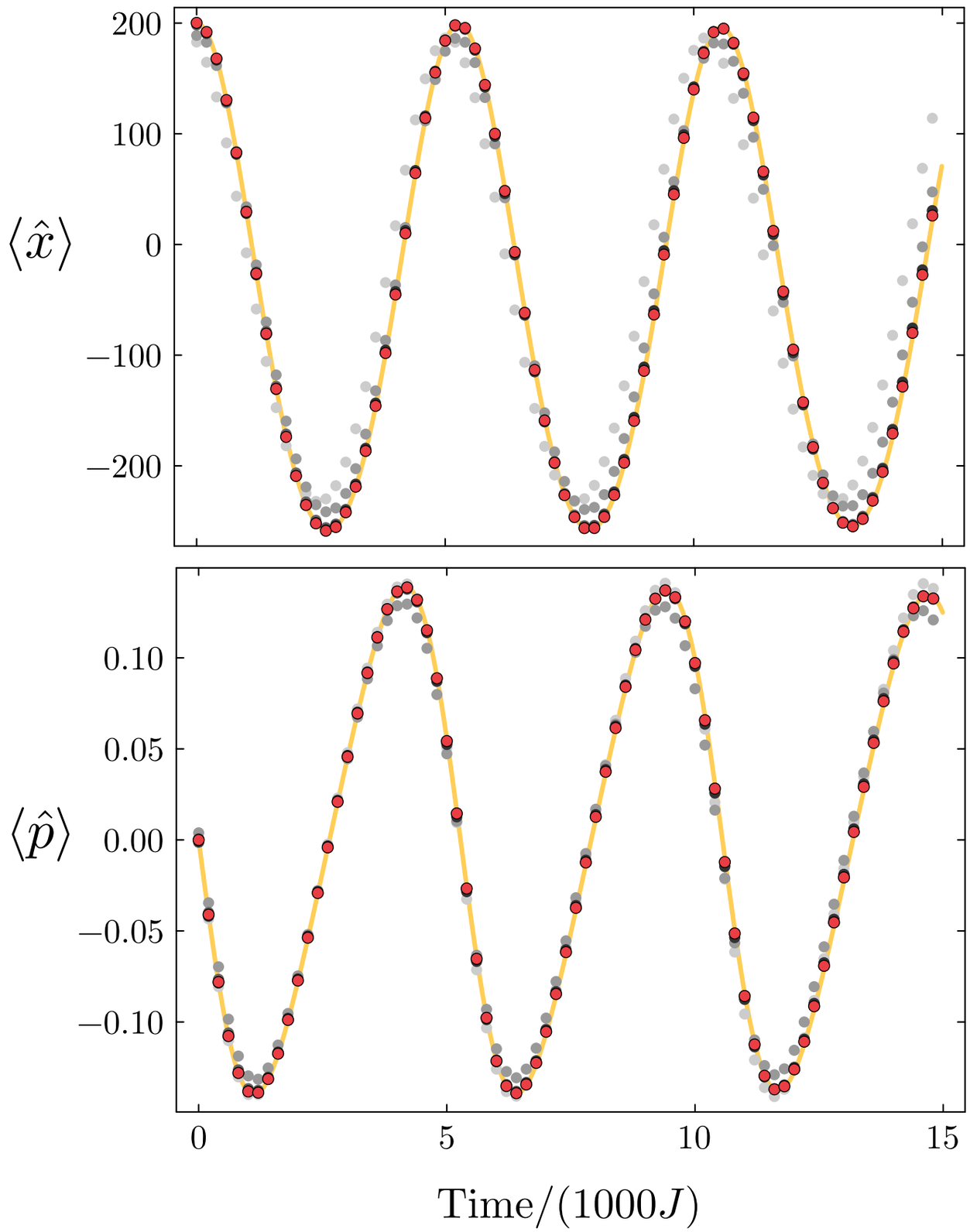
$\langle \hat{p} \rangle$ `mean(y[(nt+1):end].^2)`

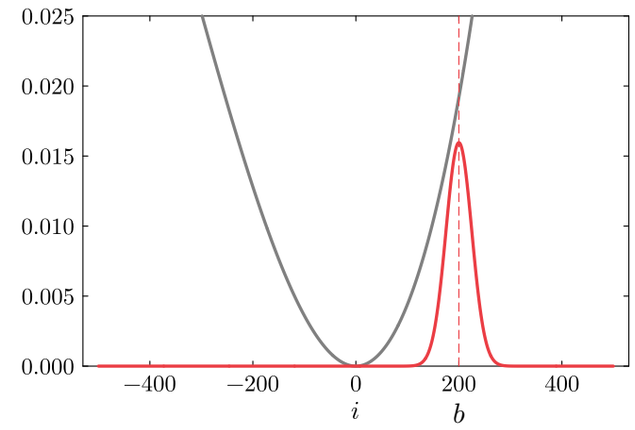
$\langle \hat{x}^2 \rangle$ `mean(y[1:nt].^2)`

$\langle \hat{p}^2 \rangle$ `mean(y[(nt+1):end])`

# Lecture 2.3 - 1D particle in anharmonic potential - ED vs. TWA

- Mean position
- Mean momentum



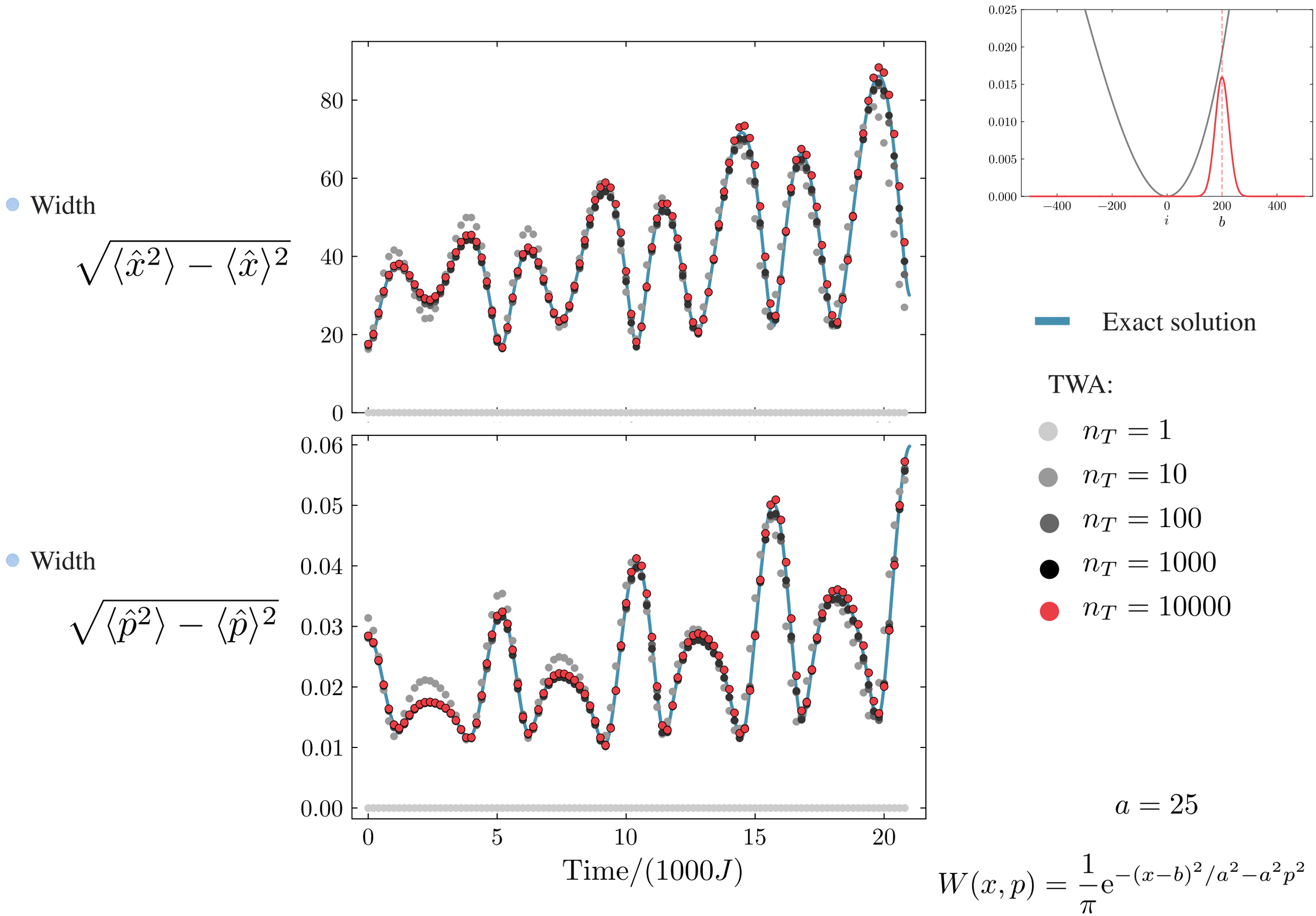




Exact solution

TWA:

- $n_T = 1$
- $n_T = 10$
- $n_T = 100$
- $n_T = 1000$
- $n_T = 10000$

# Lecture 2.3 - 1D particle in anharmonic potential - ED vs. TWA



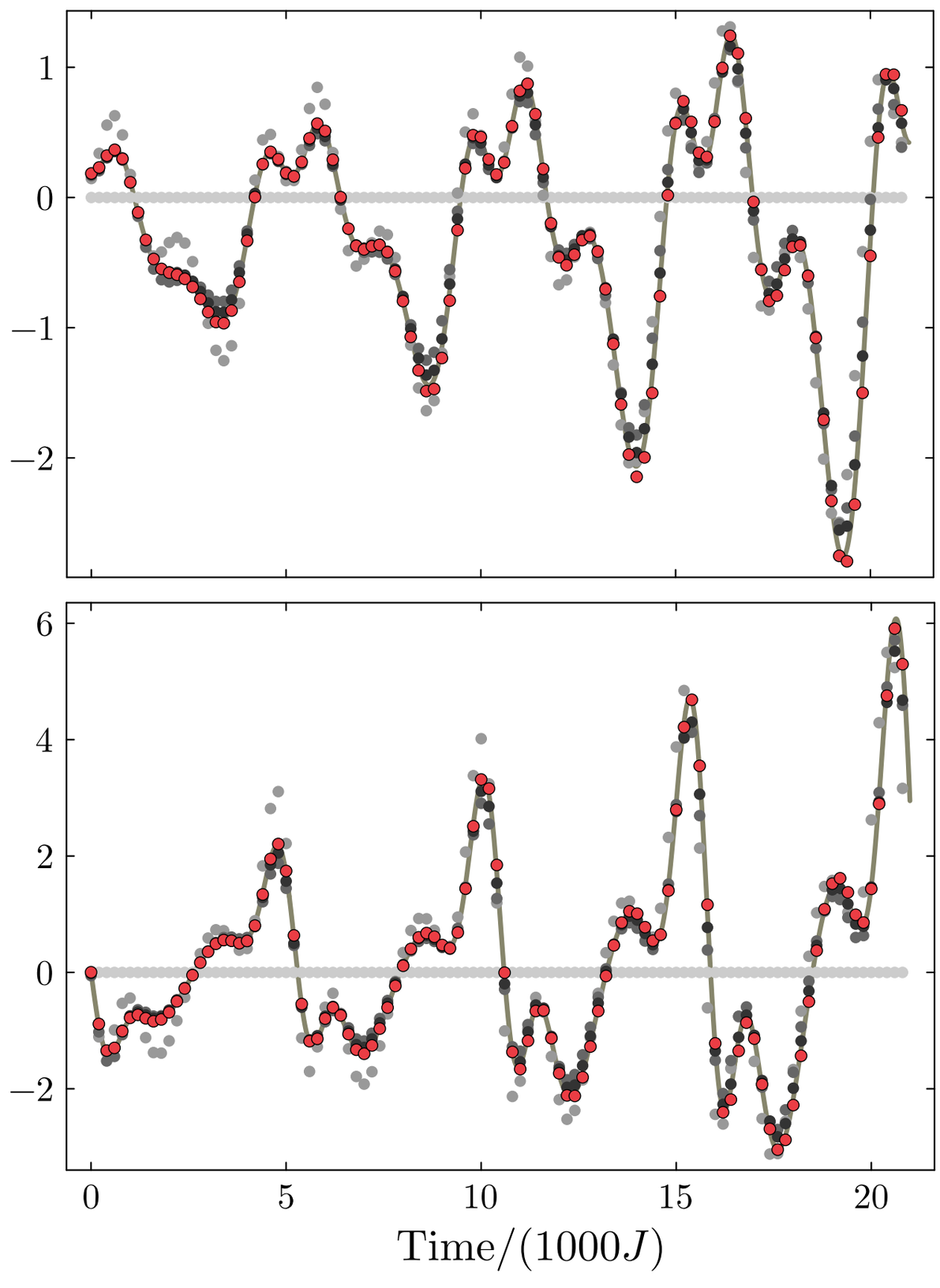
# Lecture 2.3 - 1D particle in anharmonic potential - ED vs. TWA

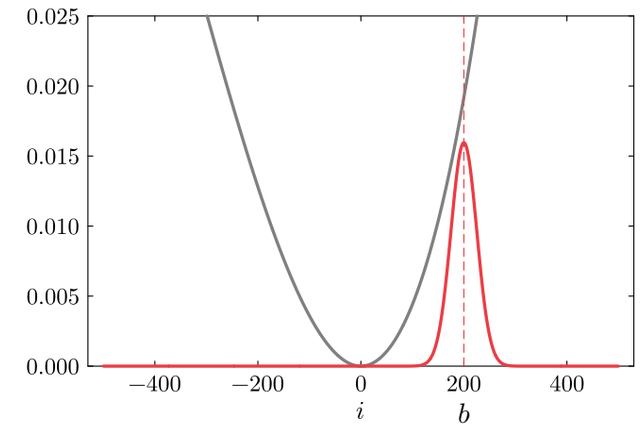
- 3rd moment

$$(\langle \hat{x}^3 \rangle - \langle \hat{x} \rangle^3)/10^6$$

- 3rd moment

$$(\langle \hat{p}^3 \rangle - \langle \hat{p} \rangle^3)\, 10^4$$




Exact solution

TWA:

- $n_T = 1$
- $n_T = 10$
- $n_T = 100$
- $n_T = 1000$
- $n_T = 10000$

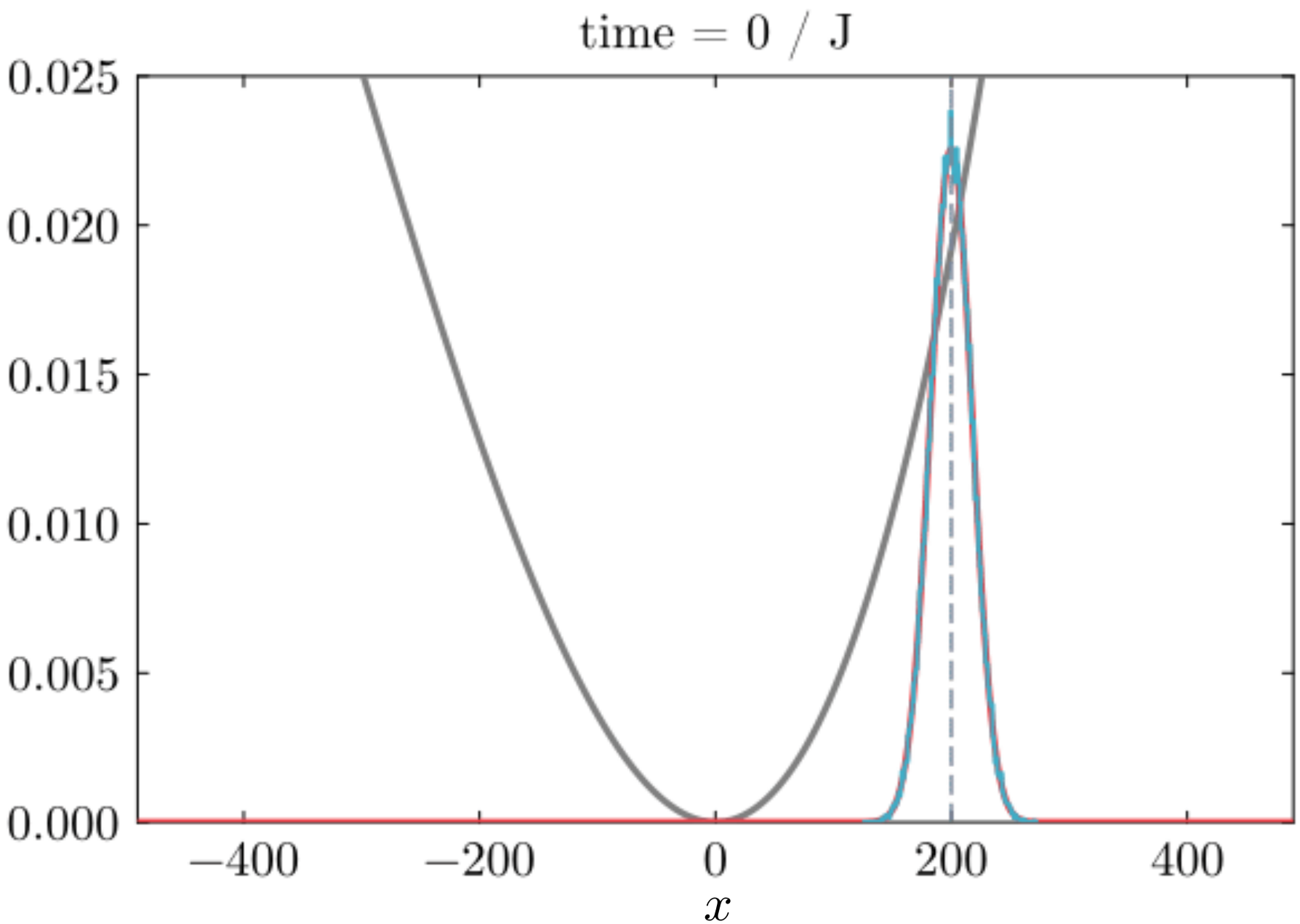
- … anharmonicity is quite small, need to go to still higher moments or longer times to see differences.

# Lecture 2.3 - 1D particle in anharmonic potential - ED vs. TWA

- Evolution of full distribution (*histogram with bins*)

$p(x)$ $|\psi(x)|^2$ Exact solution

$n_T = 10^5$



# Lecture 2 - Recap

- We introduced the phase space description of quantum mechanics.

**Hilbert space** $\Longleftrightarrow$ **Phase space**

$$\hat{O} = \int dx dp\, O_W(x,p)\hat{A}(x,p)$$

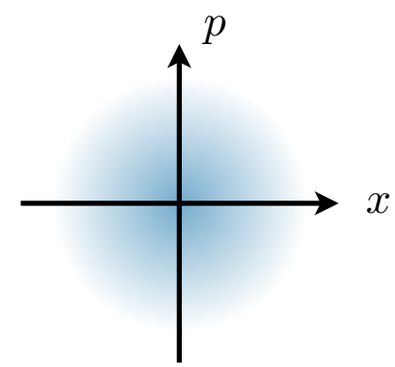
$$O_W(x,p) = \frac{1}{\mathcal{N}} \mathrm{tr}\left[\hat{A}(x,p)\hat{O}\right]$$

*Bopp representation*

$$\hat{x} \to x + \frac{\mathrm{i}}{2}\frac{\partial}{\partial p}$$
$$\hat{p} \to p - \frac{\mathrm{i}}{2}\frac{\partial}{\partial x}$$

- Instead of using matrices on Hilbert space, QM can described by functions of phase space variable (Weyl symbols)
- The transformation can be described by phase-point operators that are **normalized** and **orthogonal**
- The Weyl symbol of the density matrix is the **Wigner function**

*A quasi-probability distribution to describe any quantum state. It can have negative values!*




$$W(x,p) = \frac{1}{\pi}\mathrm{e}^{-x^2/a^2 - a^2p^2}$$

- Useful alternative picture to look at quantum states!
- Dynamics of Weyl symbols is described by Moyal brackets *(equivalent to a commutator on phase space)*

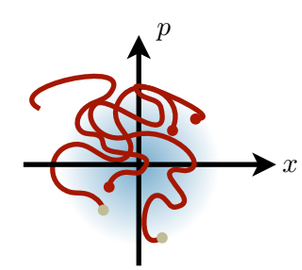
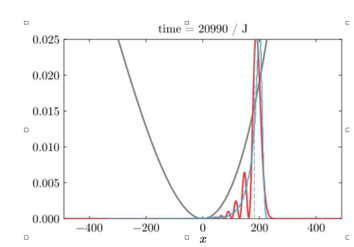
$$\frac{d}{dt}O_W = \{O_W, H_W\}_{\mathrm{MB}}$$

$$\{O_W, O'_W\}_{\mathrm{MB}} \equiv \frac{2}{\hbar} O_W \sin\left[\frac{\hbar}{2}\mathbf{\Lambda}\right] O'_W$$

- Expansion of the Moyal bracket for $\frac{\hbar}{2} \to 0$ … leads to the truncated Wigner approximation (**TWA**)

$$\frac{d}{dt}O_W \approx \{O_W, H_W\} - \frac{\hbar^2}{24}\{O_W, H_W\}^3 + \mathcal{O}\left(\frac{\hbar^4}{4!2^4}\right)$$

- TWA implies classical equations for the Weyl symbols, which means that Weyl symbols remain factorized ad all times

$$(\hat{O}_{x^n p^m})_W(t) = (\hat{x})^n_W(t)(\hat{p})^m_W(t)$$

- The TWA is useful for simulating dynamics beyond classical (beyond mean-field): Sample trajectories from (positive) Wigner functions and simulate each trajectory classically. This is exact as long as only quadratic terms are in the Hamiltonian. We tested the concept with anharmonic oscillator evolution.