Exploring Phase-Space methods and beyond for tunneling

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Motivations : SMF and inspired techniques

SMF → simple beyond mean-field method

S. Ayik and Y. Abe, Phys. Rev. C - Nucl. Phys. **64**, 246091 (2001).

Motivations : SMF and inspired techniques

SMF $\rightarrow$ simple beyond mean-field method

Mean-Field: $\rho(t_0)$ $\rightarrow$ $\rho(t)$ 1 “classical” trajectories

SMF: $\rho^{(n)}(t_0)$ $\rightarrow$ $\overline{\rho^{(n)}(t)}$ n “classical” trajectories

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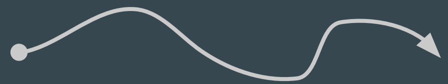
Mean-Field: $\rho(t_0)$  $\rho(t)$ 1 “classical” trajectories

SMF: $\rho^{(n)}(t_0)$  $\overline{\rho^{(n)}(t)}$ n “classical” trajectories

Mimic *initial* quantum moments with random numbers

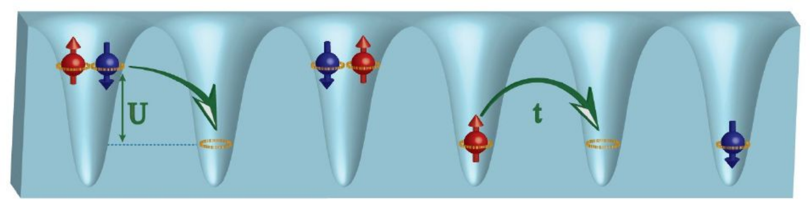
$$\overline{\delta\rho^{(n)}(t_0)} = 0$$

$$\overline{\delta\rho^{(n)}_{ij}(t_0)\delta\rho^{(n)}_{kl}(t_0)} = \frac{1}{2}\delta_{il}\delta_{jk}[n_i(1-n_k)+n_k(1-n_i)]$$

A priori Gaussian distribution

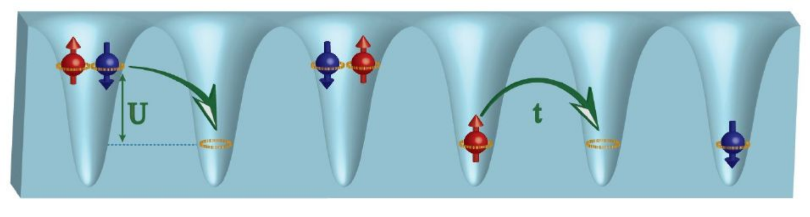
S. Ayik and Y. Abe, Phys. Rev. C - Nucl. Phys. **64**, 246091 (2001).

SMF : an illustration



Hubbard model: electrons hopping from sites to sites

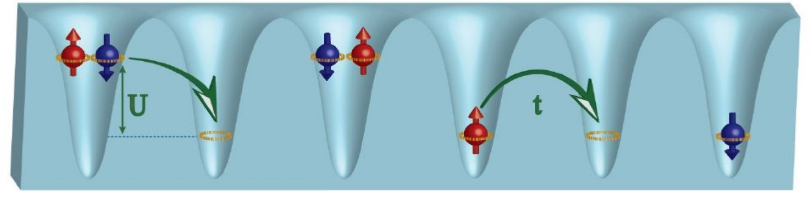
SMF : an illustration



Hubbard model: electrons hopping from sites to sites

$$\hat{H} = -J\sum_{i,\sigma}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i+1\sigma} + \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i-1\sigma}\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

SMF : an illustration



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a) 4 particles

b) 8 particles

$$i\hbar\partial_t\rho^{(n)} = \left[h_{\mathrm{MF}}\left[\rho^{(n)}\right], \rho^{(n)}\right]$$

$\rho(t_0)$  $\rho(t)$

$\rho^{(n)}(t_0)$ $\overline{\rho^{(n)}(t)}$

SMF : an illustration

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a) 4 particles
b) 8 particles

Exact (Schrödinger)

Mean-Field

SMF

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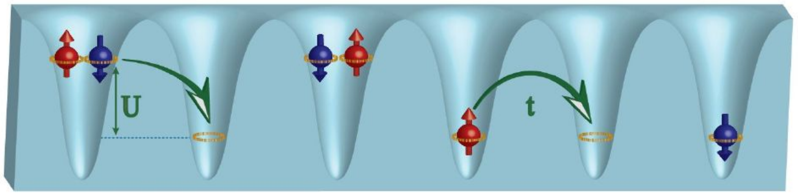
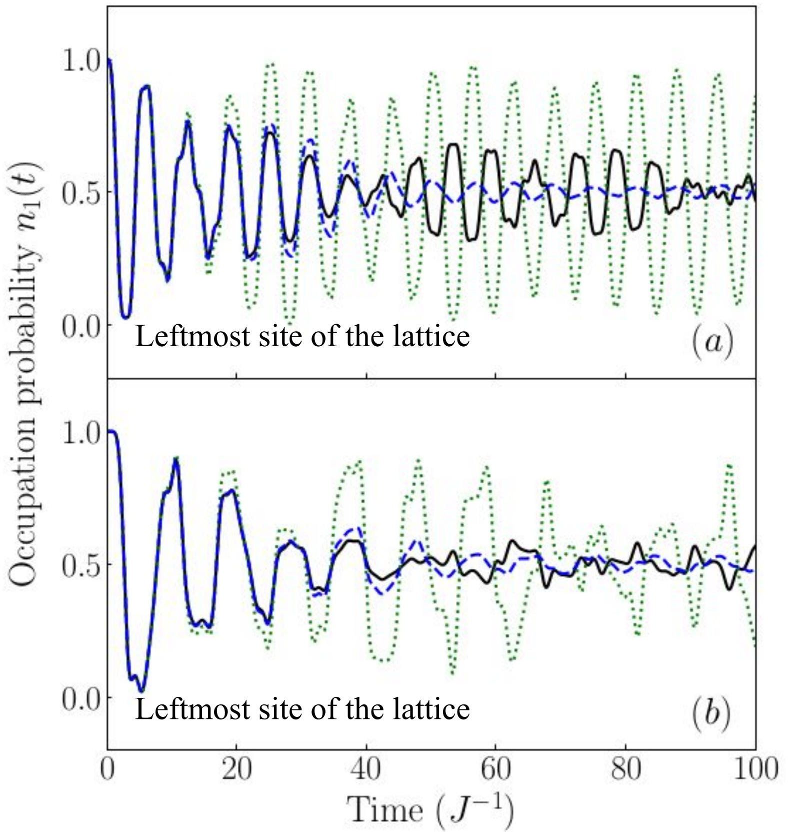
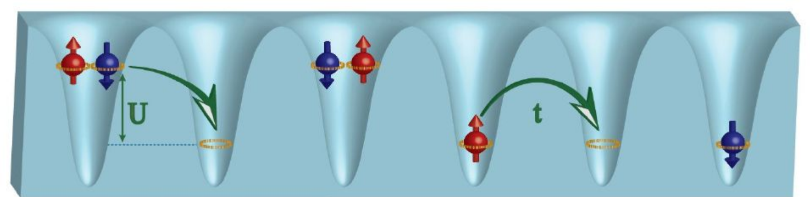




A hybrid method ? HPS

Add new correlations with a coupling to a BBGKY style hierarchy



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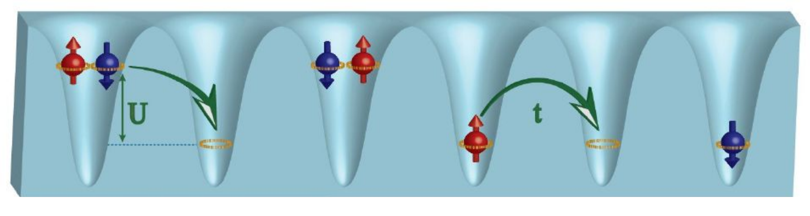
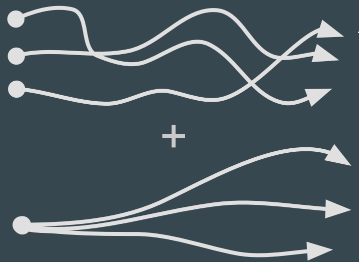


Add new correlations with a coupling to a BBGKY style hierarchy

$\rho^{(n)}(t_0)$ → $\overline{\rho^{(n)}(t)}$



$C_{12}(t_0)$ → $\overline{C_{12}^{(n)}(t)}$

$$i\hbar\partial_t \rho^{(n)} = \left[h_{\mathrm{MF}}\left[\rho^{(n)}\right], \rho^{(n)}\right]$$

$$i\hbar\partial_t C_{12}^{(n)} = \left[h_{\mathrm{MF}}\left[\rho_1^{(n)}\right] + h_{\mathrm{MF}}\left[\rho_2^{(n)}\right], C_{12}^{(n)}\right] + B_{12}\left[\rho^{(n)}\right]$$

Born term (BBGKY)

T. Czuba, D. Lacroix, D. Regnier, I. Ulgen, and B. Yilmaz, Eur. Phys. J. A 56, (2020).

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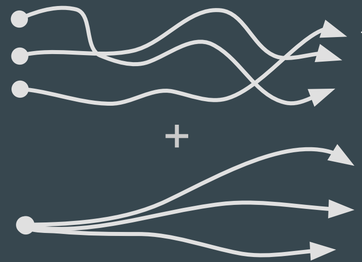
Add new correlations with a coupling to a BBGKY style hierarchy

$\rho^{(n)}(t_0)$



$\overline{\rho^{(n)}(t)}$

+

$C_{12}(t_0)$

$\overline{C_{12}^{(n)}(t)}$

HPS

$$i\hbar\partial_t\rho^{(n)} = \left[h_{\rm MF}\left[\rho^{(n)}\right], \rho^{(n)}\right]$$

$$i\hbar\partial_t C_{12}^{(n)} = \left[h_{\rm MF}\left[\rho_1^{(n)}\right] + h_{\rm MF}\left[\rho_2^{(n)}\right], C_{12}^{(n)}\right] + B_{12}\left[\rho^{(n)}\right]$$

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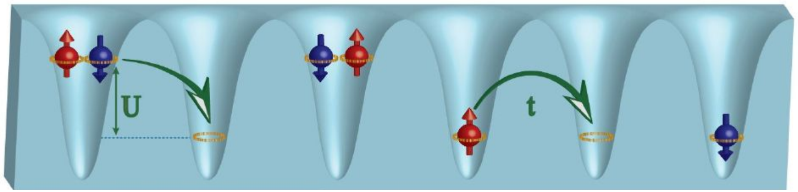
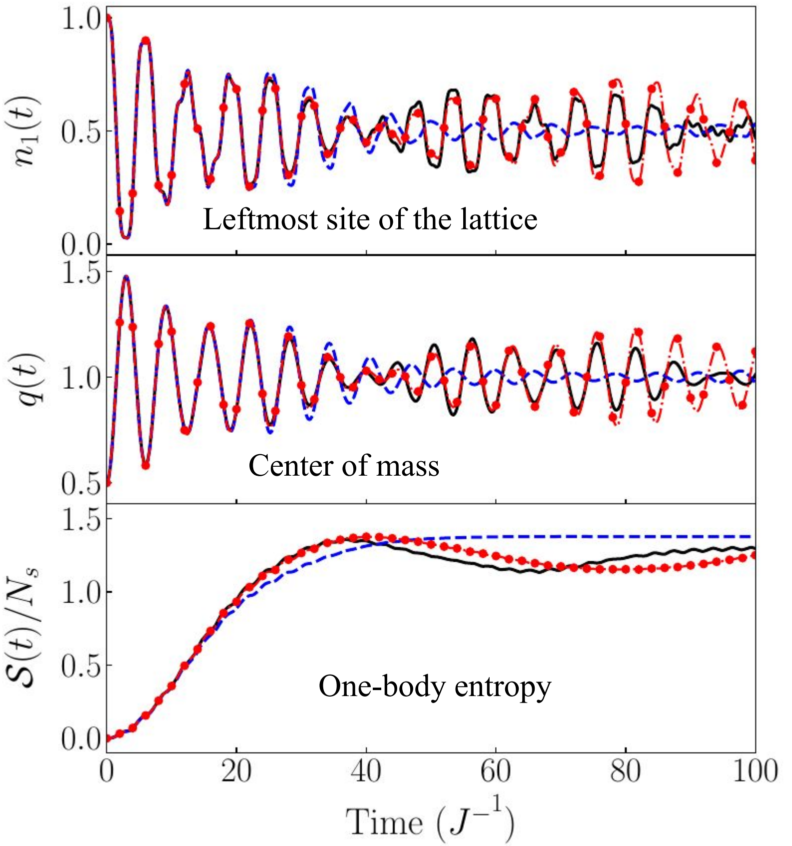
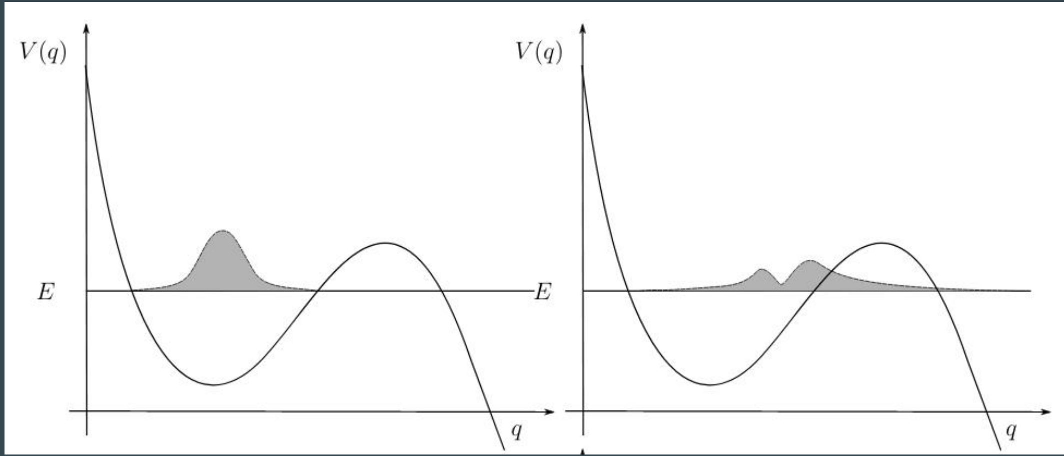




Phase-space approach: classical trajectories for tunneling

From corrected classical mechanics to fully quantum framework



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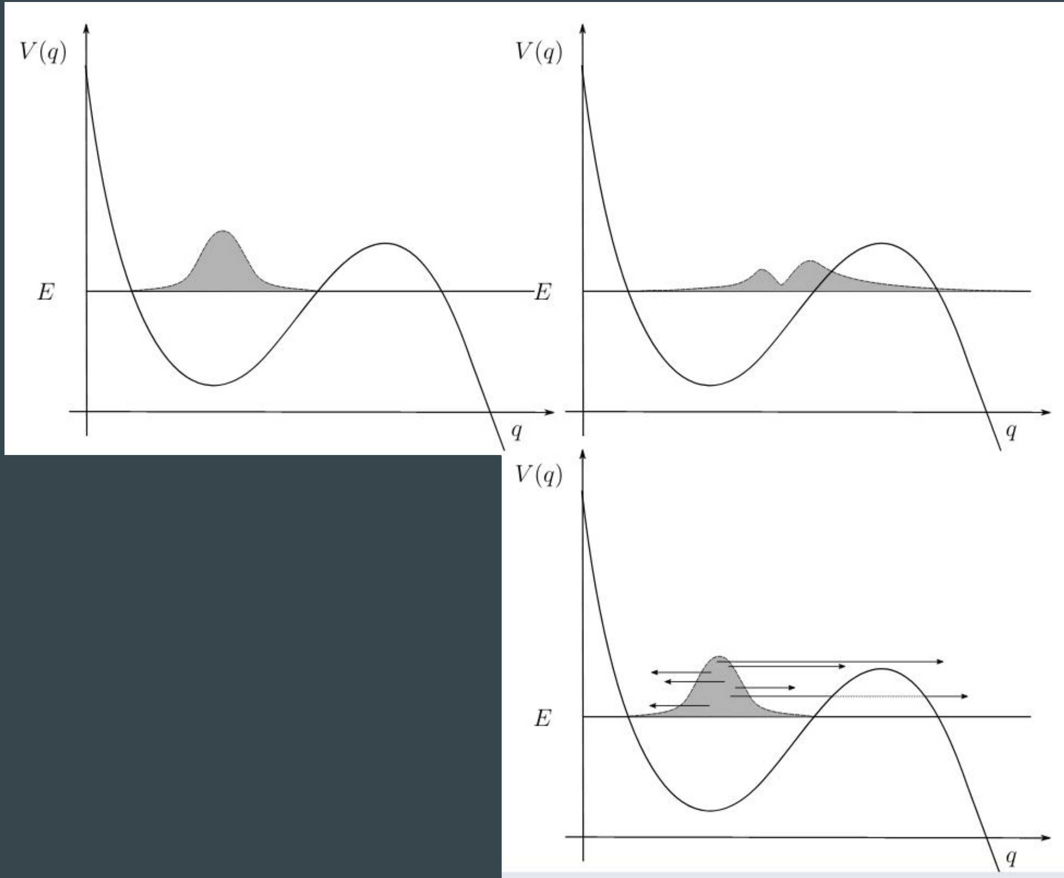
Efficient with low computational cost

Idea: trajectory-based formulation



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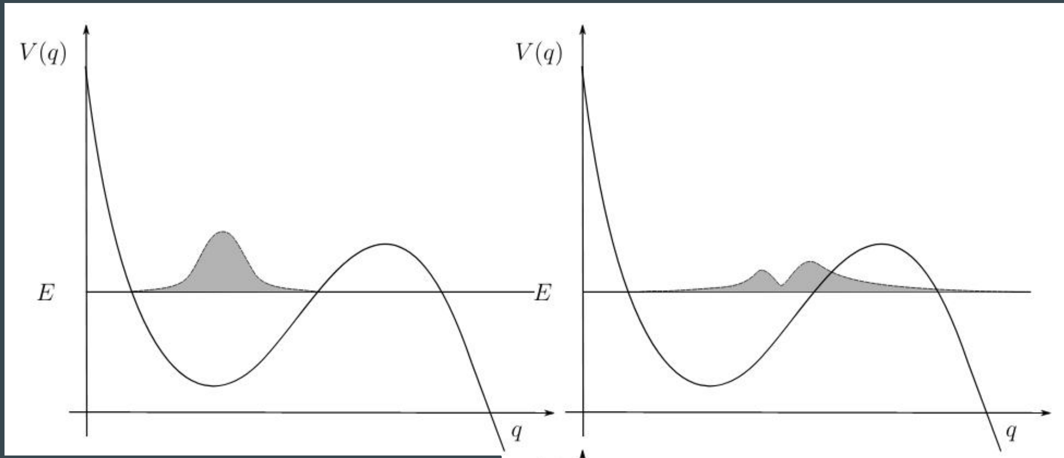
Efficient with low computational cost

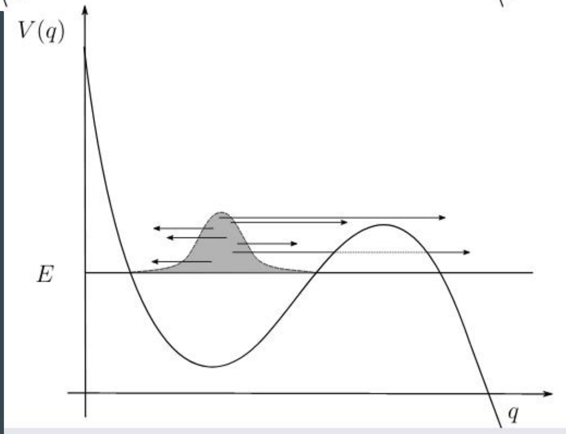
Idea: trajectory-based formulation

Goal: Average of trajectories in Phase-Space to reproduce Quantum Mechanics



Gaussian well potential

$$V(q) = \alpha_1 exp\left(-\frac{\left(q-Q_1\right)^2}{2\sigma_1^{\,2}}\right) + \alpha_2 exp\left(-\frac{\left(q-Q_2\right)^2}{2\sigma_2^{\,2}}\right)$$

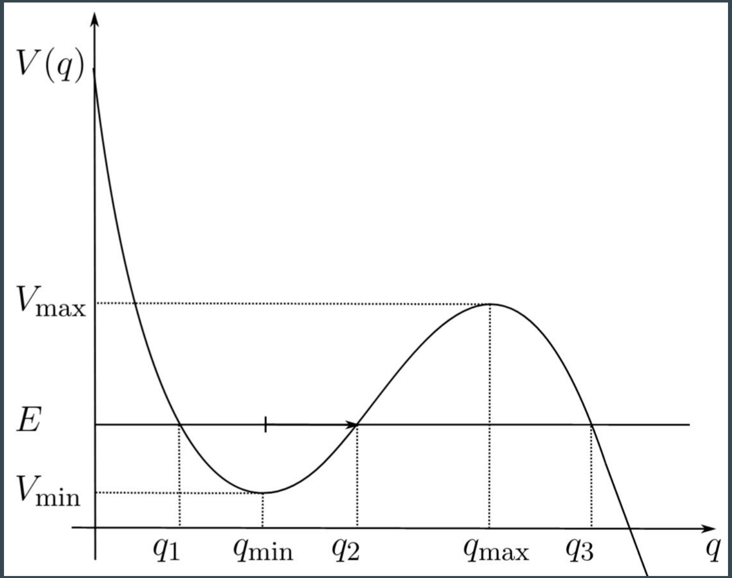


Phase-space approach: classical trajectories for tunneling

Sampling of initial conditions mimicking quantum statistics (Gaussian state):

Propagation using Classical Mechanics

$$\rho(q,t) = |\Psi(q,t)|^2 \simeq \frac{1}{N}\sum_i \delta\left(q - q_i(t)\right)$$



A. Polkovnikov, Ann. Phys. (N. Y). **325**, 1790 (2010).

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Phase-space approach: classical trajectories for tunneling

Follow the probability to detect the particle outside the well $P_{decay}(t)$

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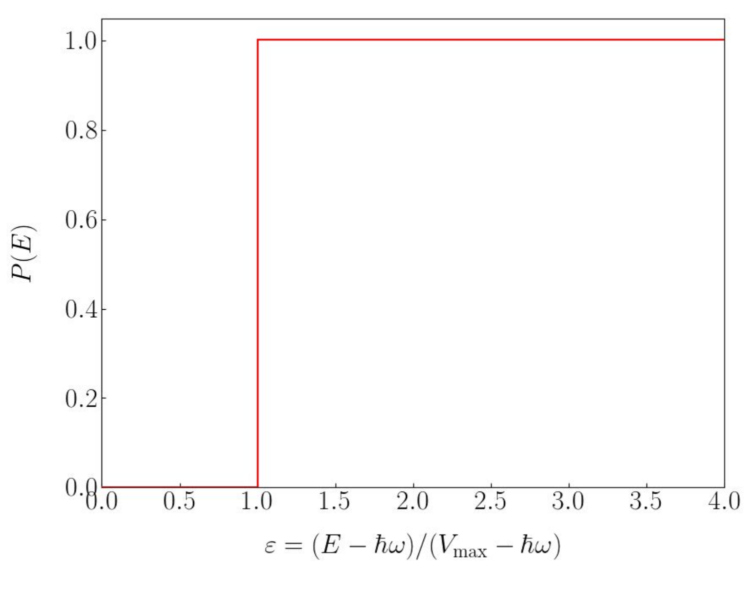

BLACK: Quantum RED: Classical

Phase-space approach: classical trajectories for tunneling

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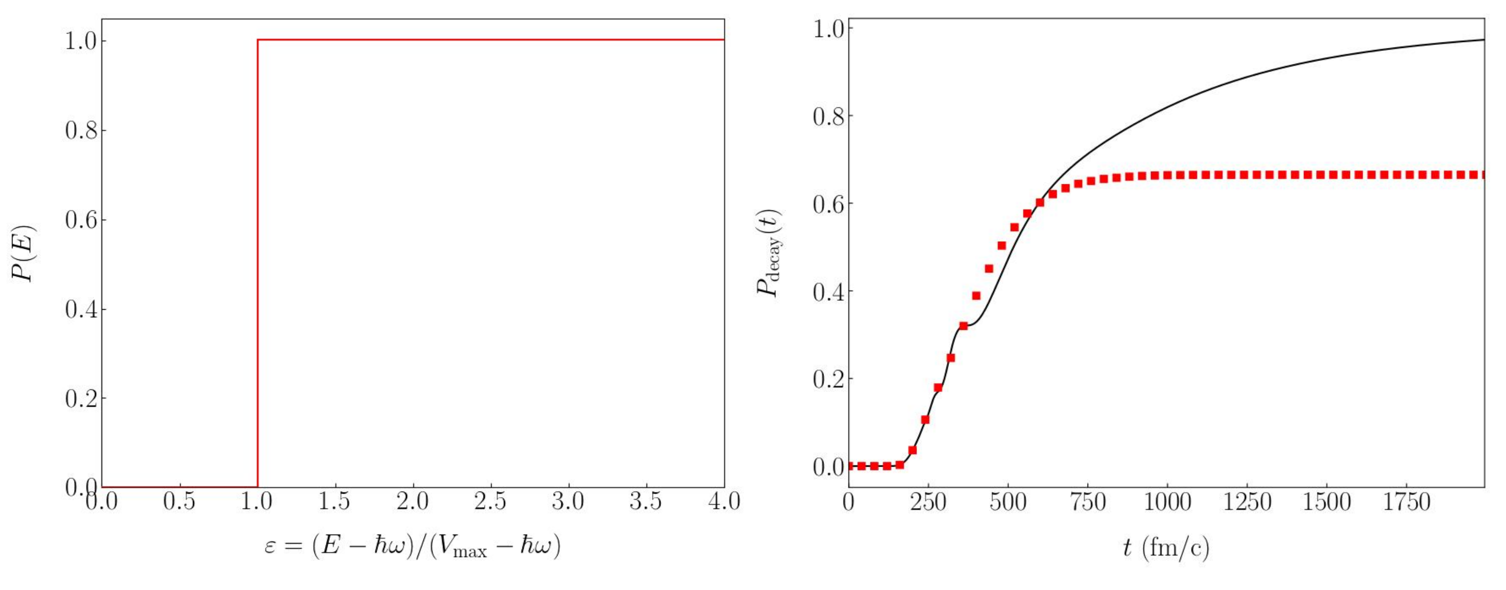

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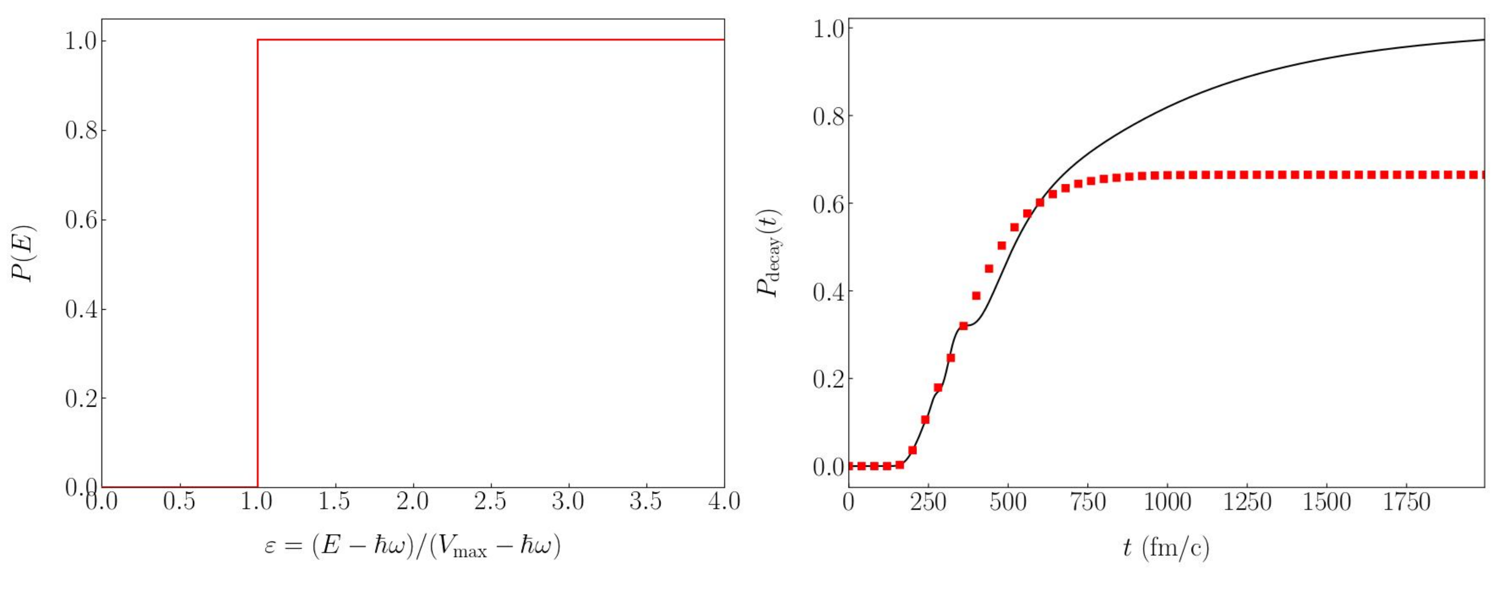


Particles of high energy escape

Wrong asymptote, wrong timescales

BLACK: Quantum RED: Classical

Classical trajectories with a jumping probability

Sampling of initial conditions mimicking quantum statistics (Gaussian state):

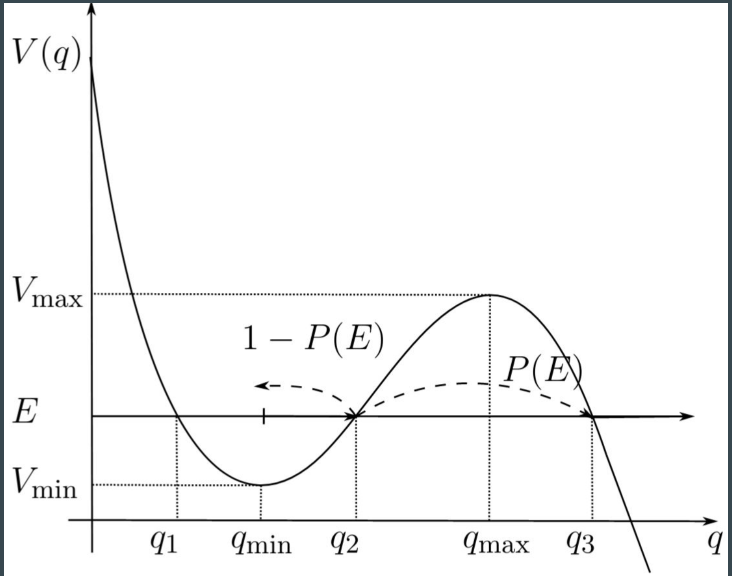
Propagation using Classical Mechanics

$$\rho(q,t) = |\Psi(q,t)|^2 \simeq \frac{1}{N}\sum_i \delta\left(q - q_i(t)\right)$$

Quantum element: jumping probability $P(E)$

First try: WKB formula

$$P(E) = e^{\frac{2i}{\hbar}\int_{q_2}^{q_3} p(q)\,\mathrm{d}q}$$



A. Polkovnikov, Ann. Phys. (N. Y). **325**, 1790 (2010).

N. Makri and W. H. Miller, J. Chem. Phys. **91**, 4026 (1989).

Classical trajectories with a jumping probability

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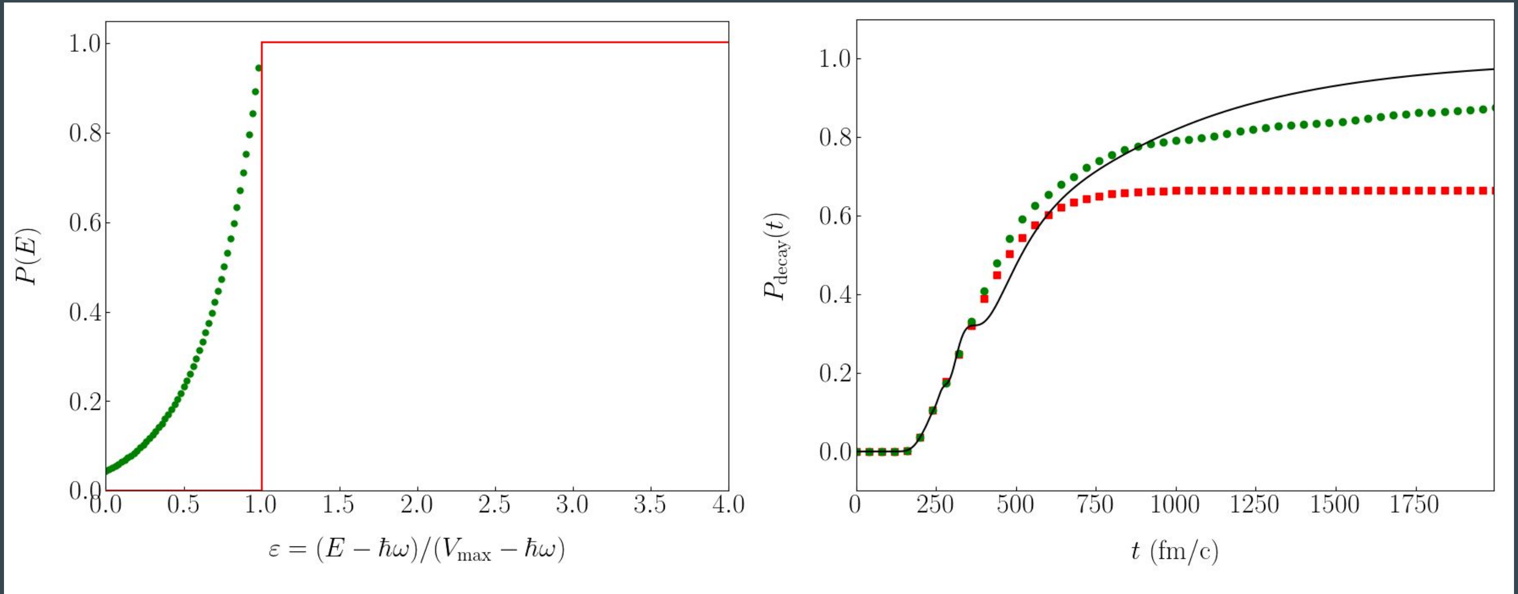

BLACK: Quantum RED: Classical GREEN: Classical + WKB

Classical trajectories with a jumping probability

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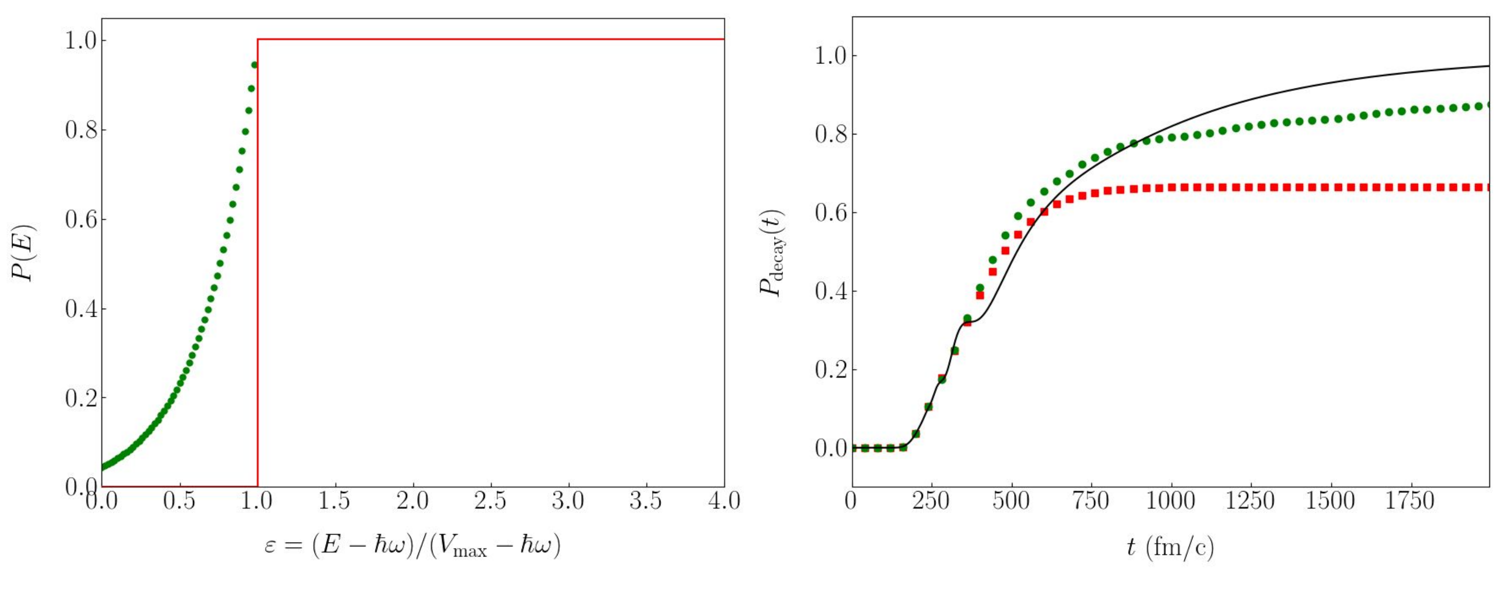

Wrong timescales!
Some particles are trapped for too long in the well.

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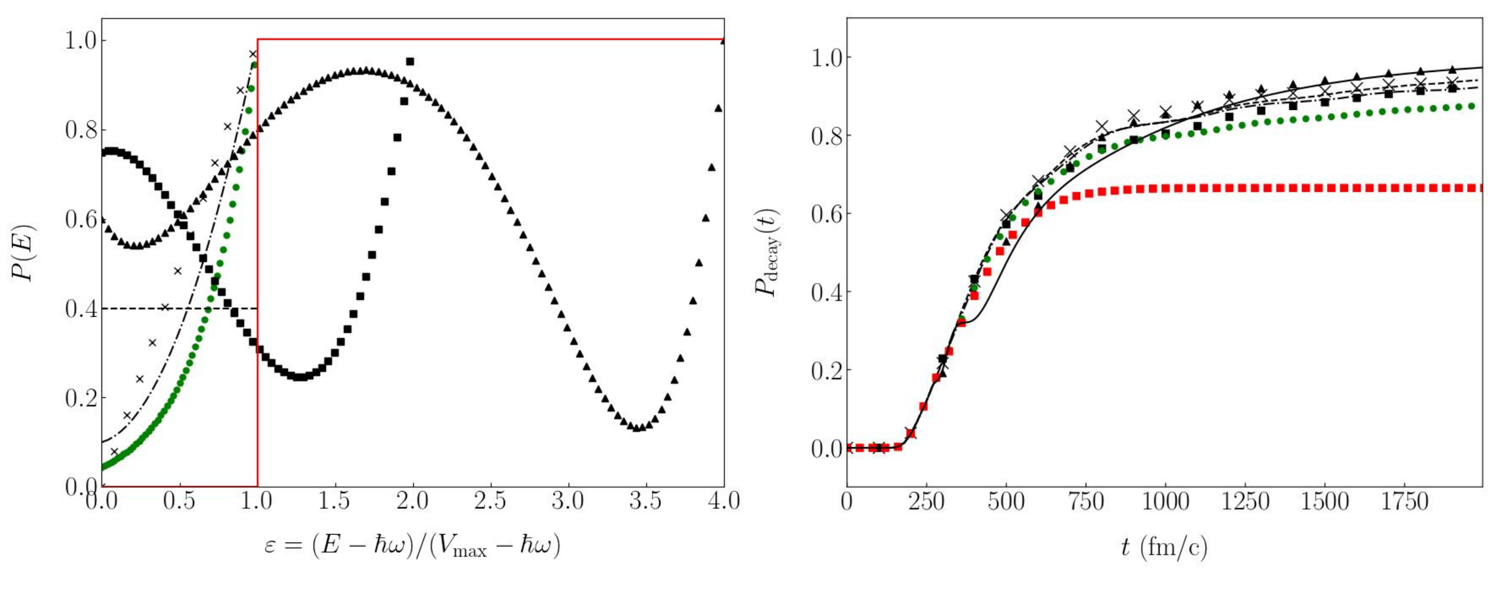
Classical trajectories with a jumping probability

Construction of $P(E)$ by inference using Lagrange polynomials



Good timescales

Need for a proper framework for defining trajectories with quantum effects

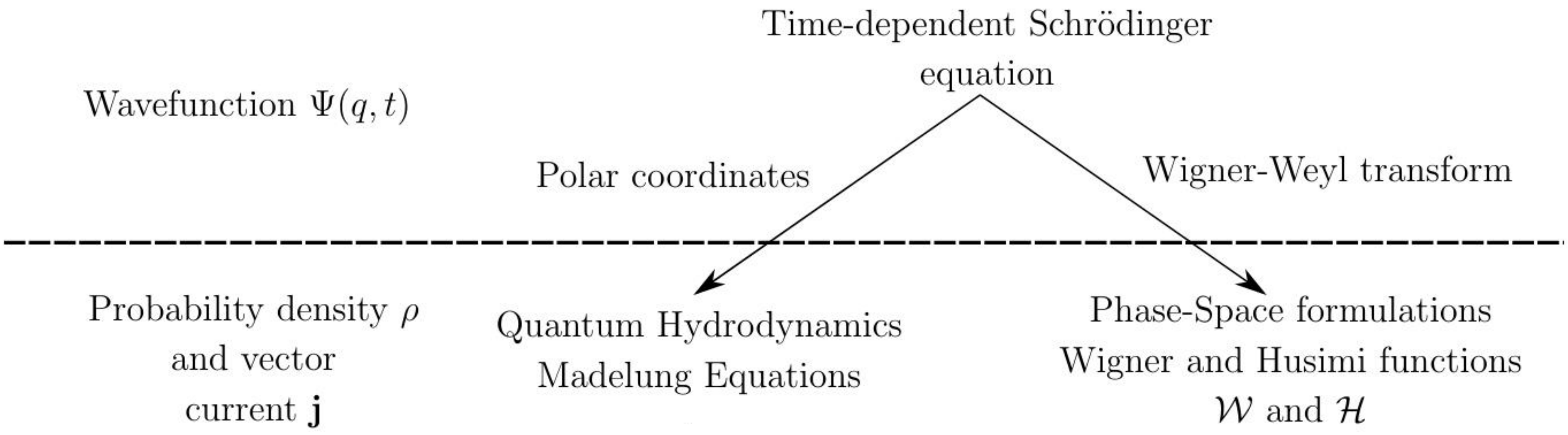
BLACK: Quantum RED: Classical GREEN: Classical + WKB

Introducing trajectories in a fully Quantum framework

Wavefunction $\Psi(q, t)$

Time-dependent Schrödinger equation

Introducing trajectories in a fully Quantum framework



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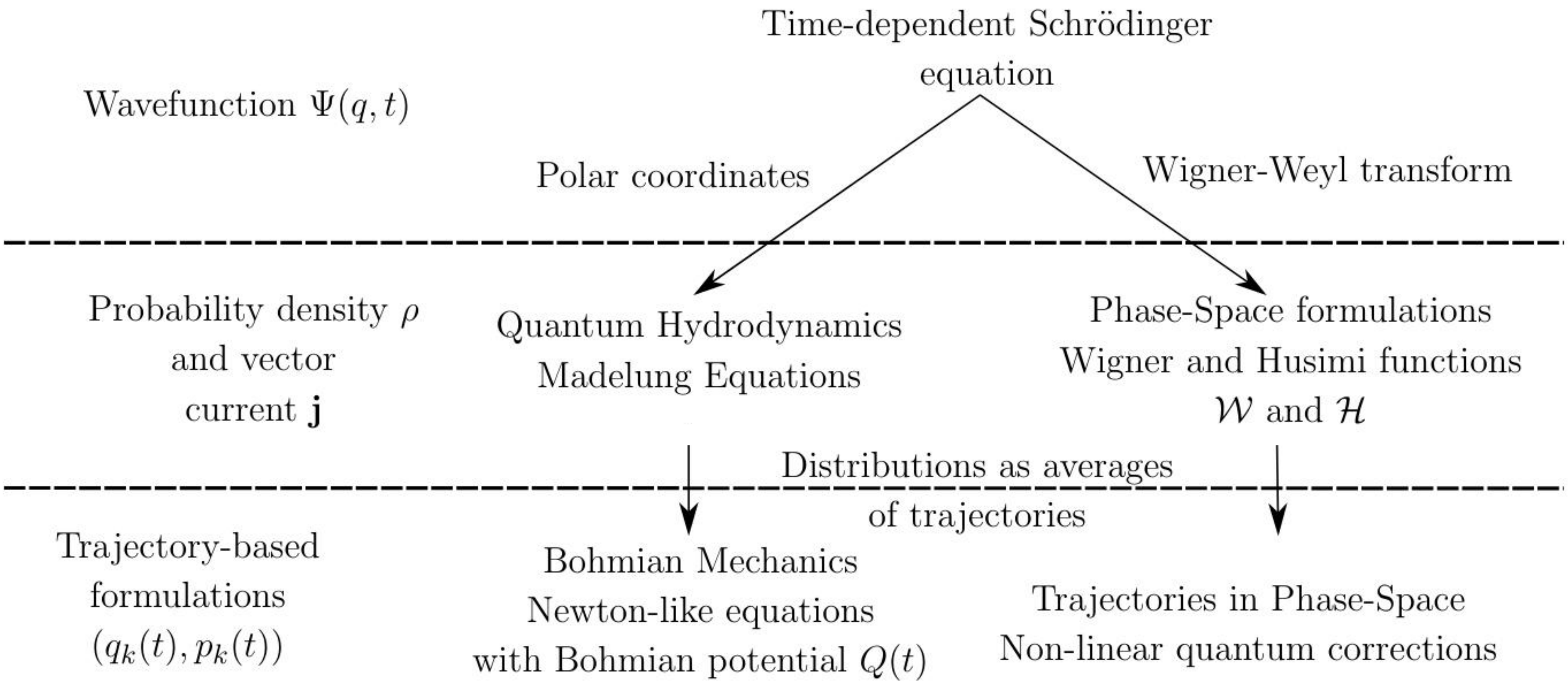

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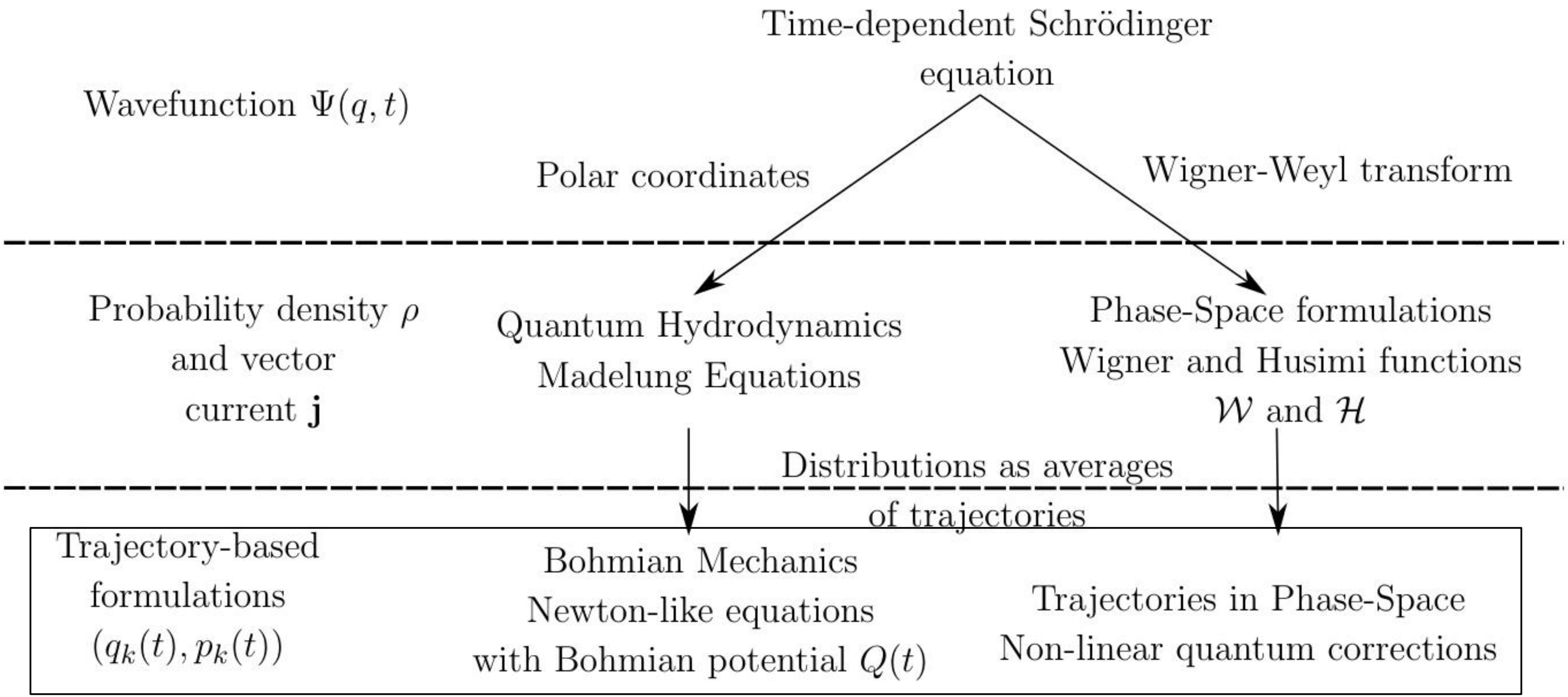

Bohmian mechanics

Wave function in polar coordinates $\Psi(q,t) = \sqrt{\rho(q,t)}e^{\frac{i}{\hbar}S(q,t)}$

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New equations of motion

$$\partial_t \rho = \frac{1}{m} \nabla \left[\rho \nabla S \right]$$

$$\partial_t S = \frac{\hbar^2}{4m} \left[\frac{\nabla^2 \rho}{\rho} - \frac{1}{2} \left(\frac{\nabla \rho}{\rho} \right)^2 \right] + \frac{(\nabla S)^2}{2m} - V\rho = -(Q+V) + \frac{(\nabla S)^2}{2m}$$

New "quantum" potential

$$Q(q,t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 \rho^{1/2}(q,t)}{\rho^{1/2}(q,t)}$$

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Depends on the wave function

Matching particle flux with probability flux: velocity field for particles!

$$\frac{\mathrm{d}}{\mathrm{d}t}mv(q_i(t),t) = -\nabla(Q(q_i(t),t) + V(q_i(t)))$$

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Depends on the wave function

Matching particle flux with probability flux: velocity field for particles!

$$\frac{\mathrm{d}}{\mathrm{d}t} m v(q_i(t),t) = -\nabla (Q(q_i(t),t) + V(q_i(t)))$$

Free Gaussian wave-packet:

$$Q(t) = -\frac{\hbar^2}{2m} \frac{1}{f(t)} \left(\frac{\left(q - q_0 - \frac{p_0}{m} t \right)^2}{f(t)} - 1 \right)$$

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Bohm in practice

MIW procedure: matching exact observable averages with trajectories averages

M. J. Hall, D.-A. Deckert, and H. M. Wiseman, Physical Review X **4**, 041013 (2014).
L. C. Rodriguez, *Trajectory-based methods for the study of ultrafast quantum dynamics*, Ph.D. thesis, Université Paul Sabatier-Toulouse III (2018).

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MIW procedure: matching exact observable averages with trajectories averages

Implies an approximation of density with N trajectories

$$\tilde{\rho}(x_i(t)) = \frac{1}{N(x_i(t) - x_{i-1}(t))}.$$

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Exact average energy = average trajectory energy

$$\tilde{Q} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\nabla\rho(x_i)}{\rho(x_i)}\right)^2$$

$$f_Q(x_i) = \frac{\hbar^2}{4m}\left[\sigma_{i+1} - \sigma_i\right]$$

$$\sigma_i = \frac{1}{(x_i - x_{i-1})^2}\left[\frac{1}{x_{i+1} - x_i} - \frac{2}{x_i - x_{i-1}} + \frac{1}{x_{i-1} - x_{i-2}}\right]$$

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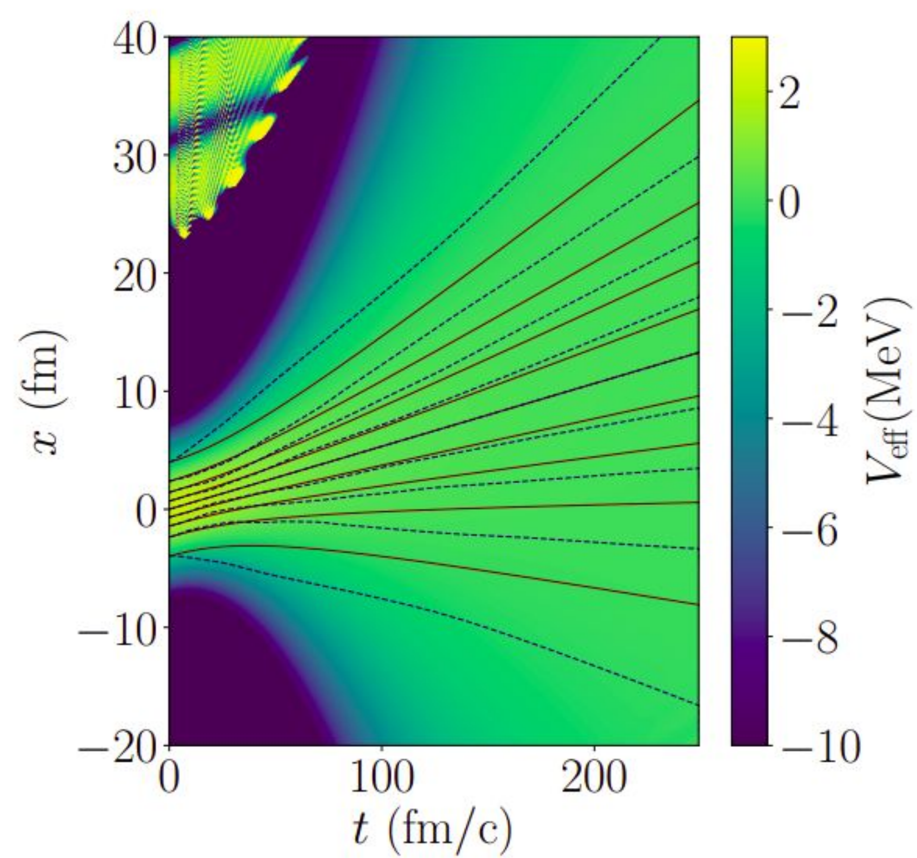

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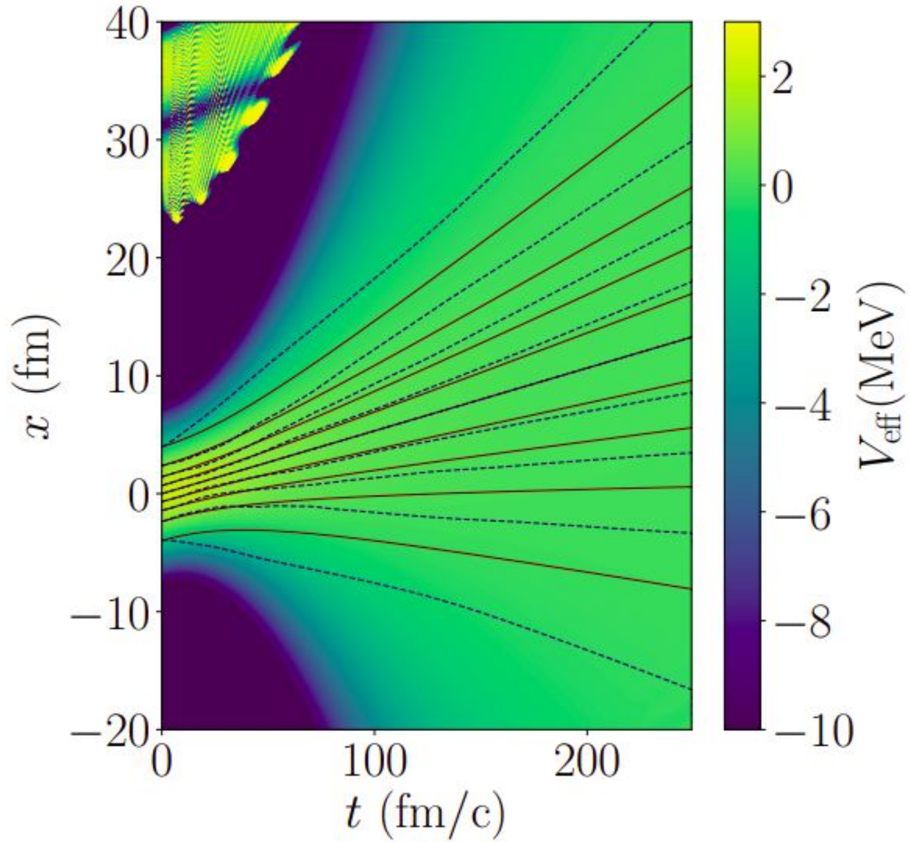
Several stages (exact):

1) Quasi-newtonian very short times



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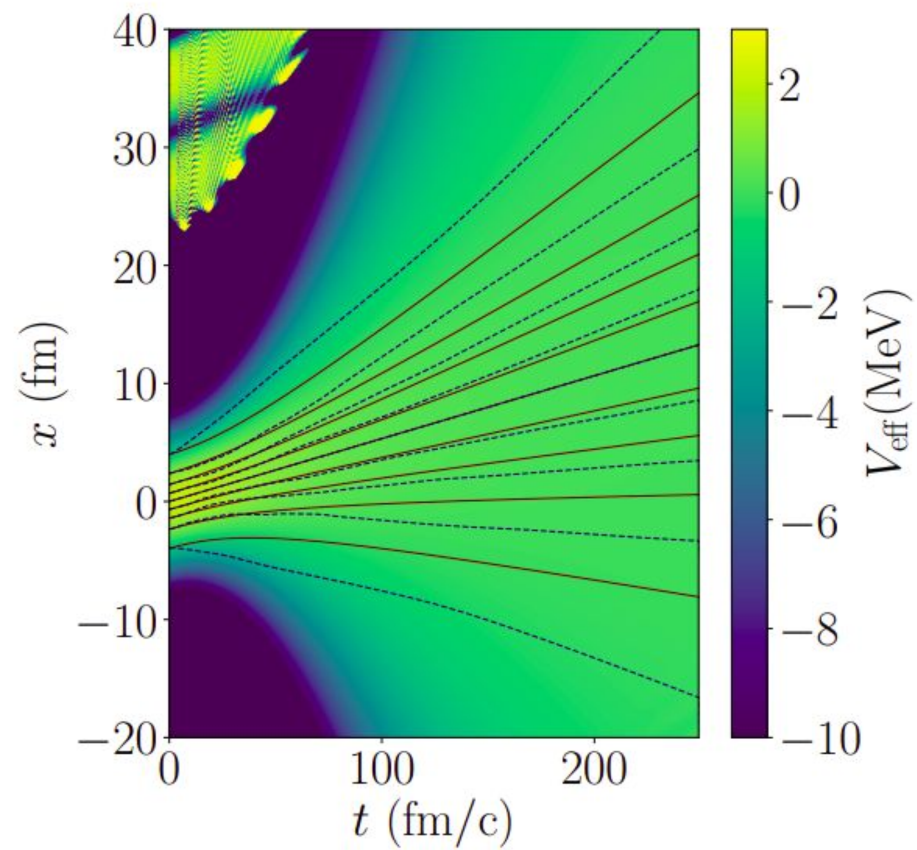
1) Quasi-newtonian very short times
2) Acceleration because of spreading

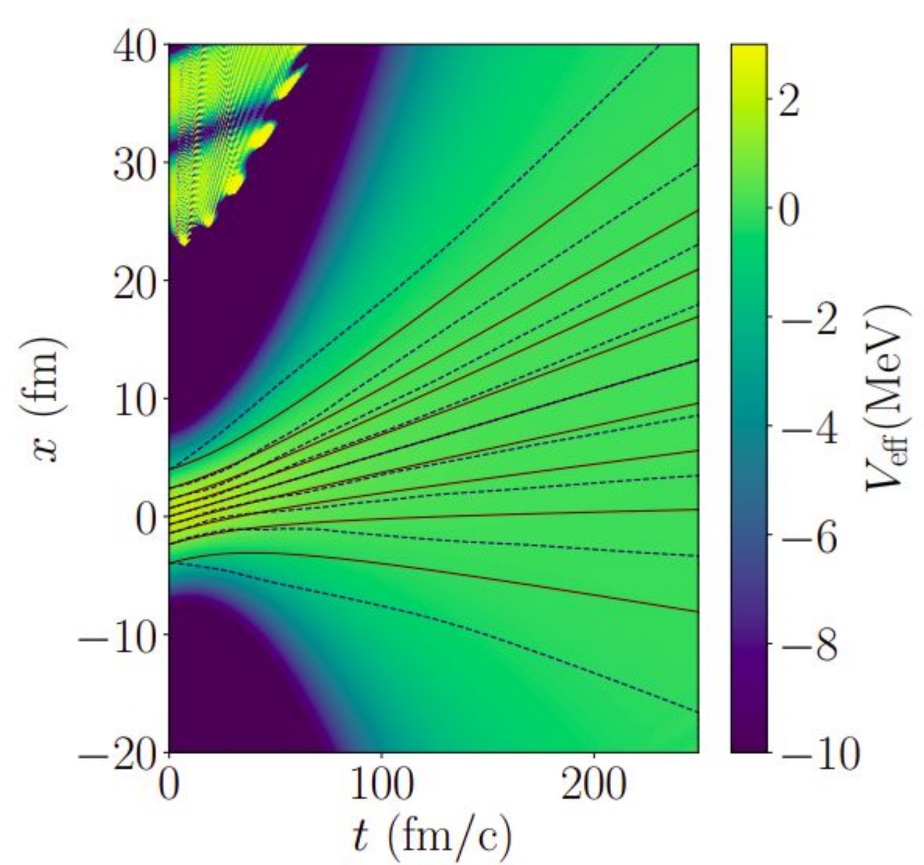


M. J. Hall, D.-A. Deckert, and H. M. Wiseman, Physical Review X **4**, 041013 (2014).
L. C. Rodriguez, *Trajectory-based methods for the study of ultrafast quantum dynamics*, Ph.D. thesis, Université Paul Sabatier-Toulouse III (2018).

Bohm in practice: free Gaussian wavepacket

Several stages (exact):

1) Quasi-newtonian very short times
2) Acceleration because of spreading
3) Linear propagation phase at long times



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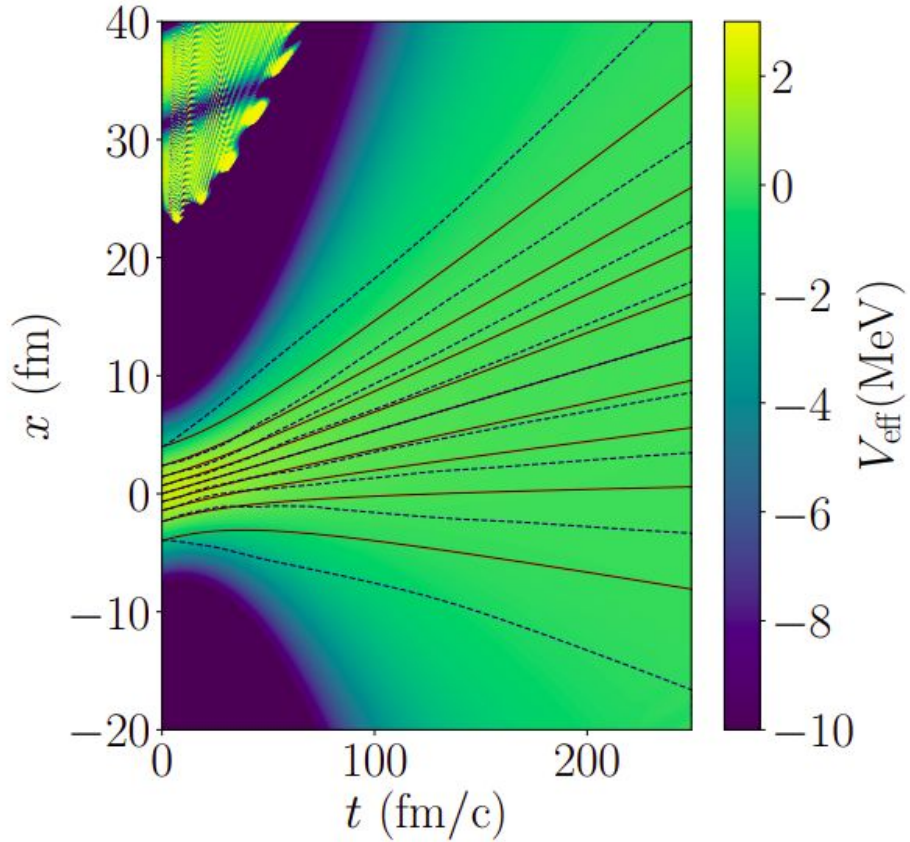
Sudden and dominant behavior of Bohm over the potential

Approximated potential: lacks of attractivity



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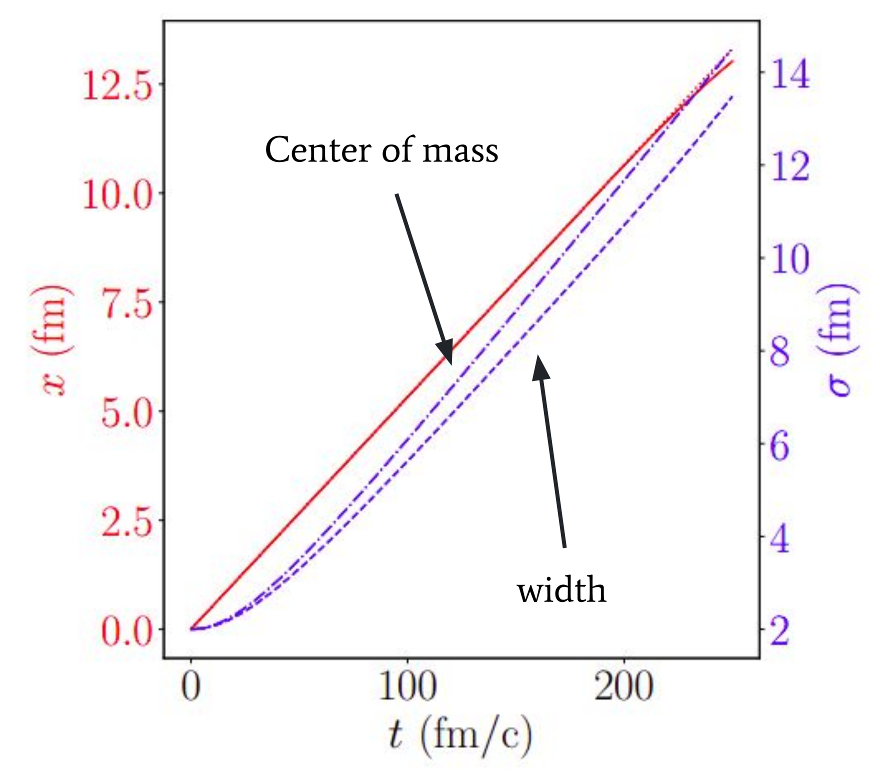

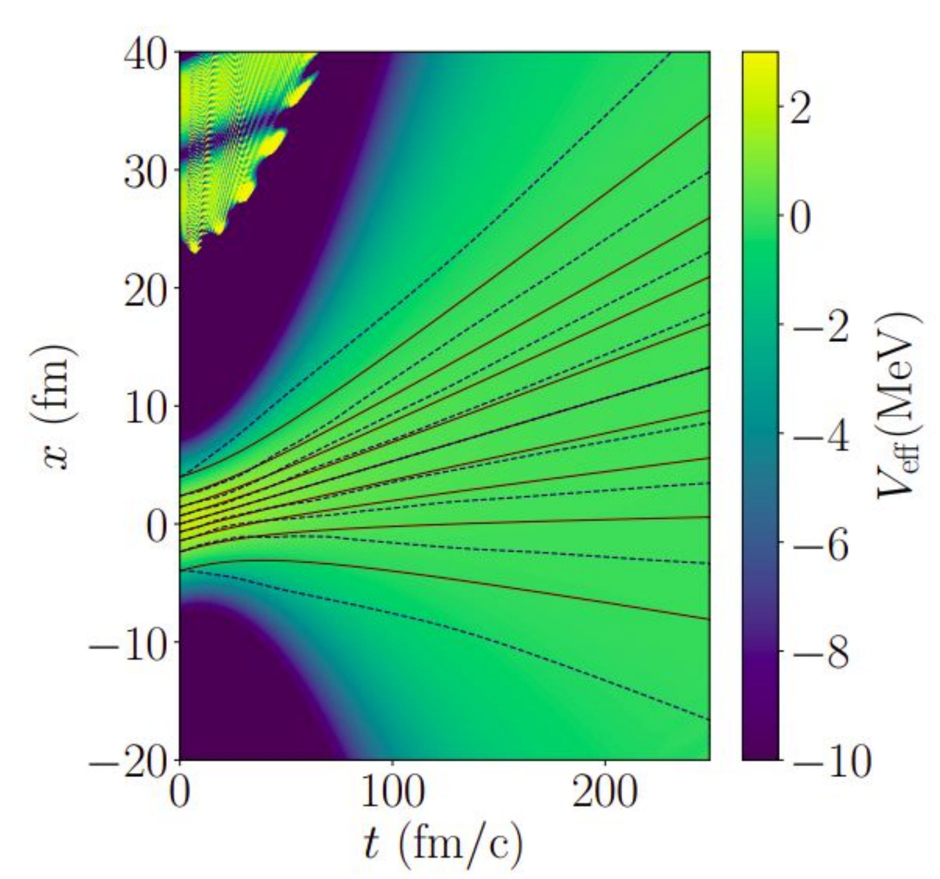

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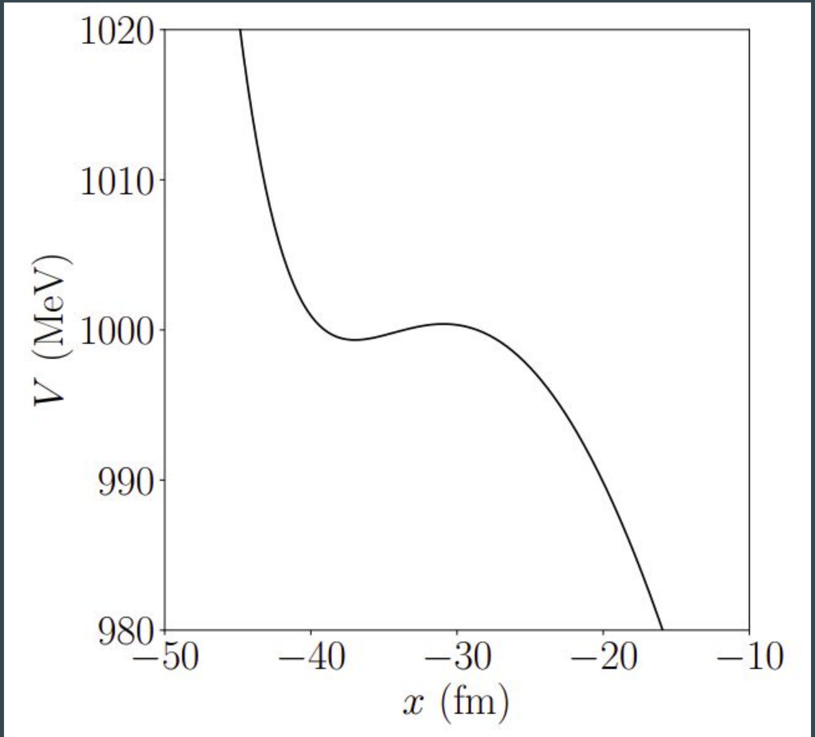
Bohm in practice: quantum tunneling

$$V(q) = \alpha_1 exp\left(-\frac{\left(q - Q_1\right)^2}{2\sigma_1^{\ 2}}\right) + \alpha_2 exp\left(-\frac{\left(q - Q_2\right)^2}{2\sigma_2^{\ 2}}\right)$$



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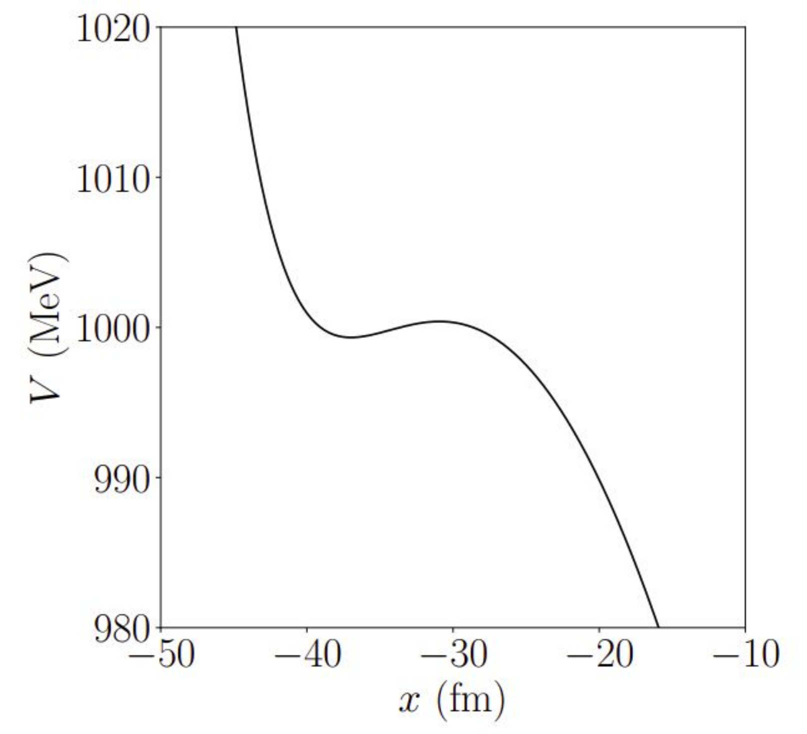

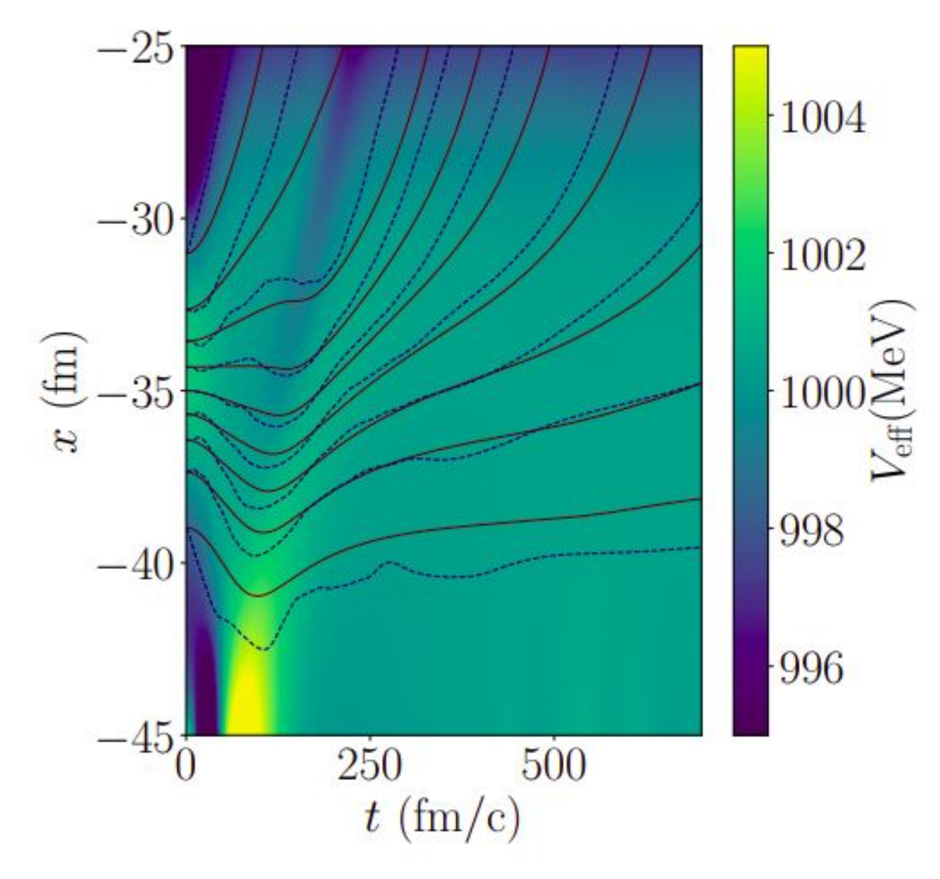

Phase-Space trajectories

Systematic correction to Classical Mechanics:

A. Polkovnikov, Ann. Phys. (N. Y). **325**, 1790 (2010).

Phase-Space trajectories

Systematic correction to Classical Mechanics:

Wigner-Weyl transform:

$$\mathcal{W}(q_w, p_w) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \rho\left(q_w - \frac{x'}{2}, q_w + \frac{x'}{2}\right) e^{\frac{i}{\hbar} p x'} \mathrm{d}x'$$

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Transformed dynamics:

$$\partial_t \mathcal{W} = -\frac{p_w}{m} \nabla_{q_w} \mathcal{W} + \frac{i}{2\pi\hbar} \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}\eta \mathrm{d}z \left(V\left(q_w + \frac{z}{2}\right) - V\left(q_w - \frac{z}{2}\right)\right) e^{-\frac{i}{\hbar} z(\eta - p_w)} = -\nabla \cdot \mathbf{j}$$

Probability flux

Explicit non-locality

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Trajectories: matching prob. flux with particle flux

$$\dot{q}_i(t) = \frac{p_i(t)}{m}$$

$$\dot{p}_i(t) = \frac{i}{2\pi\hbar\mathcal{W}(q_i, p_i, t)}\int_{\mathbb{R}} \mathrm{d}z \mathrm{d}p' \left[V\left(q_i - \frac{z}{2}\right) - V\left(q_i + \frac{z}{2}\right)\right] e^{\frac{i}{\hbar}z(p_i - p')}\mathcal{W}(q_i, p', t) = -\nabla_q V(q_i(t)) + \dots$$

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Classical mechanics + corrections

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Need for Wigner function reconstruction

Phase-Space trajectories

Not that easy ! Wigner distribution can be negative !

A. Wang, Y. Zheng, C. C. Martens, and W. Ren, Phys. Chem. Chem. Phys. 11, 1588 (2009).
L. Wang, Q. Zhang, F. Xu, X. D. Cui, and Y. Zheng, Int. J. Quantum Chem. 115, 208 (2015).

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Idea: smooth it using Gaussian functions ϕ with width h

$$\mathcal{W}(q,p,t) \approx \frac{1}{N_{\mathrm{evt}}} \sum_i \phi(q - q_i(t))\phi(p - p_i(t))$$

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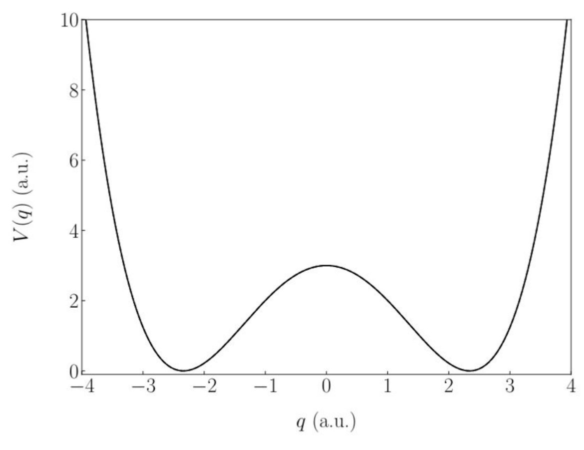
Test on quartic potential



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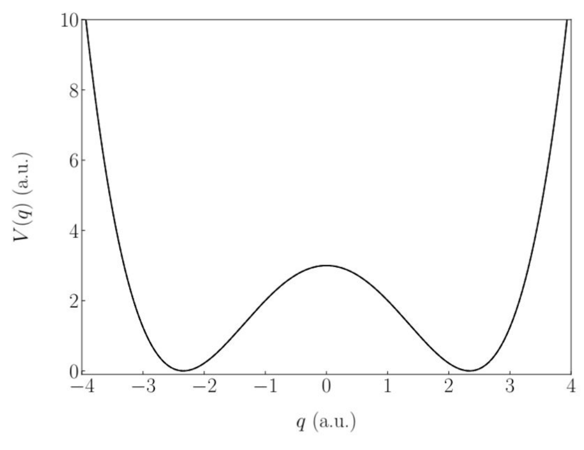
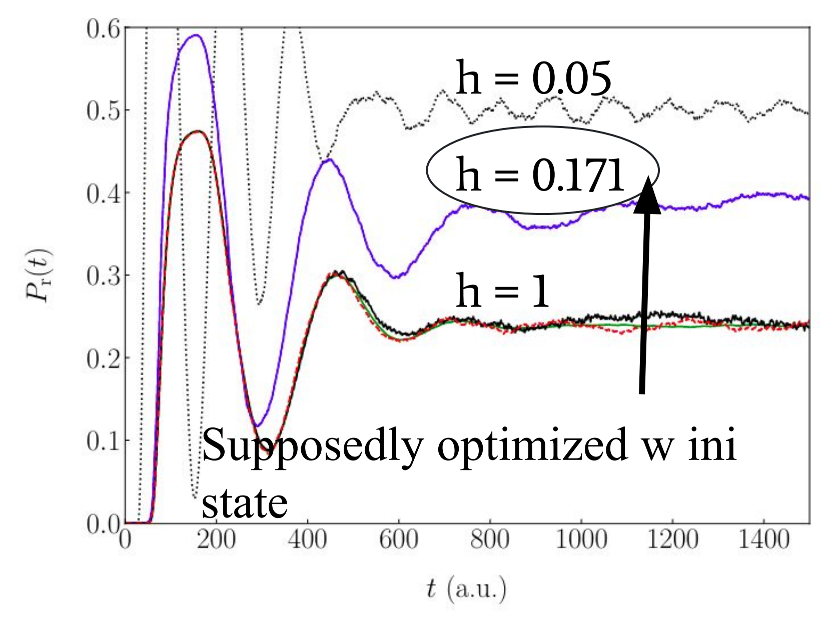


New method
+
Exact and SMF equivalent (TWA)

Results are degraded…



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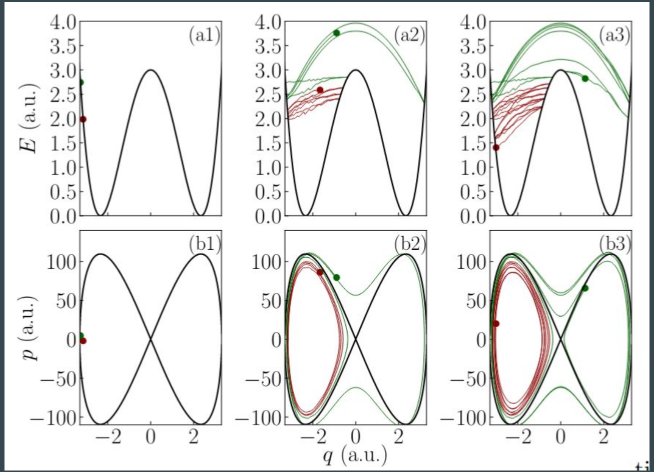


Example of trajectories

Exchange of energy between trajectories of similar momentum

A. Wang, Y. Zheng, C. C. Martens, and W. Ren, Phys. Chem. Chem. Phys. 11, 1588 (2009).
L. Wang, Q. Zhang, F. Xu, X. D. Cui, and Y. Zheng, Int. J. Quantum Chem. 115, 208 (2015).

Phase-Space trajectories

Gaussian convolution: Husimi function, not Wigner !

New equations of motion…

$$\partial_t \mathcal{H}(q_h, p_h, t) = -\frac{p_h}{M} \nabla_{Q_2} \mathcal{H}(Q_2, p_h, t)\big|_{Q_2=q_h} - \frac{h_p^2}{M} \nabla_{Q_2} \nabla_{P_2} \mathcal{H}(Q_2, P_2)\big|_{Q_2=q_h, P_2=p_h}$$
$$+ \left\{-2b + 6ch_q^2 q_h^2\right\} \left\{q_h \nabla_{P_2} + h_q^2 \nabla_{Q_2} \nabla_{P_2}\right\} \mathcal{H}(Q_2, P_2, t)\big|_{Q_2=q_h, P_2=p_h}$$
$$+ 4cq_h^3 \nabla_{P_2} \mathcal{H}(q_h, P_2)\big|_{P_2=p_h} + 4ch_q^6 \nabla_{Q_2}^3 \nabla_{P_2} \mathcal{H}(Q_2, P_2, t)\big|_{Q_2=q_h, P_2=p_h}$$
$$+ 12ch_q^2 \left(q_h \nabla_{Q_2}^2 \nabla_{P_2} + q_h^2 \nabla_{Q_2} \nabla_{P_2}\right) \mathcal{H}(Q_2, P_2, t)\big|_{Q_2=q_h, P_2=p_h}$$
$$+ c\hbar^2 \left(h_q^2 h_p^2 \nabla_{Q_2} \nabla_{P_2}^4 + q_h \nabla_{P_2}^3\right) \mathcal{H}(Q_2, P_2, t)\big|_{Q_2=q_h, P_2=p_h} ,$$

Not really simple…

Higher order crossed derivatives

A. Wang, Y. Zheng, C. C. Martens, and W. Ren, Phys. Chem. Chem. Phys. 11, 1588 (2009).
L. Wang, Q. Zhang, F. Xu, X. D. Cui, and Y. Zheng, Int. J. Quantum Chem. 115, 208 (2015).

H. López, C. C. Martens, and A. Donoso, J. Chem. Phys. **125**, (2006).

Conclusion

Trials of trajectory-based methods:

1) SMF + inspired method (HPS): catching higher order correlations (HPS can be expensive)
2) Trajectory inspired descriptions of tunneling

- Empirical methods: classical trajectories with probability jump, proba can be found using by inference, lack of a grounded theoretical framework

- More grounded trajectories: Bohm (configuration space) and Wigner (phase-space)

Bohm: well-defined (newtonian) trajectories with new effective potential, numerically challenging but tackled by the MIW, to be generalized for more complex systems (3D…)

Wigner: phase-space dynamics, classical trajectories + quantum corrections, Wigner function can be negative, reconstruction of Wigner function, optimized width to change with time ?

Need the wavefunction, difficulties otherwise

THANKS FOR LISTENING

Conclusion

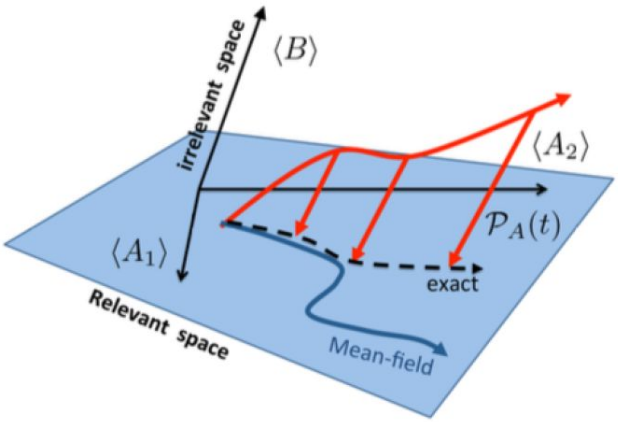
What can be done in the future ?

1) Stabilization of Bohm using new methods

2) Development of a momentum based equivalent to Bohmian Mechanics

3) Apply SMF / HPS on quantum tunneling problems

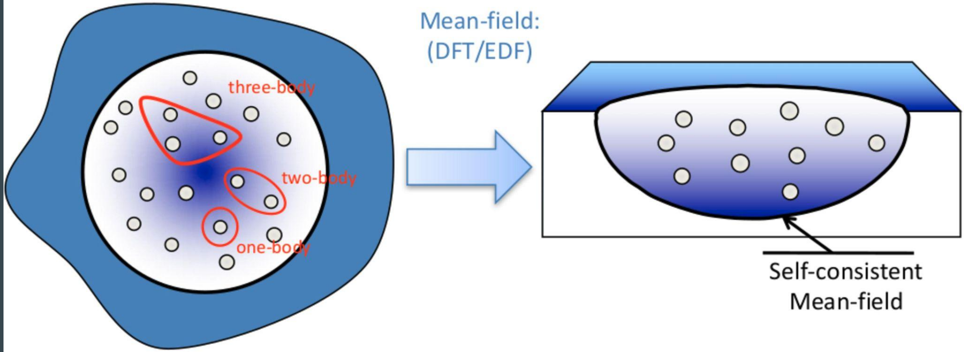
Usual approach: mean-field theories



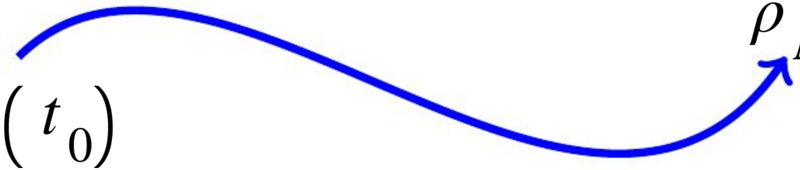
Time-Dependent Hartree-Fock theory (1-body DOFs):

1) Effective Hamiltonian $h_{MF}(\rho)$
2) Self-consistent equations of motion

$$i\hbar \frac{\partial \rho}{\partial t} = \left[h_{MF}(\rho), \rho \right]$$



$\rho(t_0)$



$\rho_{MF}(t)$

Beyond Mean-Field theories ?

Trajectory-based approach: Stochastic mean-field (SMF)

Phase-space:

1) sampling of initial conditions mimicking quantum correlations

$$\rho^{(n)}(t_0) = \rho(t_0) + \delta\rho^{(n)}(t_0)$$

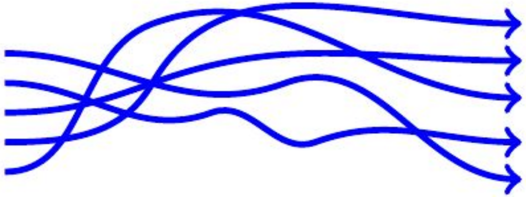
2) Mean-Field-like propagation

$$i\hbar \frac{\partial \rho^{(n)}}{\partial t} = \left[h_{MF}(\rho^{(n)}), \rho^{(n)} \right]$$

3) Average over trajectories

$$\bar{\rho} = \frac{1}{N} \sum_{n}^{N} \rho^{(n)}$$

$\rho^{(n)}(t_0)$



$\bar{\rho}(t)$

- Low energy dissipation
- Spontaneous symmetry breaking
- Applications to fission
- …

S. Ayik, Phys. Lett. B **658**, 174 (2008).
D. Lacroix and S. Ayik, Eur. Phys. J. **A50**, 95 (2014).

Quantum hydrodynamics and PS trajectories

Hydrodynamical equations of motion

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = -\nabla \mathbf{j}(\mathbf{r},t),$$

$$\partial_t \mathbf{j}(\mathbf{r},t) = -\frac{\rho(\mathbf{r},t)}{m}\nabla\left[V(\mathbf{r}) + Q(\mathbf{r},t)\right] - \nabla\left[\frac{\mathbf{j}(\mathbf{r},t)}{\sqrt{\rho(\mathbf{r},t)}}\right]^2.$$

Trajectories in PS

$$\begin{cases} \dfrac{\mathrm{d}q_i(t)}{\mathrm{d}t} = \dfrac{p_i(t)}{m}, \\ \dfrac{\mathrm{d}p_i(t)}{\mathrm{d}t} = -\dfrac{1}{\mathcal{W}(q_i(t),p_i(t),t)}\displaystyle\int_{\mathbb{R}} \Theta(q_i(t),p_i(t)-p')\mathcal{W}(q_i(t),p',t)\mathrm{d}p', \\ \quad = -\left.\nabla_x V(x)\right|_{x=q_i(t)} + \displaystyle\sum_{\substack{s>0 \\ 2s+1}}^{+\infty}\left(\frac{\hbar}{2}\right)^{2s}\frac{(-1)^{s+1}}{(2s+1)!}\left(\left.\nabla_x^{2s+1}V(x)\right|_{x=q_i(t)}\right)\left(\frac{\left.\nabla_p^{2s}\mathcal{W}(q_i(t),p)\right|_{p=p_i(t)}}{\mathcal{W}(q_i(t),p_i(t))}\right), \end{cases}$$

with

$$\Theta(q_w,p_w) = \frac{i}{2\pi\hbar}\int_{\mathbb{R}}\left[V\left(q_w+\frac{z}{2}\right) - V\left(q_w-\frac{z}{2}\right)\right]\exp\left[-\frac{i}{\hbar}zp_w\right]\mathrm{d}z.$$

Trajectories in PS for gaussian in quartic potential

$$\dot{q}_k = \frac{p_k}{M}$$

$$\dot{p}_k = 2bq_k - 4cq_k^3 + \hbar^2\frac{cq_k}{h_p^2}\frac{\sum_i \phi(q_k(t)-q_i(t),p_k(t)-p_i(t))\left[\frac{(p_k(t)-p_i(t))^2}{h_p^2} - 1\right]}{\sum_j \phi(q_k(t)-q_j(t),p_k(t)-p_j(t))}.$$

Full resolution of the Wigner problem

$$\mathcal{W}(q_w, p_w, t + \mathrm{d}t) = \mathcal{L}\mathcal{W}(q_w, p_w, t),$$
$$\mathcal{L} = -\frac{p_w}{m}\nabla_q + \frac{i}{\hbar}\left[V^- - V^+\right] = \mathcal{L}_1 + \mathcal{L}_2$$

$$V^\pm = V\left(q_w \pm \frac{i\hbar}{2}\nabla_p\right),$$
$$\mathcal{L}_1 = -\frac{p_w}{m}\nabla_q,$$
$$\mathcal{L}_2 = \frac{i}{\hbar}\left[V^- - V^+\right].$$

$$e^{\mathrm{d}t(\mathcal{L}_1+\mathcal{L}_2)} \approx e^{\frac{\mathrm{d}t}{2}\mathcal{L}_1} e^{\mathrm{d}t\mathcal{L}_2} e^{\frac{\mathrm{d}t}{2}\mathcal{L}_1}$$

Fast Fourier Transform algorithm

Quartic potential Gaussian wavepacket