Searching for simple modelization of quantum dynamical effects

Thomas CZUBA
Supervisor: Denis LACROIX

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Give an accurate description of the dynamical properties of mesoscopic systems (A = 1 to A ~ 300 particles)

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Idea: replace a realistic complex quantum problem with several simpler ones through Phase-Space methods

Phase-Space approach

Broad spectrum of possibilities: corrected classical mechanics to a fully quantum framework

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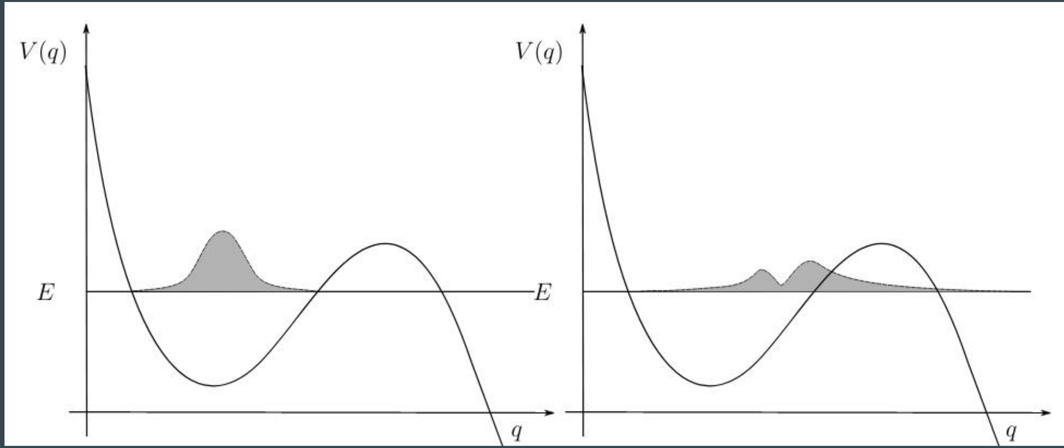
Efficients with low computational cost



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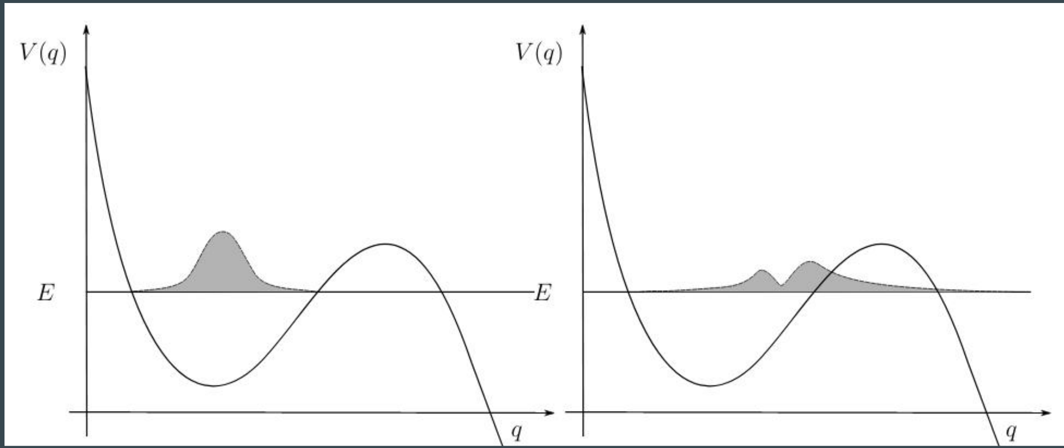

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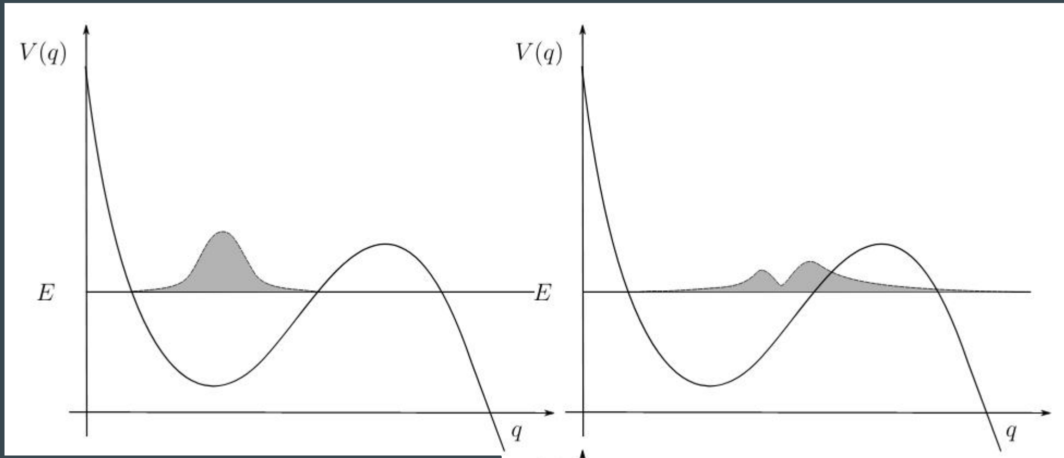

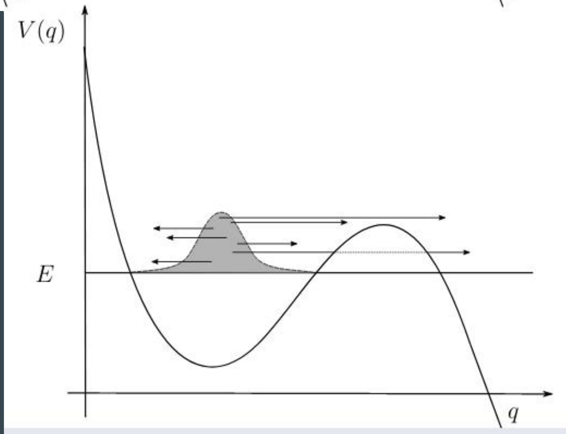

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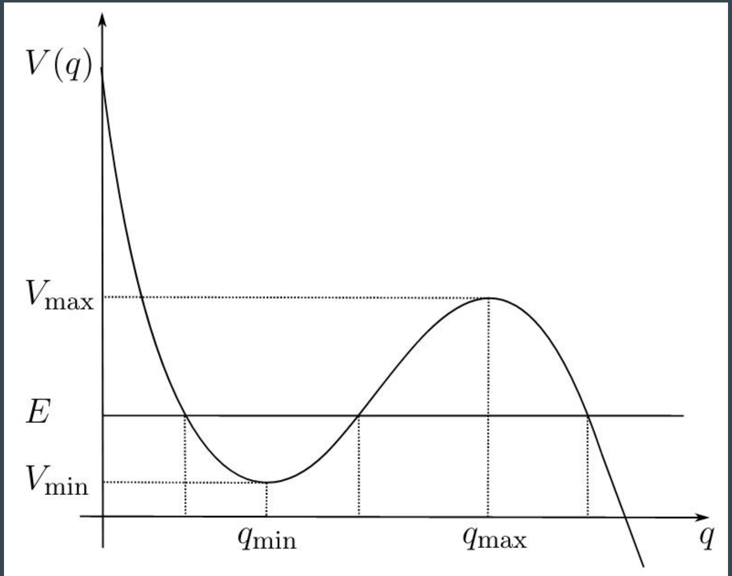
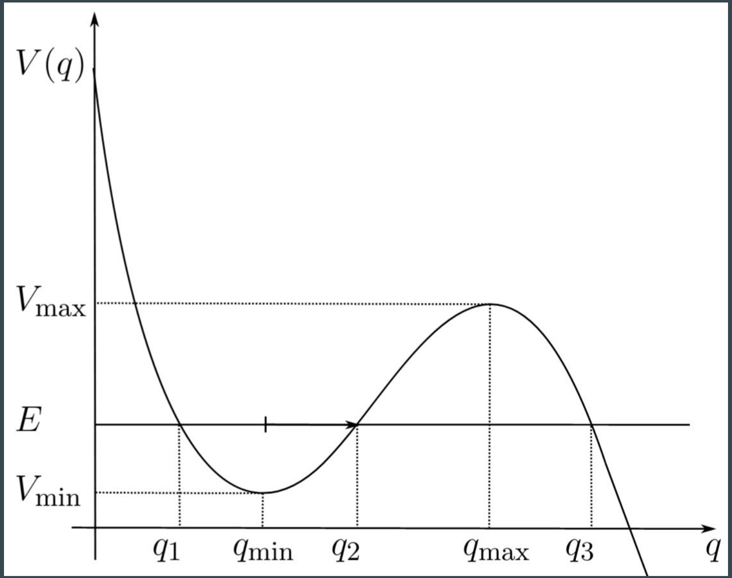


Classical trajectories with a jumping probability

Sampling of initial conditions mimicking quantum statistics (Gaussian state) [1]:



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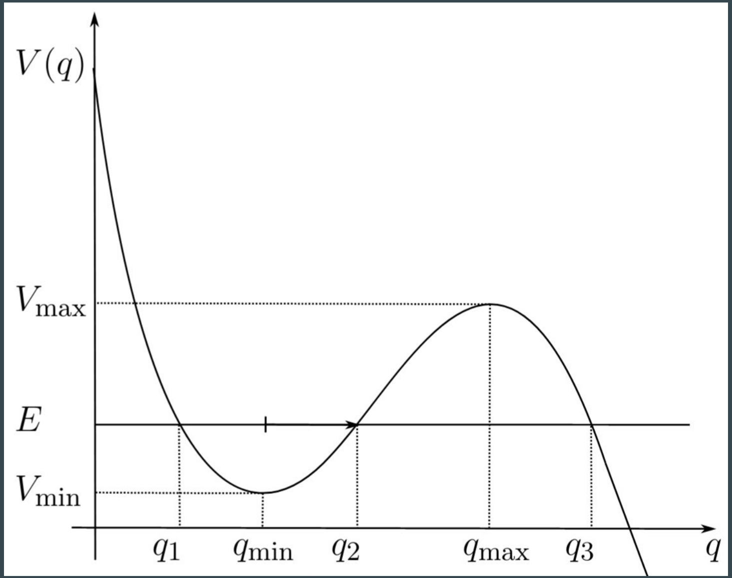
Propagation using Classical Mechanics

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



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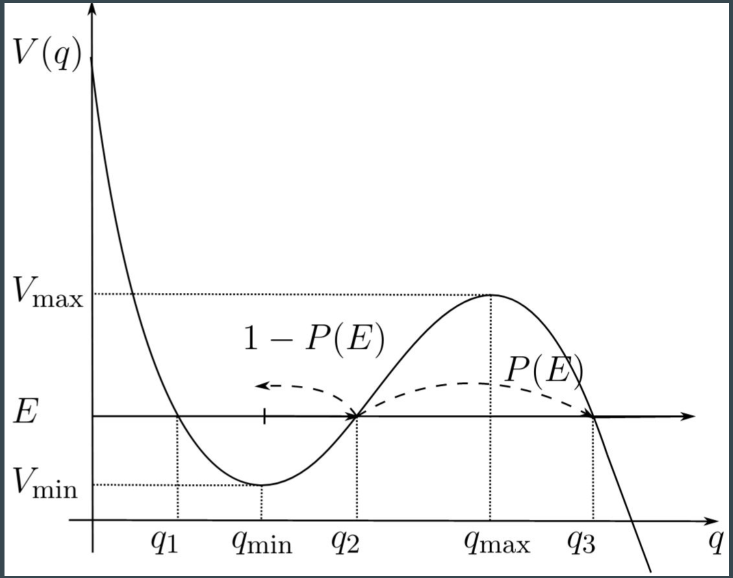
Quantum element: jumping probability $P(E)$ [2]

First try: WKB formula

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



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

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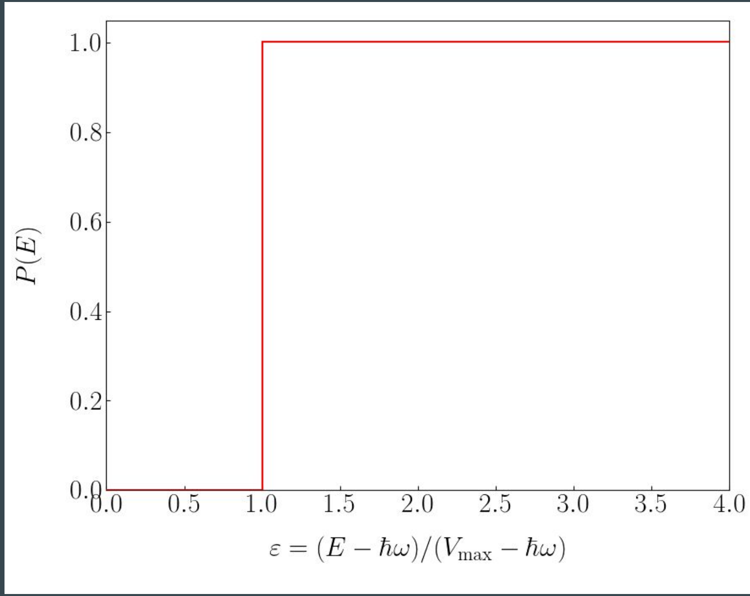

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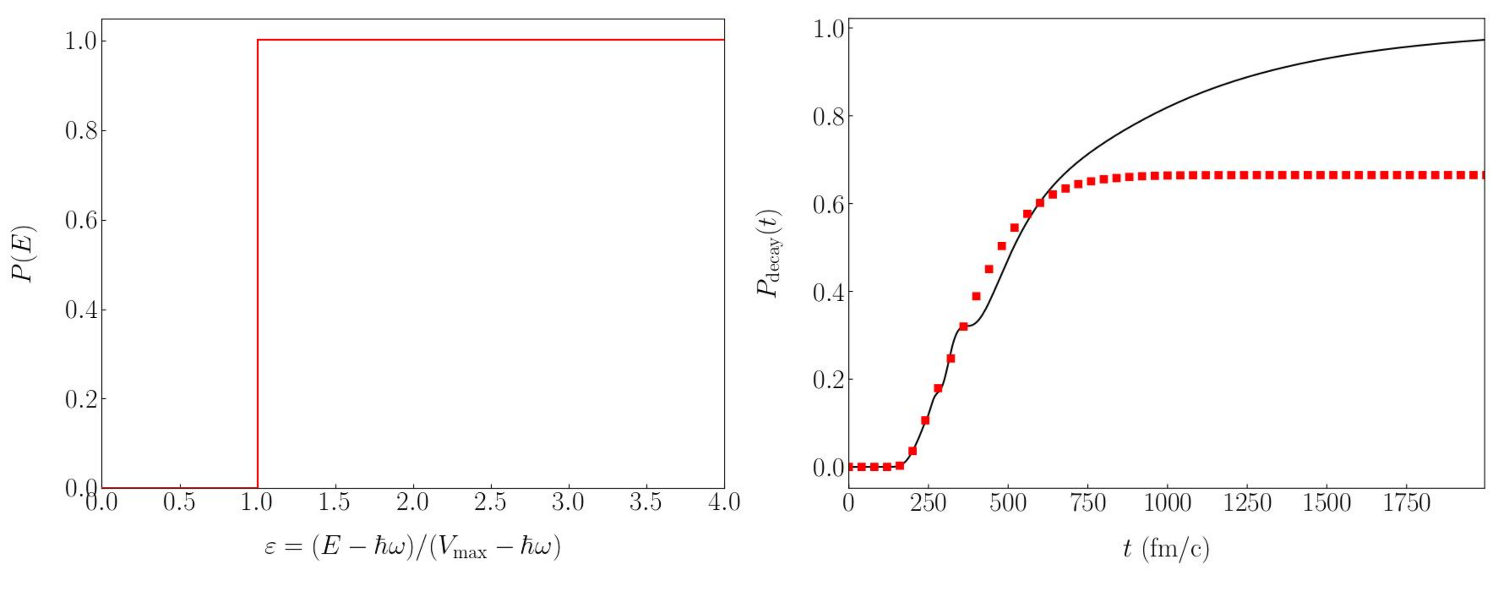

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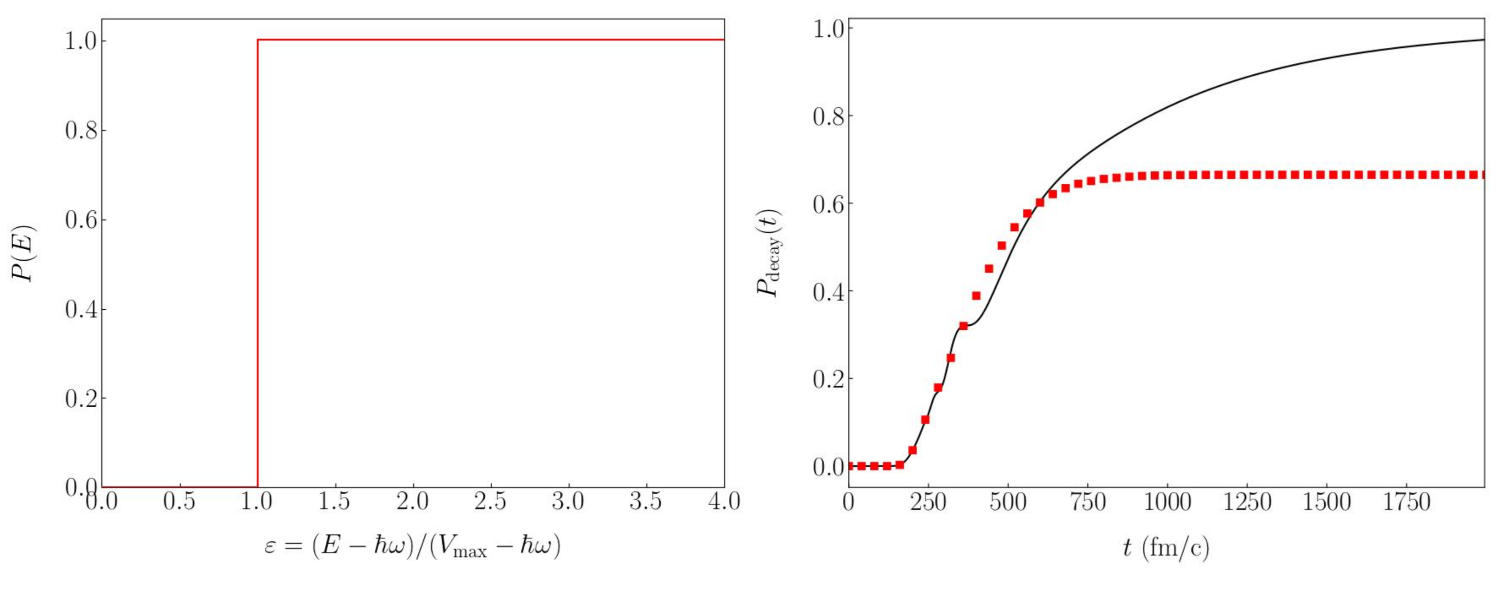

Particles of high energy escape

But wrong asymptote !

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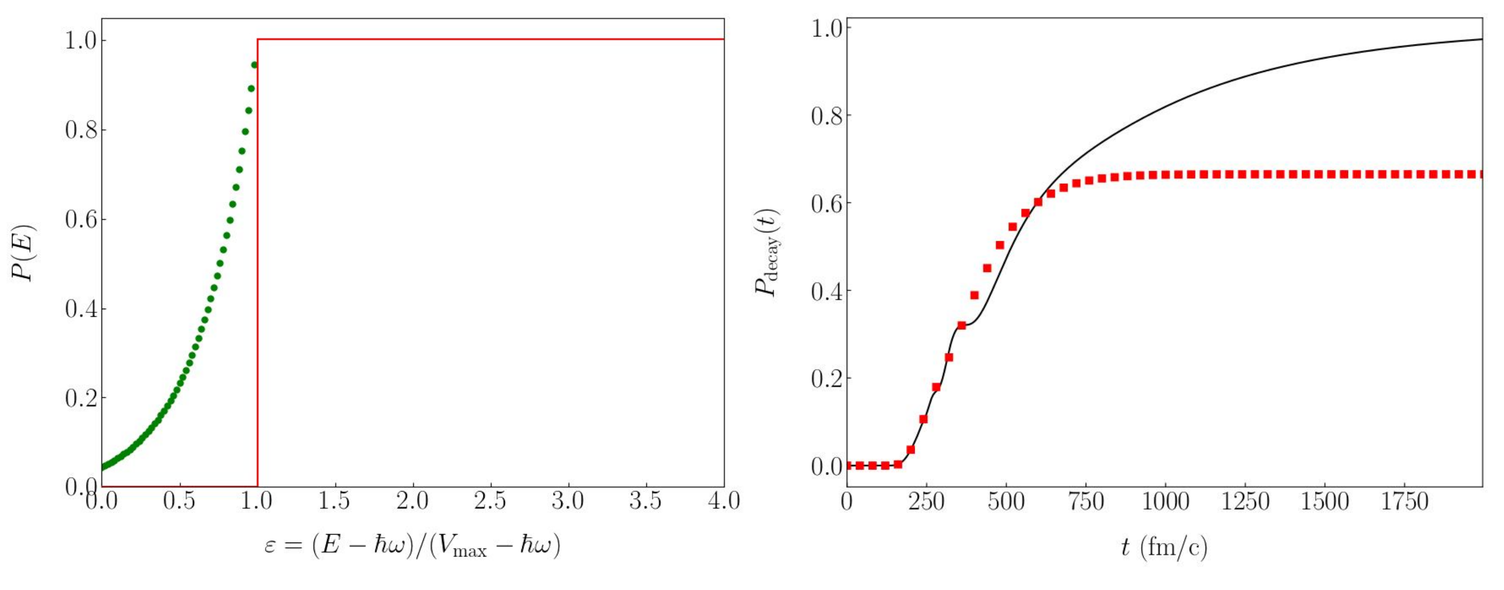

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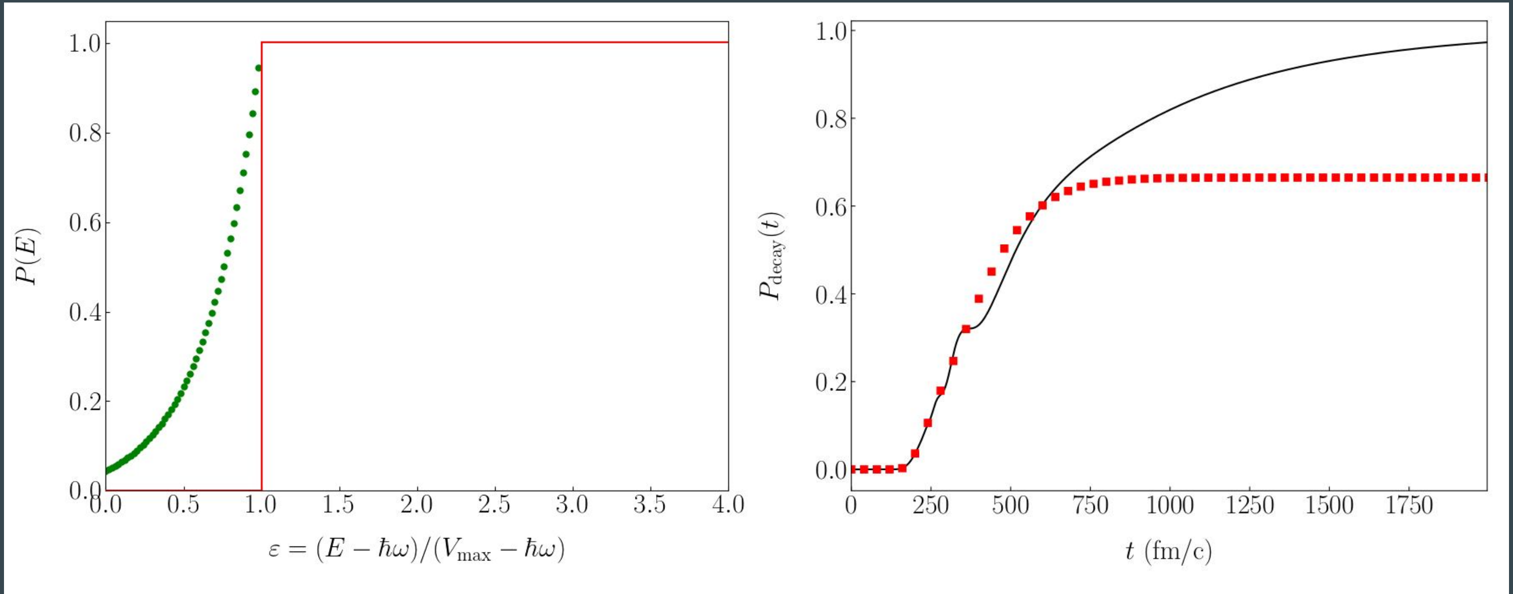

Better but wrong timescales !
Some particles are trapped for too long in the well.

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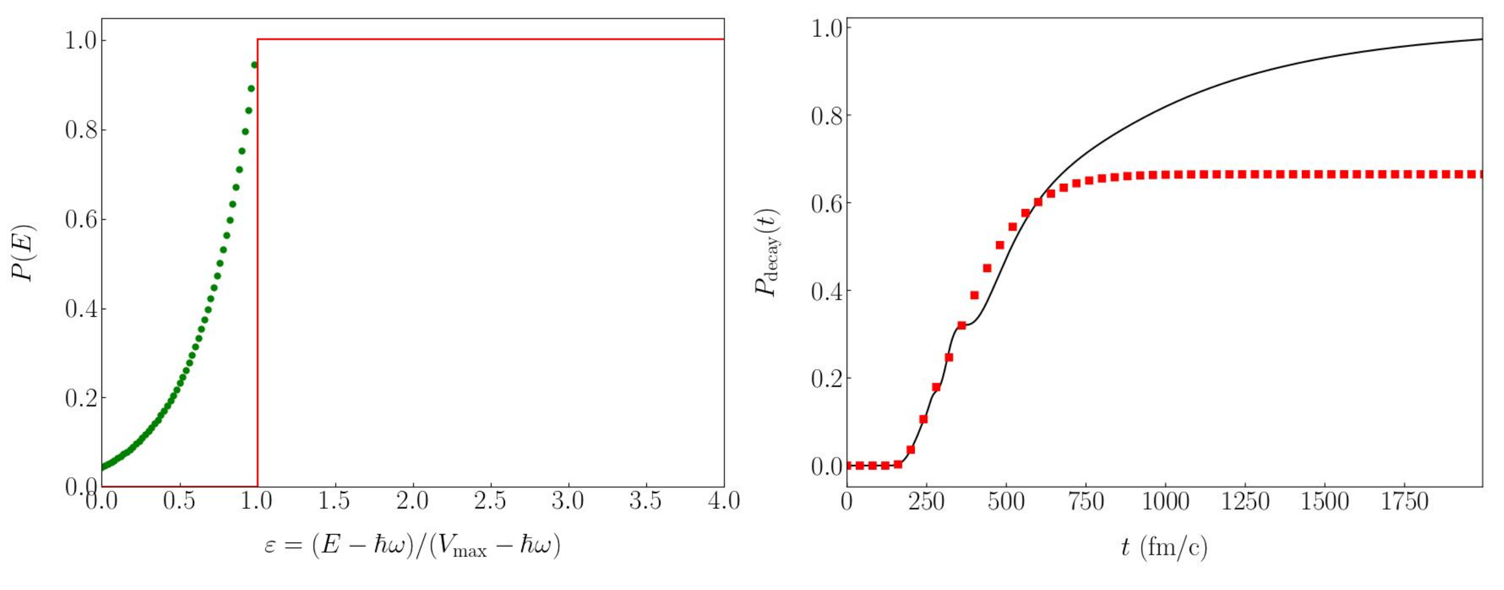

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Can a good probability distribution even be constructed ?

Investigation by inference

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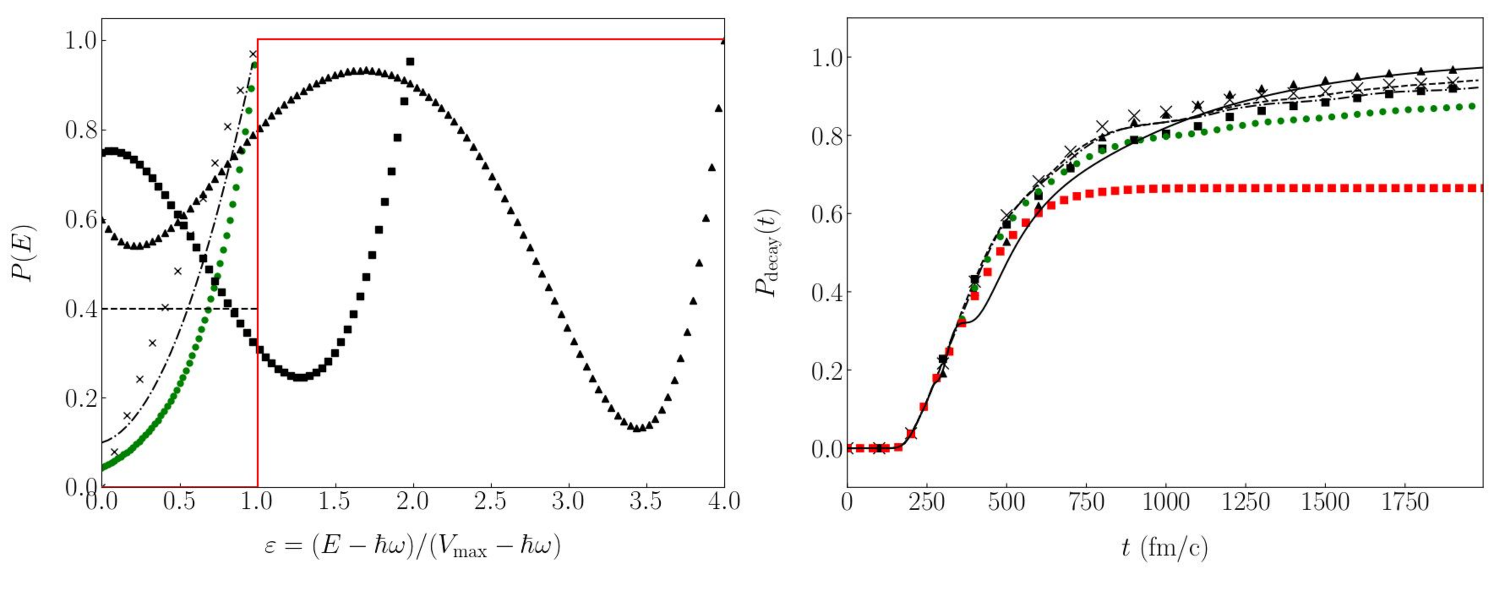
Construction of $P(E)$ by inference using Lagrange polynomials



It works, but possibly unphysical...

Need for a more proper way of defining trajectories along with quantum effects

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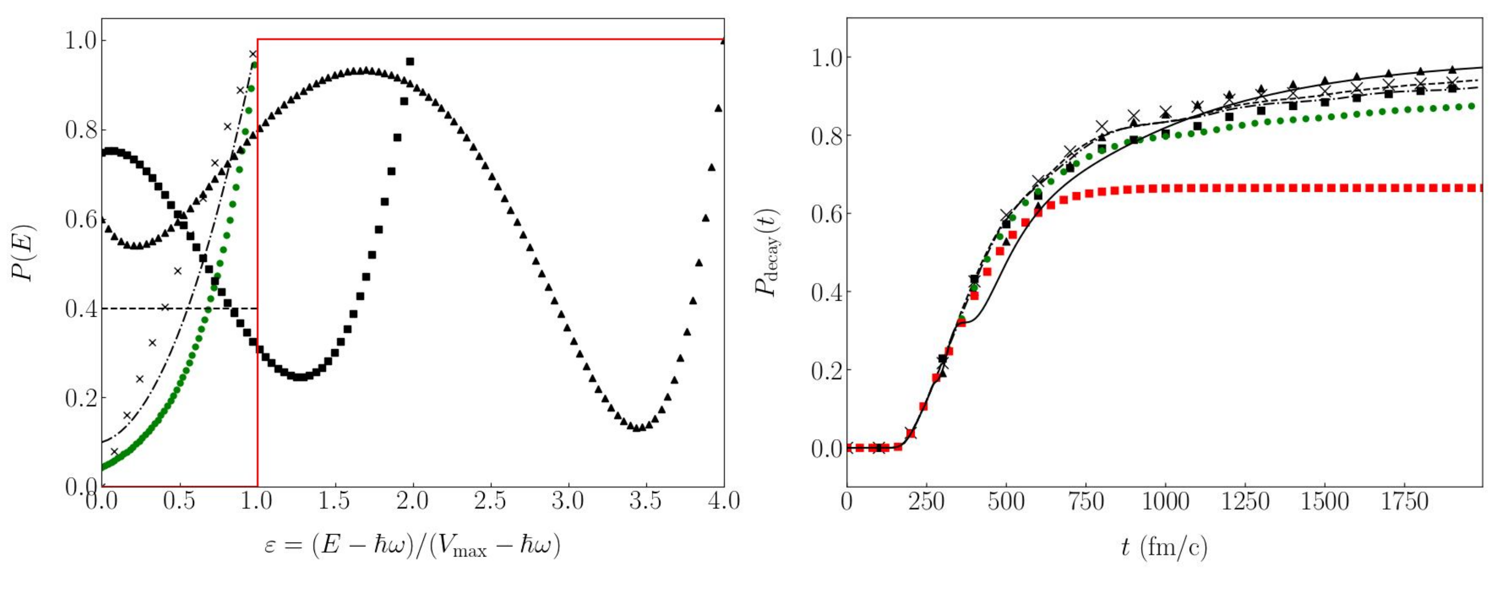

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Empirical method

Several other ways to explore:

1) Phase-Space formulations

2) Bohmian Mechanics

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Introducing trajectories in a fully Quantum framework

Time-dependent Schrödinger equation

Wavefunction $\Psi(q, t)$

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Probability density ρ and vector current $\mathbf{j}$

Quantum Hydrodynamics
Madelung Equations

$$\partial_t \rho = -\nabla [\rho v]$$

$$\partial_t S = -\frac{1}{m}\nabla \left[V + Q(t)\right]$$

Distributions as averages of trajectories

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Distributions as averages of trajectories

Trajectory-based formulations $(q_k(t), p_k(t))$

Bohmian Mechanics
Newton-like equations
with Bohmian potential $Q(t)$

$$m\frac{d}{dt}v(q(t),t) = -\nabla\left(V(q) + Q[\rho(t)]\right)$$

$$Q(t) = -\frac{\hbar^2}{2m}\frac{\nabla\sqrt{\rho}}{\sqrt{\rho}}$$

Bohmian mechanics

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

High density of probability: repulsive force

$f(t)$ spreading of wave packet

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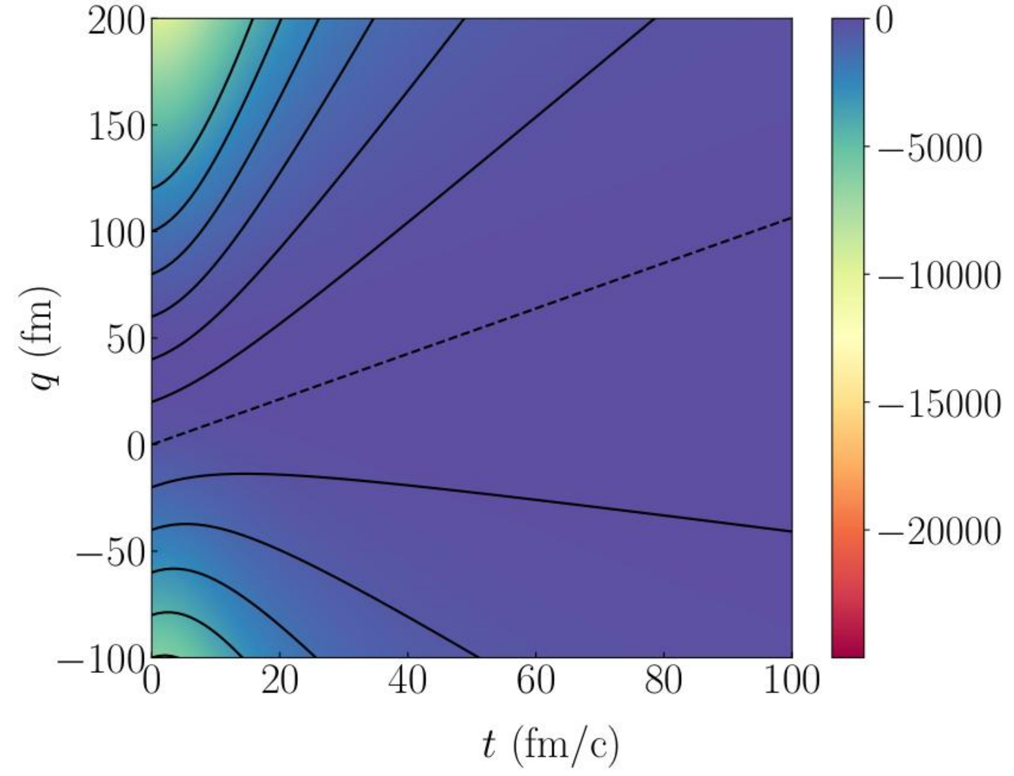
Sudden and dominant behavior of Bohm over the potential



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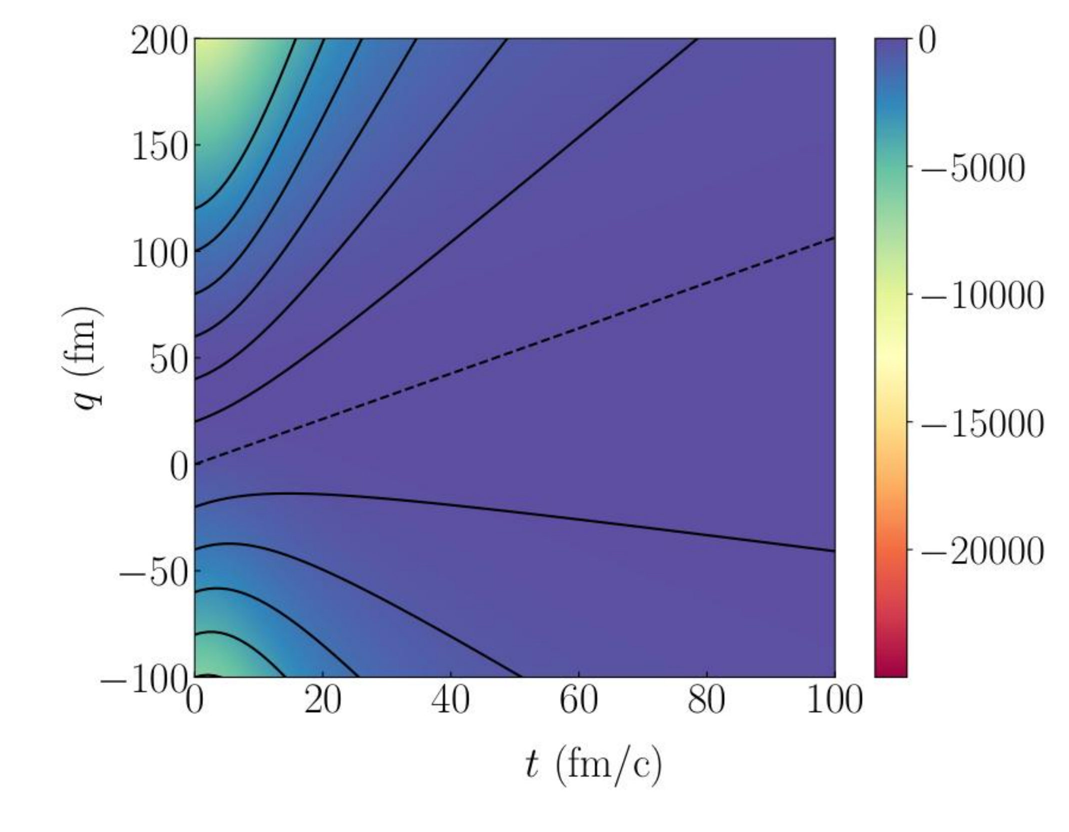

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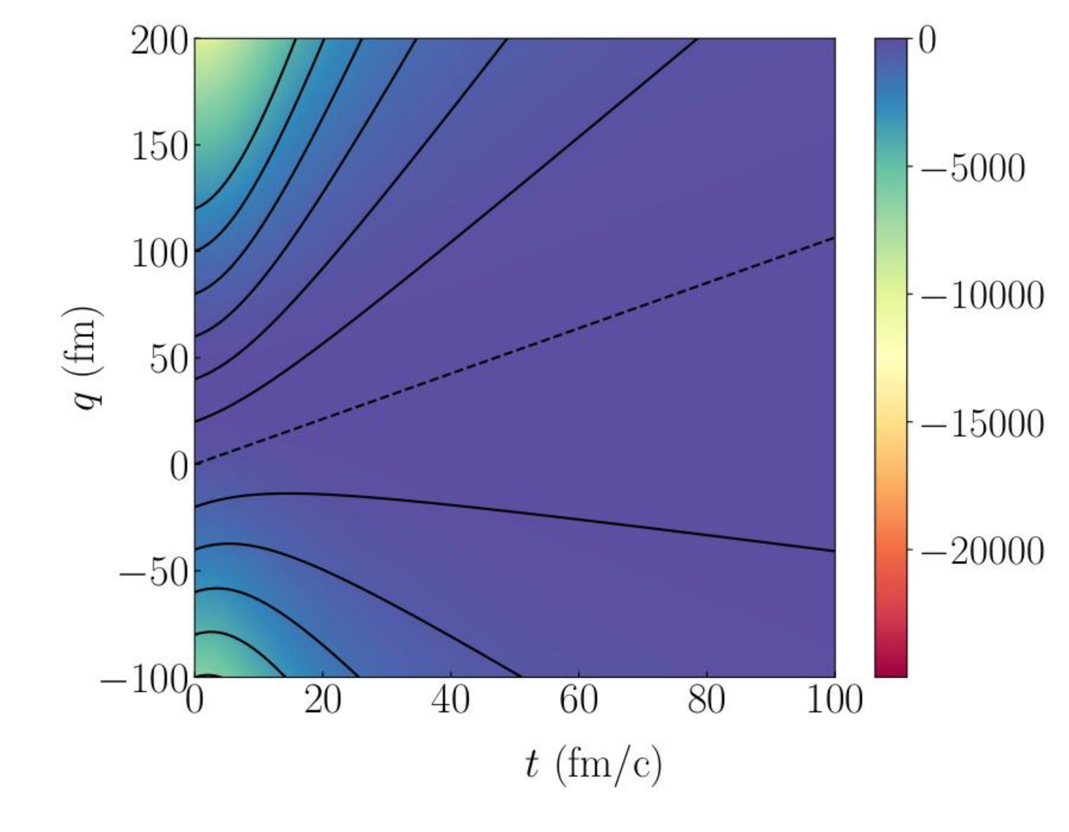

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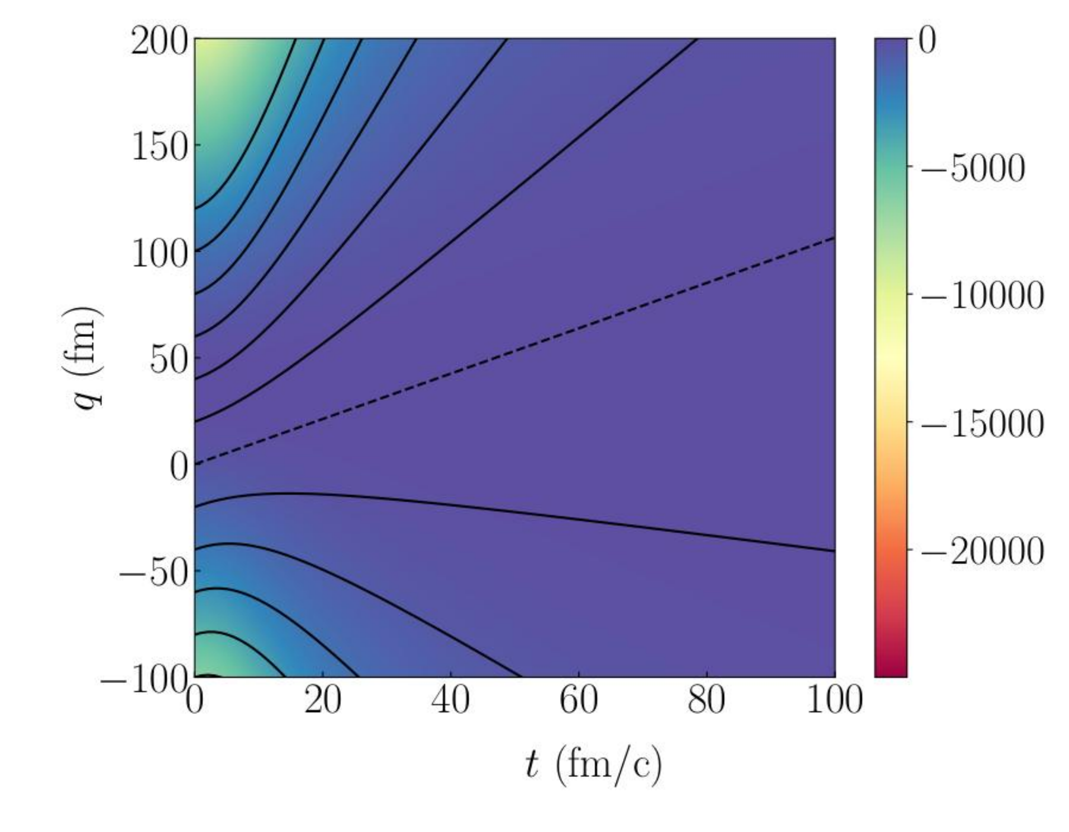

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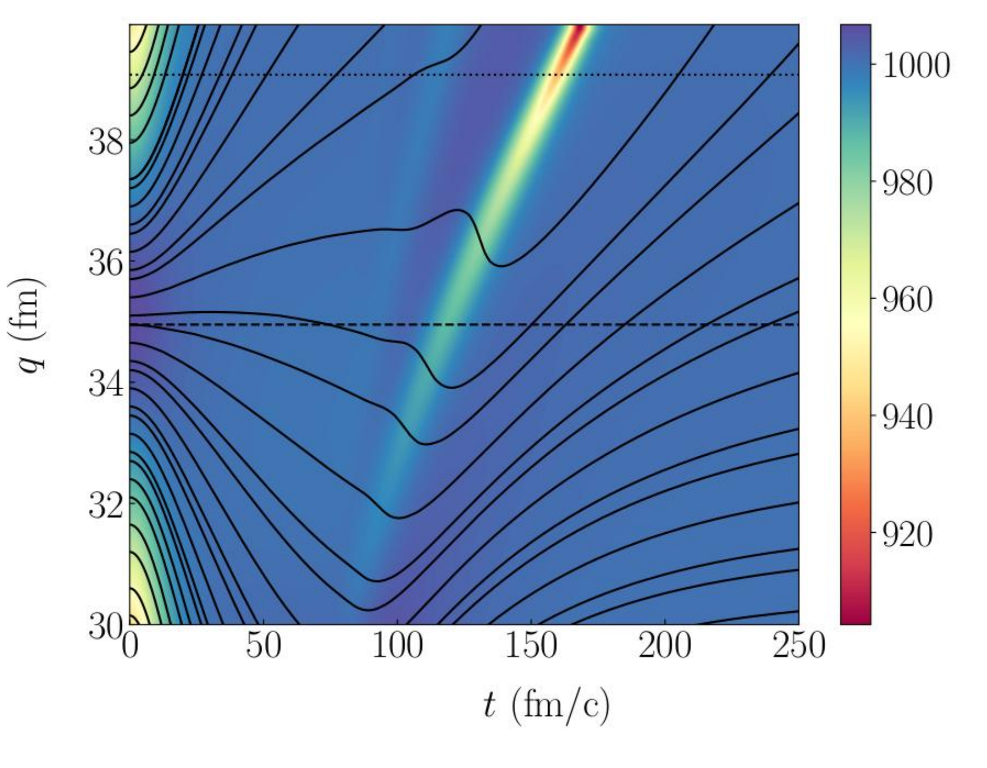

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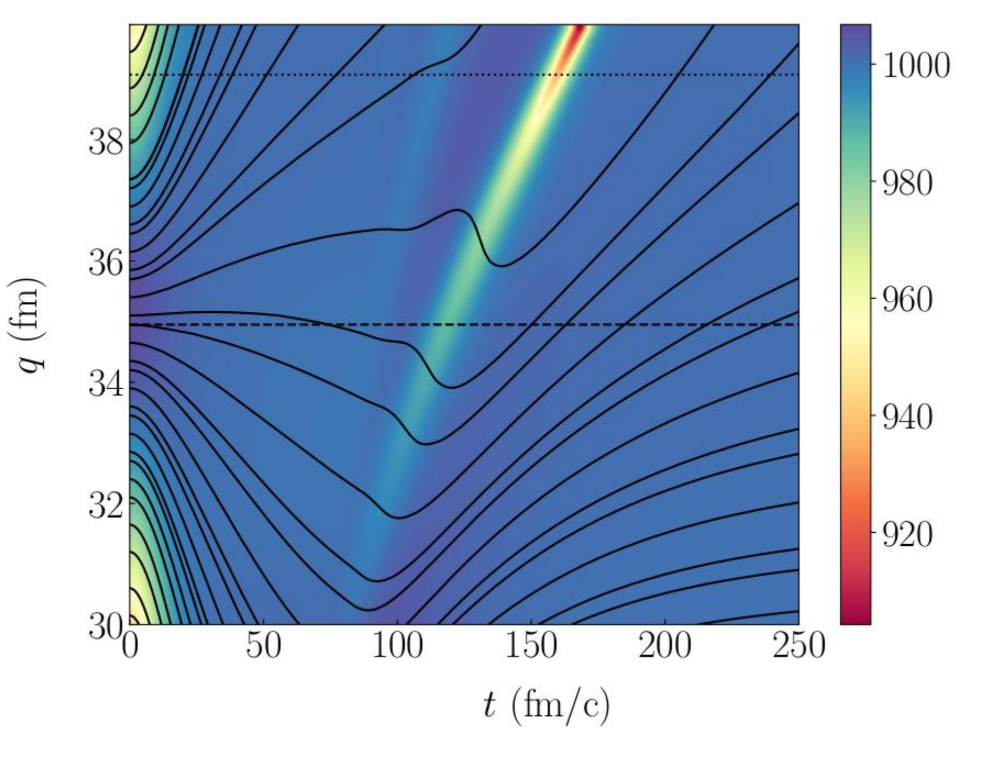

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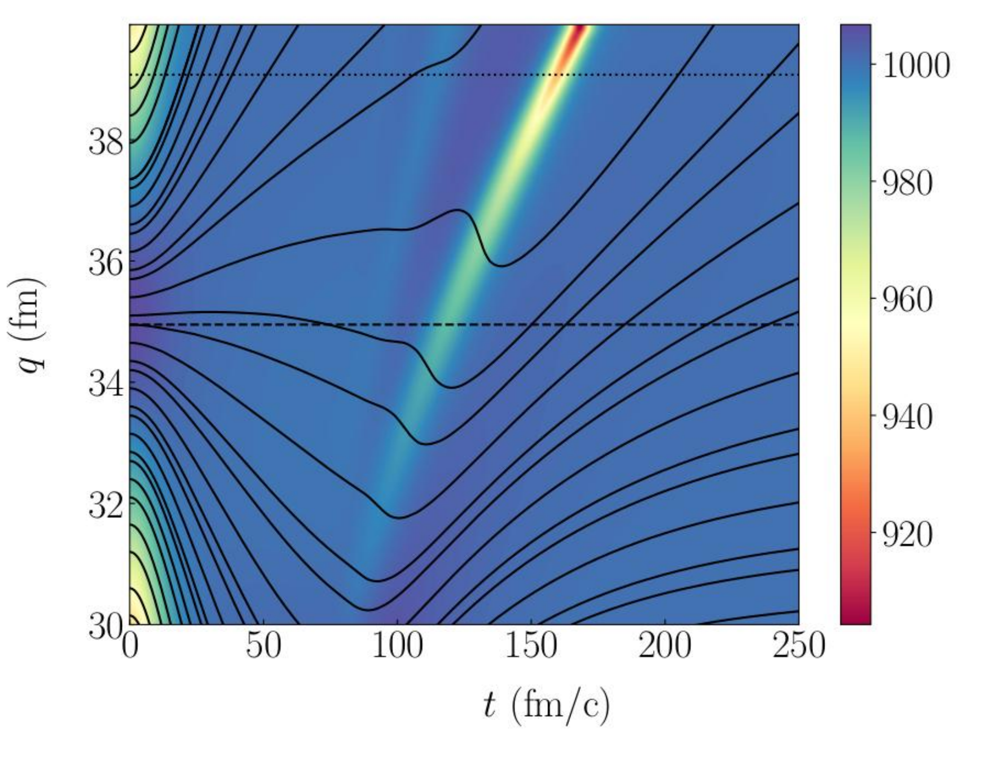

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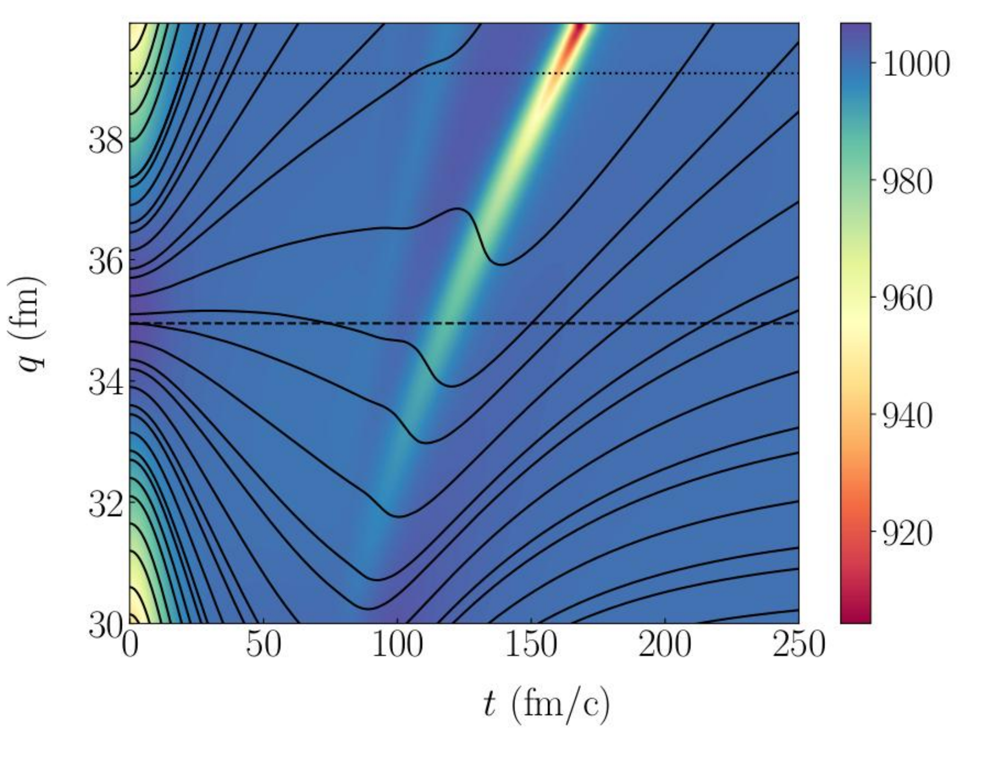

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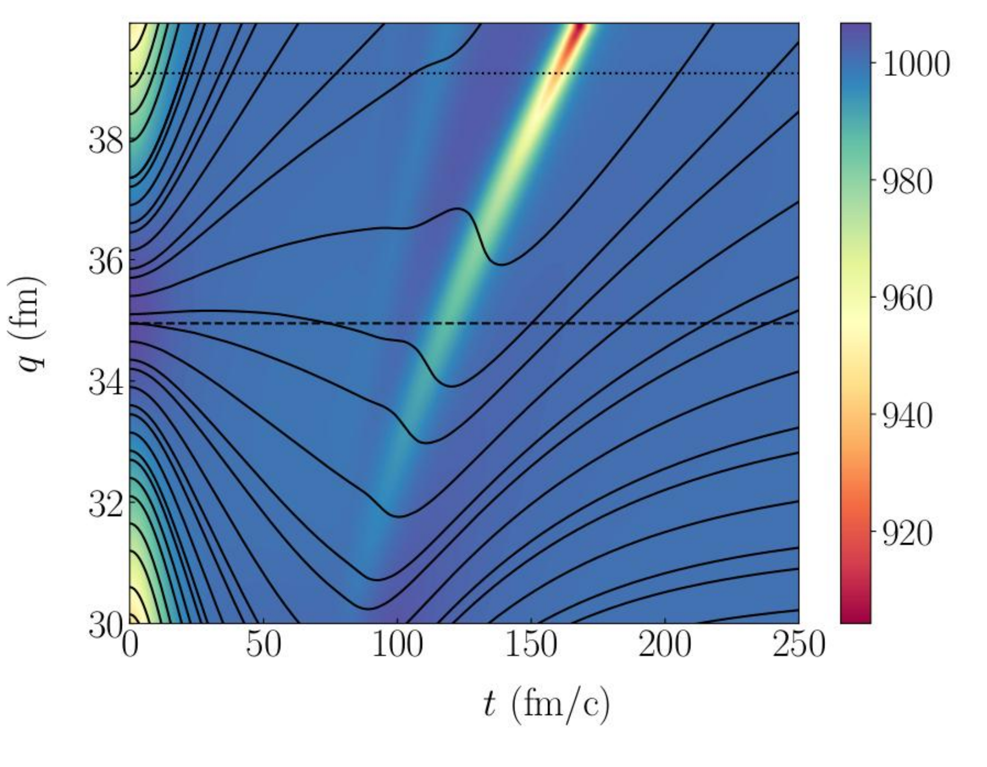
Bohm: lowers the potential barrier to allow the particles escape



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2) Simplifications of HPS for realistic applications
3) Implementation of collisional integrals in realistic applications (e.g. spallation)

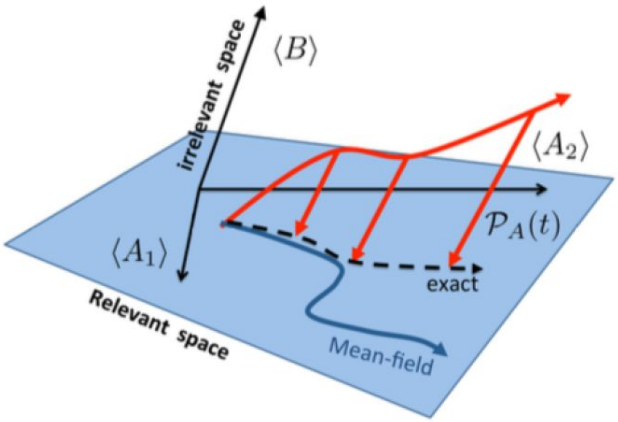
THANKS FOR LISTENING

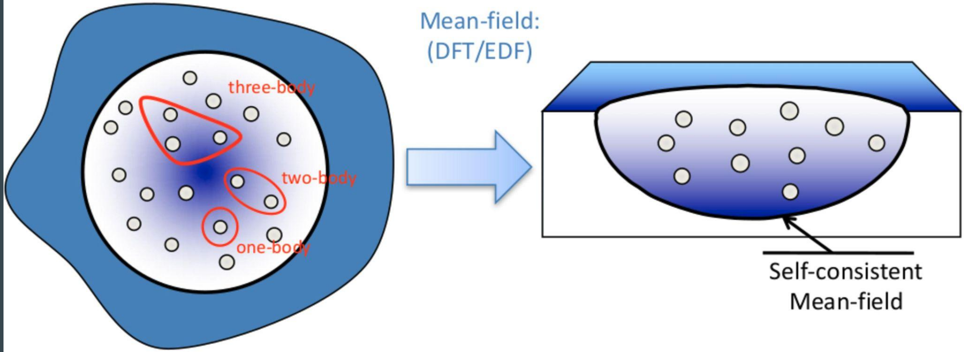
Usual approach: mean-field theories

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

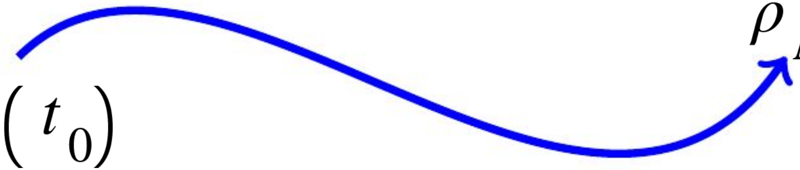
1) Effective Hamiltonian $h_{MF}(\rho)$
2) Self-consistent equations of motion

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





$\rho(t_0)$



$\rho_{MF}(t)$

Beyond Mean-Field theories ?

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

Phase-space:

1) sampling of initial conditions mimicking quantum correlations

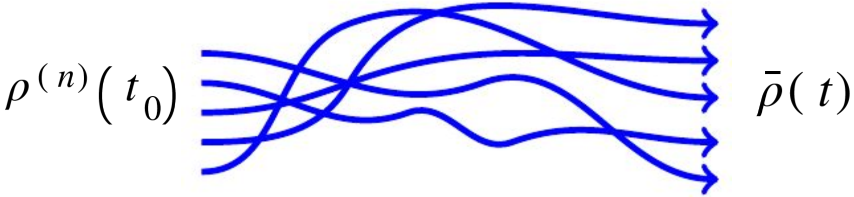
$$\rho^{(n)}(t_0) = \rho(t_0) + \delta\rho^{(n)}(t_0)$$

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

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



- 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).

Introducing trajectories in a fully QM framework