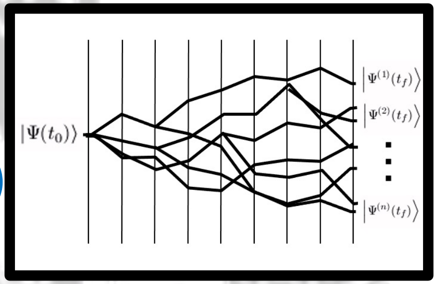
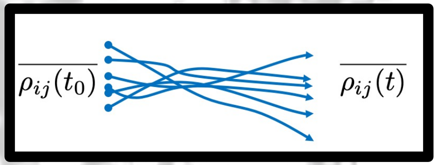
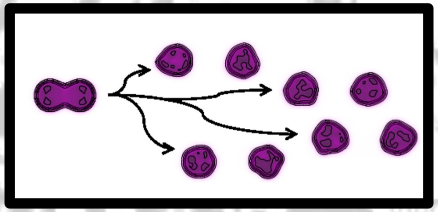
Quantum Stochastic methods for the N-body "Nuclear" problem

Denis Lacroix [IJCLab-Orsay]

- Exact quantum jump method in real-time (Hubbard-Stratonovich)
- Approximate quantum jump method for in-medium collisions
- Phase-space approaches for Fermi systems
- Applications







General strategy

S. Levit, PRC21 (1980) 1594.

Given a Hamiltonian and an initial State

$$|\Phi(t+\Delta t)\rangle = \exp\left(\frac{\Delta t}{i\hbar} H\right)|\Phi(t)\rangle$$

Write H into a quadratic form

$$H|\Phi\rangle = \left(H_1 - O^2\right)|\Phi\rangle$$

The many-body problem

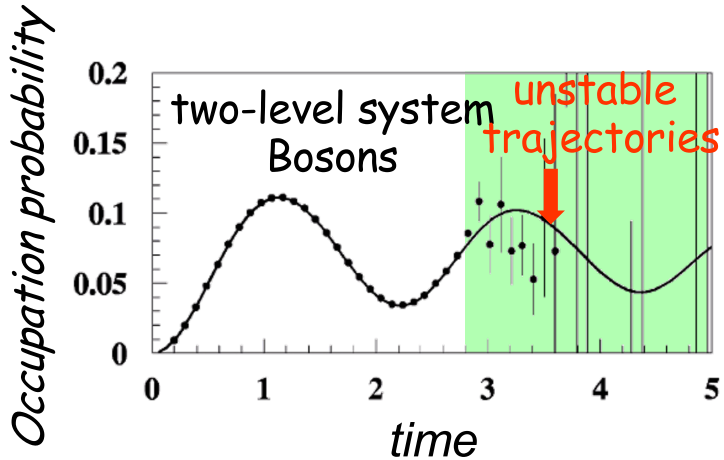
$$H = \sum_{ij} T_{ij} a_i^+ a_j + \frac{1}{4}\sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k$$

O_{ij} $\qquad$ $O_{il}\, O_{jk}$

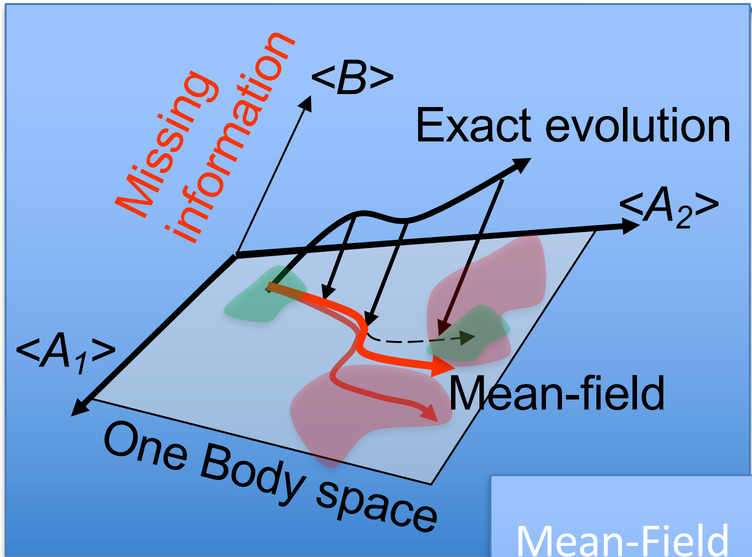
- The method is general.
  the SSE are deduced easily

  ➡ extension to Stochastic TDHFB
  DL, arXiv nucl-th 0605033
- The mean-field appears naturally and the interpretation is easier
- the numerical effort can be reduced by reducing the number of observables

but…



D. Lacroix, Ann. of Phys. 322 (2007).



Mean-Field
State: Slater det, QP vacuum
information: one-body DOFs

Correct for the improper
Evolution of initial quantum
Fluctuations with
Phase-space approaches

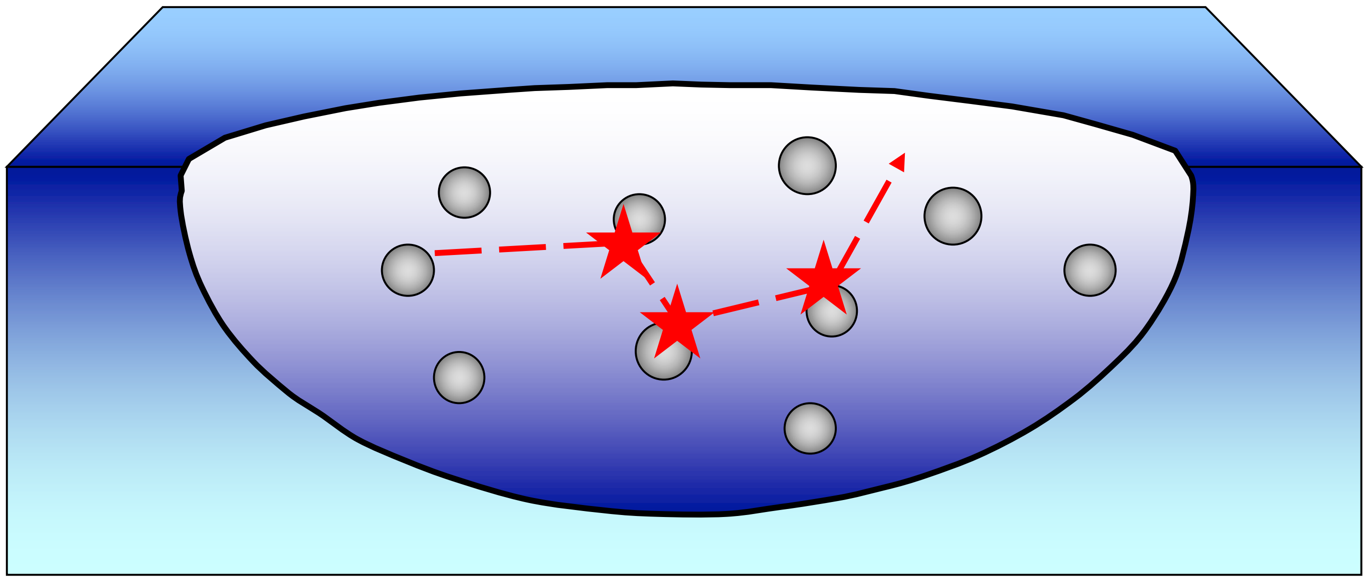
Correlation that built up in time

Ex: BBGKY
$(\rho_1, \rho_2, \cdots)$

Stochastic
unraveling

Replace the initial complex problem by an
ensemble of simpler problem
(mean-field like)

Correlations that built-up in time: in medium collisions



GOAL: Restarting from an uncorrelated (Slater) state $D = |\Phi_0\rangle\langle\Phi_0|$ we should:

1-have an estimate of $D = |\Psi(t)\rangle\langle\Psi(t)|$

2-interpret it as an average over jumps between “simple” states

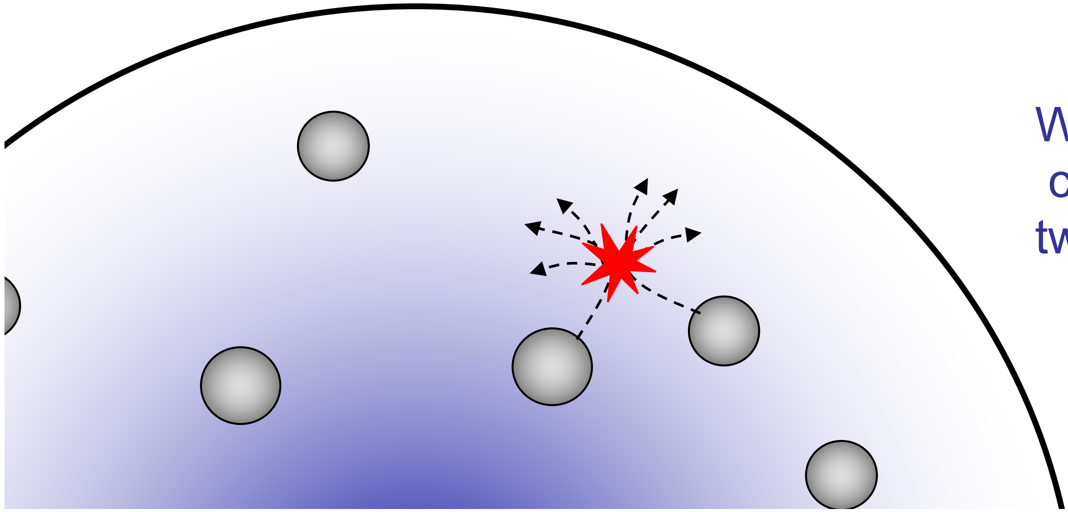
Weak coupling approximation : perturbative treatment

Reinhard and Suraud, Ann. of Phys. 216 (1992)

$$|\Psi(t')\rangle = |\Phi(t')\rangle - \frac{i}{\hbar}\int \delta v_{12}(s)|\Phi(s)\rangle\, ds - \frac{1}{2\hbar^2}T\left(\int\int \delta v_{12}(s)\delta v_{12}(s')\,ds\,ds'\right)|\Phi(s)\rangle$$

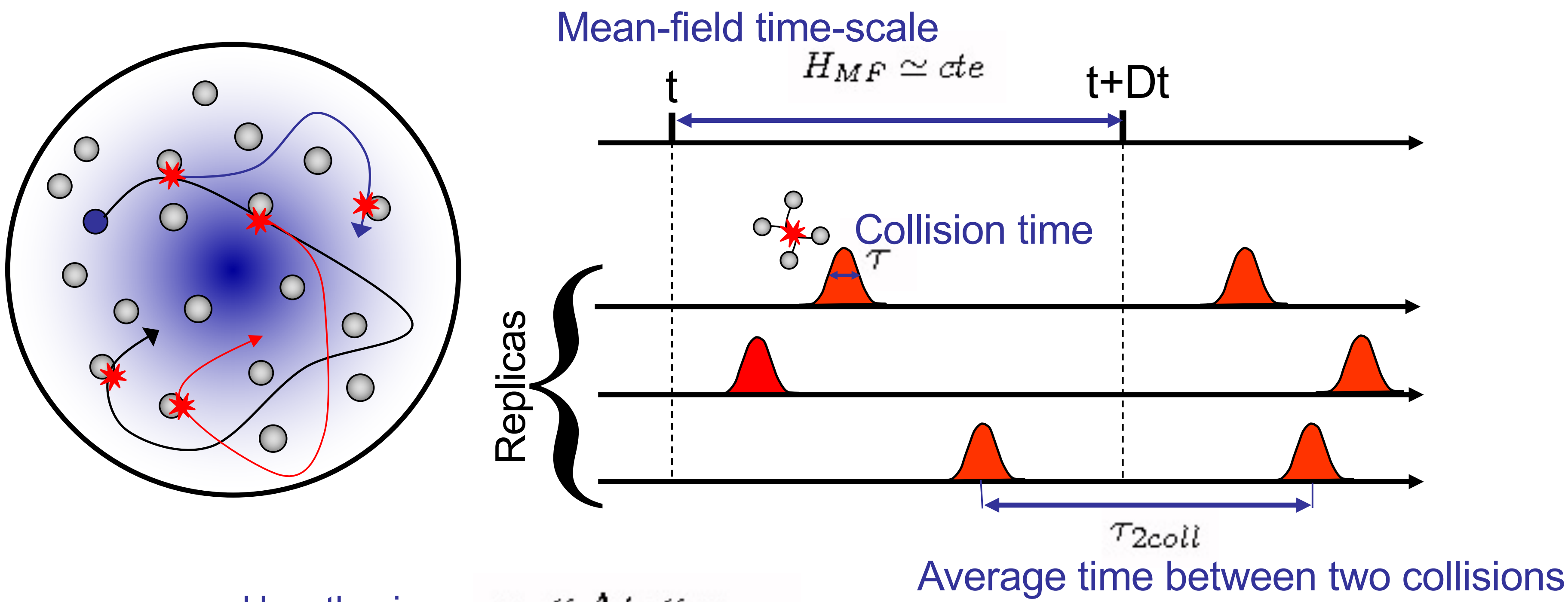
Residual interaction in the mean-field interaction picture

Statistical assumption in the Markovian limit :



We assume that the residual interaction can be treated as an ensemble of two-body interaction:

$$\begin{cases} \overline{\delta v_{12}(s)} = 0 \\ \overline{\delta v_{12}(s)\delta v_{12}(s')} \propto \overline{\delta v_{12}^2(s)}\, e^{-(s-s')^2/2\tau^2} \end{cases}$$



Hypothesis : $\tau \ll \Delta t \ll \tau_{2coll}$

Average Density Evolution:

$$\overline{\Delta D} = \frac{\Delta t}{i\hbar}[H_{MF}, D] - \frac{\tau \Delta t}{2\hbar^2}\overline{[\delta v_{12}, [\delta v_{12}, D]]}$$

One-body density
Master equation
step by step

$$\overline{\Delta D} = \frac{\Delta t}{i\hbar}[H_{MF}, D] - \frac{\tau \Delta t}{2\hbar^2}\overline{[\delta v_{12}, [\delta v_{12}, D]]}$$

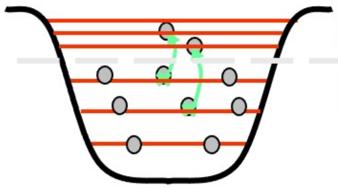
Initial simple state

$$D = |\Phi\rangle\langle\Phi|$$
$$\rho = \sum_\alpha |\alpha\rangle\langle\alpha|$$

$$i\hbar\frac{d}{dt}\rho = [h_{MF}, \rho] - \frac{\tau}{2\hbar^2}\mathcal{D}(\rho)$$

with $\langle j|\mathcal{D}|i\rangle = \overline{\left\langle\left[\left[a_i^+ a_j, \delta v_{12}\right], \delta v_{12}\right]\right\rangle}$

2p-2h nature
of the interaction



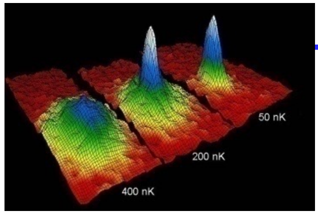
$$\mathcal{D}(\rho) = Tr_2\,[v_{12}, C_{12}]$$

with
$$C_{12} = (1-\rho_1)(1-\rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2 v_{12}(1-\rho_1)(1-\rho_2)$$

Separability of the interaction $v_{12} = \sum_\lambda O_\lambda(1) O_\lambda(2)$

$$\mathcal{D}(\rho) = \sum_k \gamma_k\,(A_k A_k \rho + \rho A_k A_k - 2A_k \rho A_k)$$

- Dissipation contained in Extended TDHF is included
- The master equation is a Lindblad equation
- Associated SSE *DL, PRC73 (2006)*



Application to Bose-Einstein condensates

1D bose condensate with gaussian two-body interaction

N-body density: $D = |N:\alpha\rangle\langle N:\alpha|$

SSE on single-particle state :

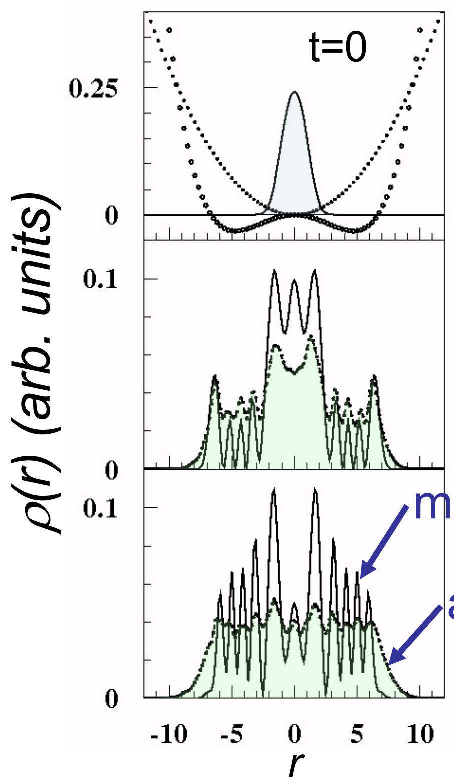
$$d|\alpha\rangle = \left\{ \frac{dt}{i\hbar} h_{MF}(\rho) + \sum_k dW_k (1-\rho) A_k - \frac{dt\tau}{2\hbar^2} \sum_k \gamma_k \left[A_k^2 \rho + \rho A_k \rho A_k - 2 A_k \rho A_k \right] \right\} |\alpha\rangle$$

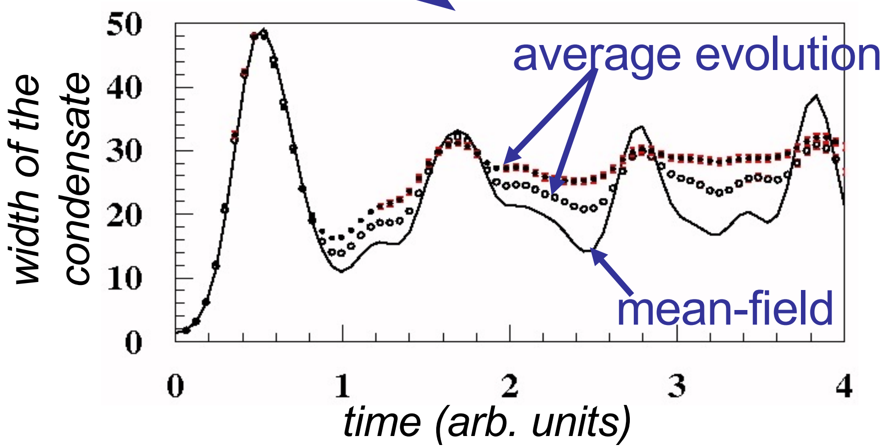
with $dW_k dW_{k'} = -\frac{dt\tau}{\hbar^2} \gamma_k \delta_{kk'}$

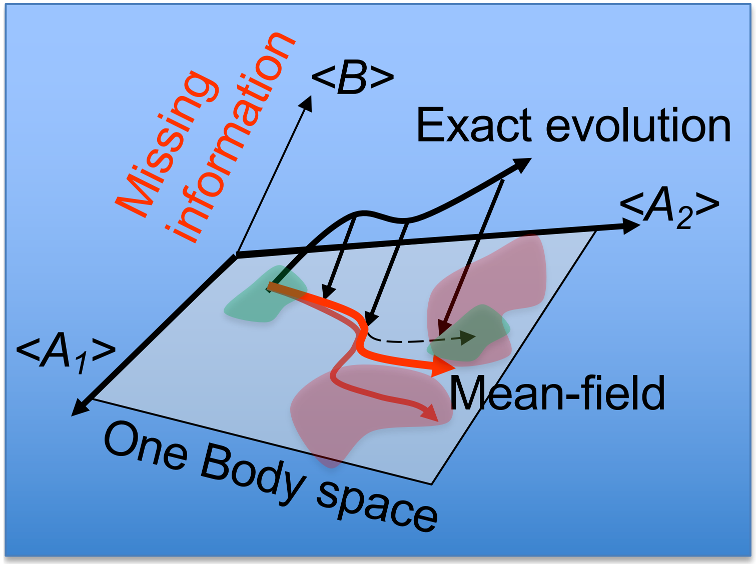
The numerical effort is fixed by the number of A_k

Density evolution

Condensate size

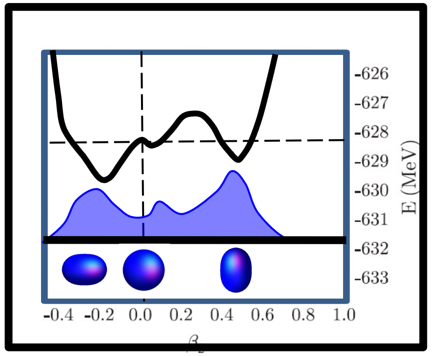






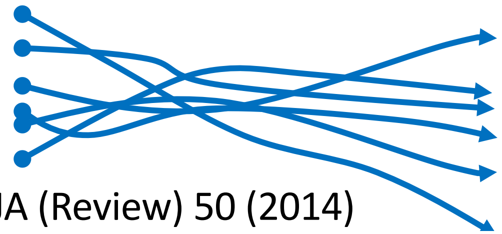
Correlations that are here initially and propagates can play a major role

A typical example in nuclear physics: deformation



Phase-space approach for Fermi systems

$\overline{\rho_{ij}(t_0)}$

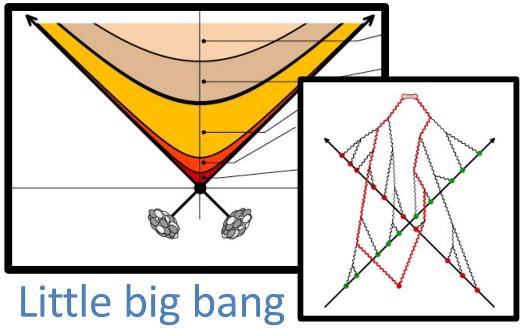


$\overline{\rho_{ij}(t)}$

Lacroix, Ayik, EPJA (Review) 50 (2014)

Note that phase-space approach are used in many fields of physics

Particle physics



Little big bang

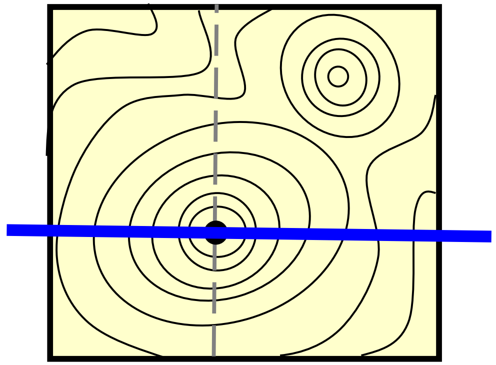
Gelis, Schenke, arxiv 2016

Cold atoms: the truncated Wigner approach

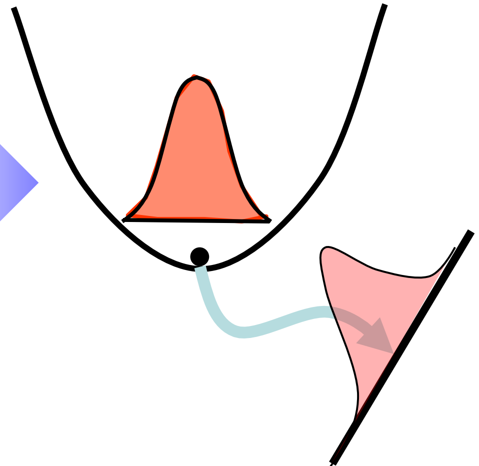
Sinatra, Lobo, Castin, J. Phys. B 35 (2002)

What is the idea behind phase-space methods?

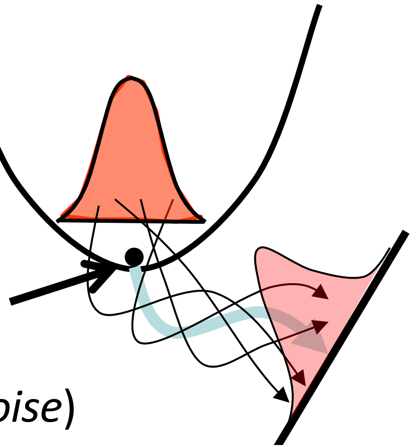
Collective energy landscape



Wave evolution



Many-classical trajectories



NB: there are many Phase-space Methods, especially for Bosons

(see Gardiner, Zoller, *Quantum noise*)

Illustration

Solution 1: Schroedinger Eq.

$$i\hbar \frac{d|\phi\rangle}{dt} = h|\phi\rangle$$

Ex: Wigner transform

$$f(r,p,t)$$

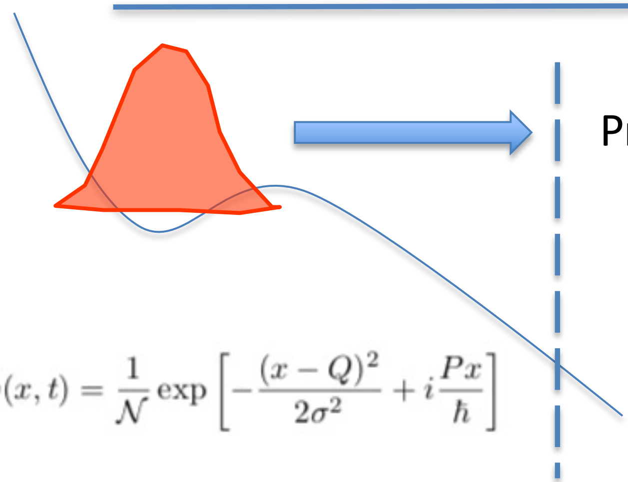
+ dynamical evolution

Classical mechanics With random initial fluctuations

$$\dot{r}^{\lambda} = p^{\lambda}/m$$

$$\dot{p}^{\lambda} = -\partial_r V(r^{\lambda})$$

Example: decay properties

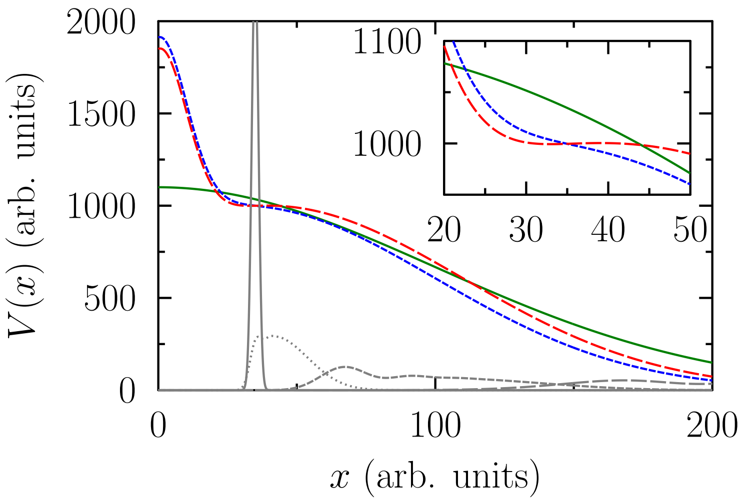


$$\varphi(x,t) = \frac{1}{\mathcal{N}} \exp\left[-\frac{(x-Q)^2}{2\sigma^2} + i\frac{Px}{\hbar} \right]$$

Probability to decay?

Quantum mechanics

$$i\hbar\dot{\varphi}(x,t) = H(x)\varphi(x,t)$$



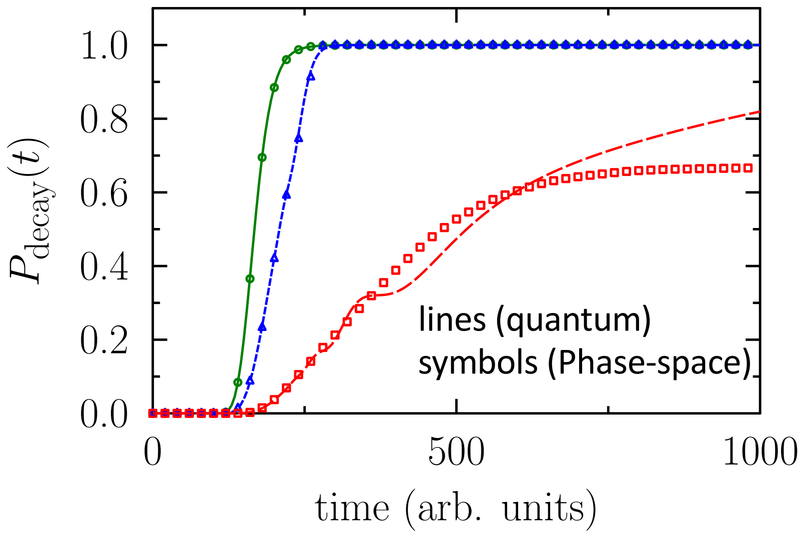
Phase-space equivalent

Sampling according to:

$$W(q,p) = \frac{1}{(2\pi\sigma_p\sigma_q)} \exp\left\{ -\frac{(q-q_0)^2}{2\sigma_p^2} - \frac{(p-p_0)^2}{2\sigma_p^2} \right\}$$

Followed by a set of classical evolution

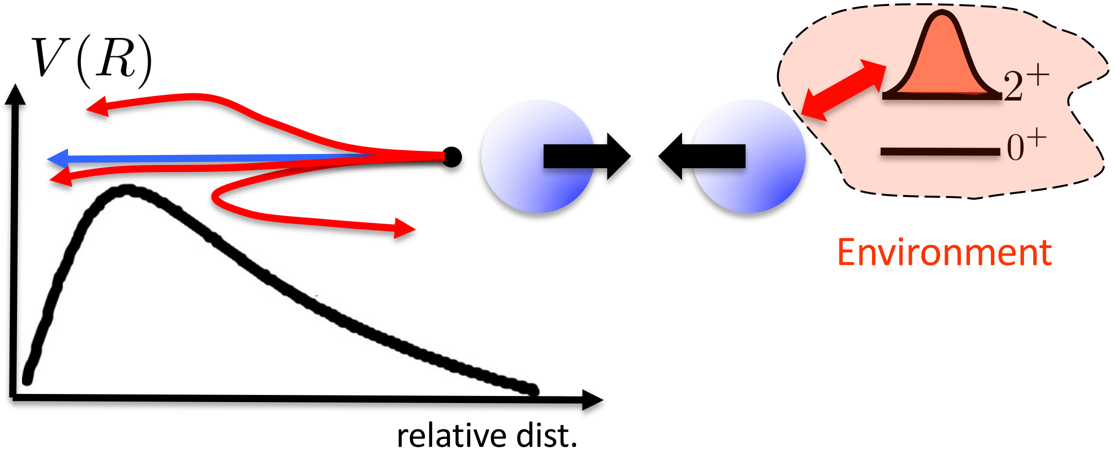
$$\begin{cases} \dot{Q}^{(n)} = P^{(n)}(t)/m \\ \dot{P}^{(n)}(t) = F(P^{(n)}(t), Q^{(n)}(t)) \end{cases}$$

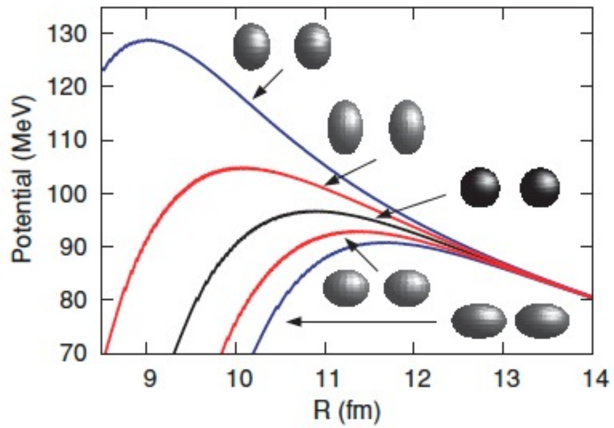


(see talk T. Czuba)

This works surprisingly well if "true" quantum effects have a weak effect !

Stochastic semi-classical treatment of discrete channels



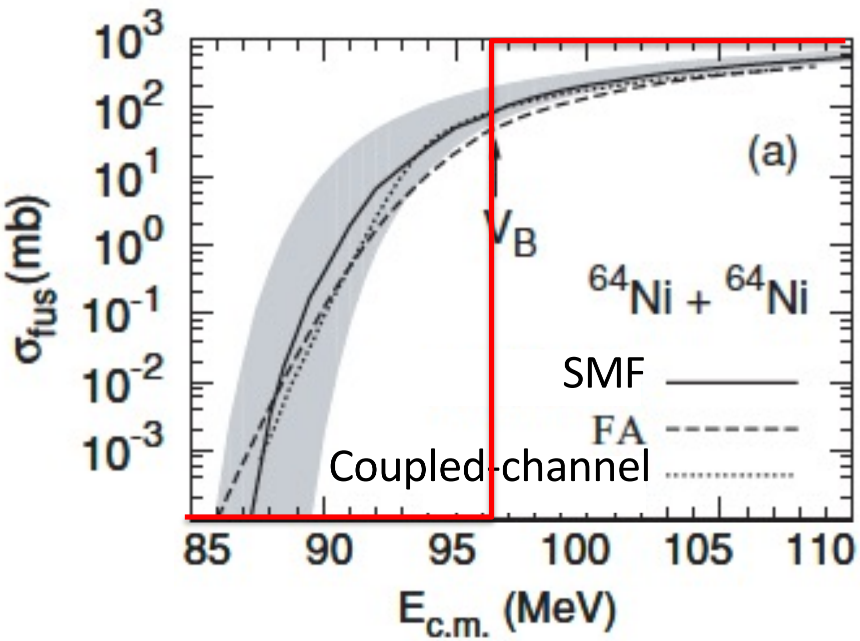


Collective Motion + Coupling

$$H = \frac{P^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu R^2} + V_C(R) + V_N(R, \Omega, \alpha_{i\lambda})$$
$$+ \sum_{i=1}^{2} \sum_{\lambda=0}^{N-1} \left[\frac{\Pi_{i\lambda}^2}{2D_{i\lambda}} + \frac{1}{2} C_{i\lambda} \alpha_{i\lambda}^2 \right],$$

Discrete Channels

Esbensen et al, PRL 41 (1978)



Ayik, Yilmaz, Lacroix, PRC81 (2010)

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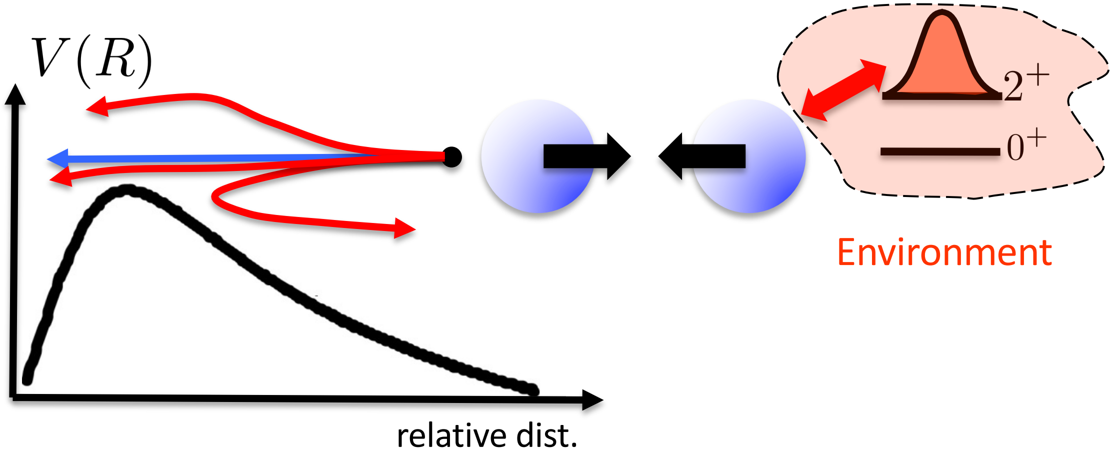

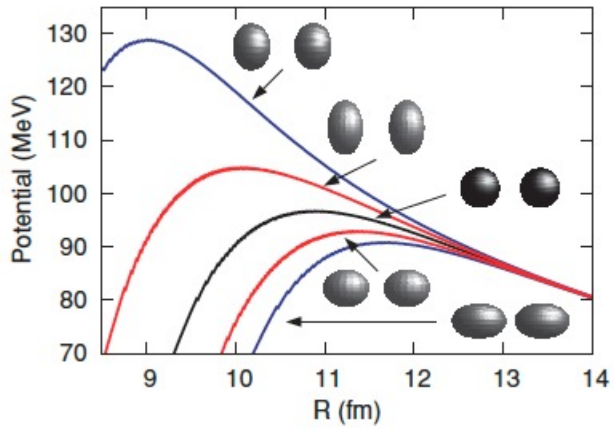

Collective Motion

+ Coupling

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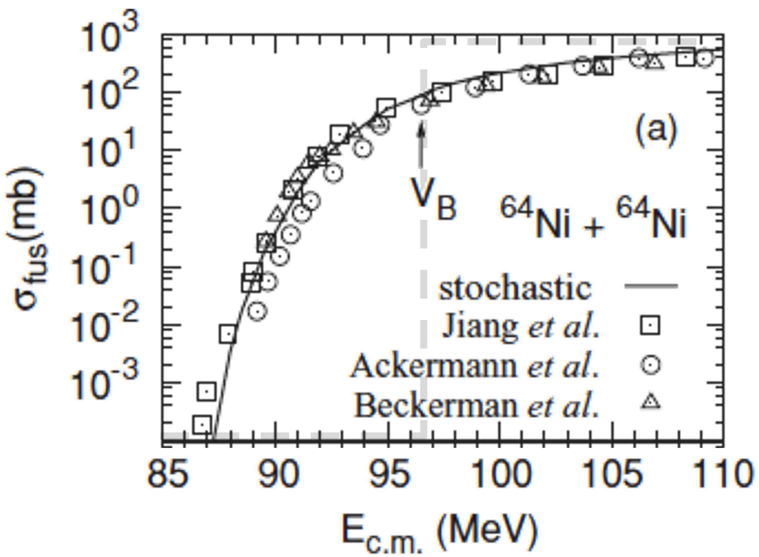
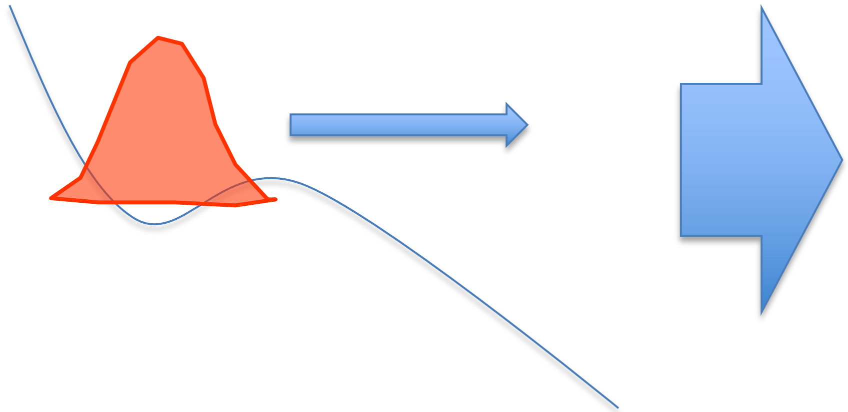


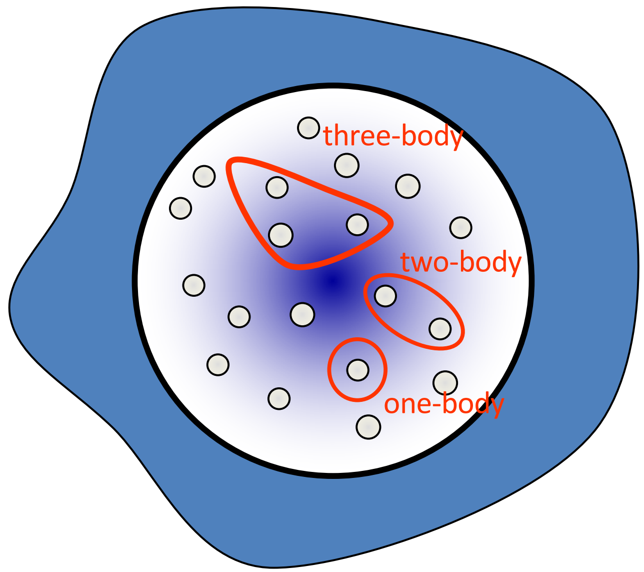
Ayik, Yilmaz, Lacroix, PRC81 (2010)

Exporting Phase-space methods to the many-body problem

Simple quantum problems

Complex quantum many-body systems





Important questions/constraints:

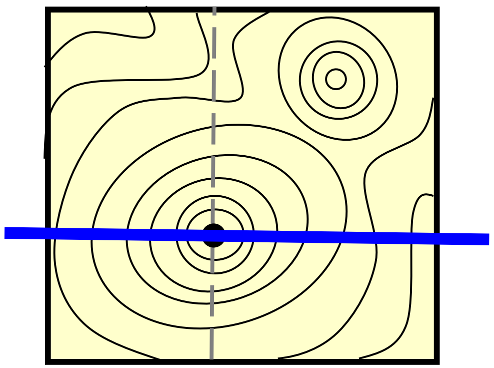
How to design the initial fluctuations ?

Initial fluctuations should reproduce in average quantum fluctuations.

What is the equivalent to classical mechanics ?

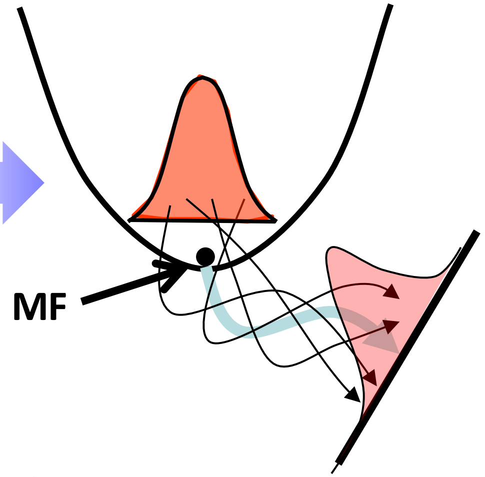
Time-dependent Hartree-Fock theory is a good candidate of “classical like” limit.

Collective phase-space



Ayik, Phys. Lett. B 658, (2008).

Quantum fluctuations



The dynamics is described by a set of mean-field evolutions with random initial conditions

Mean-Field theory

$$\frac{d\langle A_\alpha \rangle}{dt} = \mathcal{F}\left(\{\langle A_\beta \rangle\}\right)$$ at all time $\sigma_Q^2 = \langle A^2 \rangle - \langle A \rangle^2$

Stochastic Mean-Field

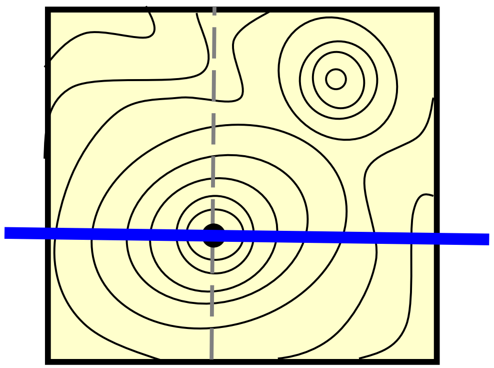
$$\frac{dA_\alpha^{(n)}}{dt} = \mathcal{F}\left(\{A_\beta^{(n)}\}\right)$$

$$\{A_\alpha^{(n)}\}$$

at all time $\Sigma_C^2 = \overline{A^{(n)} A^{(n)}} - \overline{A^{(n)}}^2$

Constraint: $\Sigma_C^2(t=0) = \sigma_Q^2(t=0)$

The stochastic mean-field (SMF) concept applied to many-body problem



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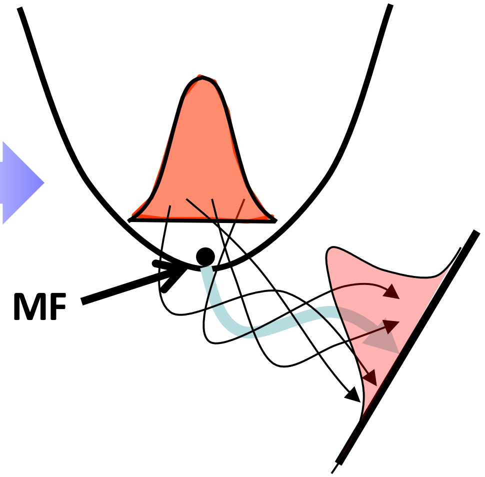


The dynamics is described by a set of mean-field evolutions with random initial conditions

The average properties of initial sampling should identify with properties of the initial state.

SMF in density matrix space

$$\rho(\mathbf{r},\mathbf{r}',t_0) = \sum_i \Phi_i^*(\mathbf{r},t_0) n_i \Phi_j(\mathbf{r}',t_0)$$

$$\Downarrow$$

$$\rho^\lambda(\mathbf{r},\mathbf{r}',t_0) = \sum_{ij} \Phi_i^*(\mathbf{r},t_0) \rho_{ij}^\lambda \Phi_j(\mathbf{r}',t_0)$$

$$\Rightarrow$$

$$\overline{\rho_{ij}^\lambda} = \delta_{ij} n_i$$

$$\overline{\delta\rho_{ij}^\lambda \delta\rho_{j'i'}^\lambda} = \frac{1}{2}\delta_{jj'}\delta_{ii'}\left[n_i(1-n_j) + n_j(1-n_i)\right].$$

SMF in collective space

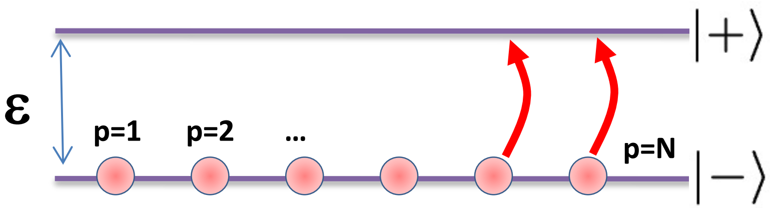
$$Q(t_0) \Downarrow Q^\lambda(t_0)$$

$$\Rightarrow$$

$$\overline{Q}^\lambda(t_0) = Q(t_0)$$

$$\sigma_Q(t_0) = \overline{\left(Q^\lambda(t_0) - \overline{Q^\lambda(t_0)}^{\,2}\right)}$$

Lipkin Model



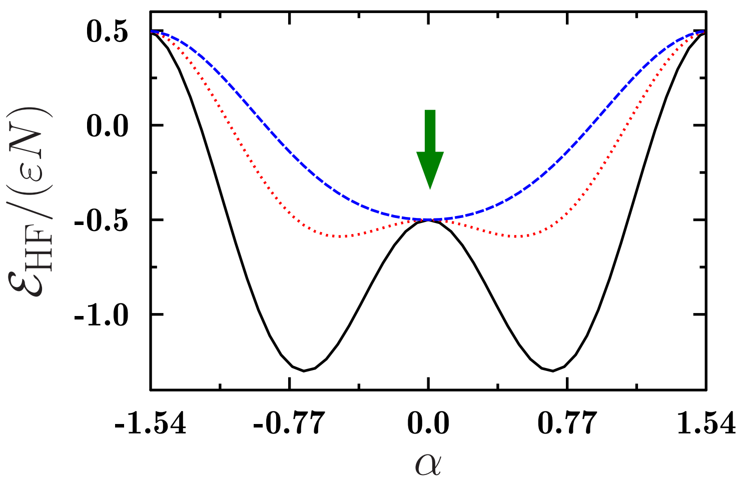
See for instance : Ring and Schuck book
Severyukhin, Bender, Heenen, PRC74 (2006)

$$H = \varepsilon J_0 - \frac{V}{2}(J_+J_+ + J_-J_-)$$

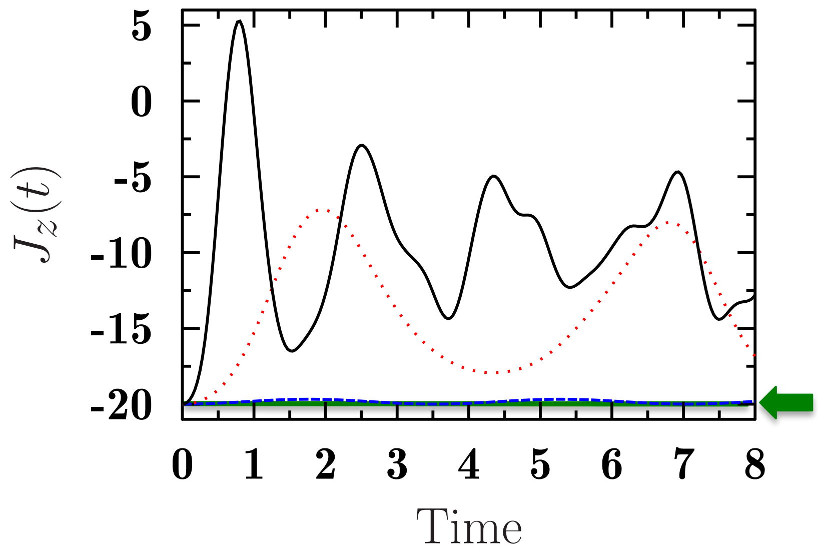
$$J_0 = \frac{1}{2}\sum_{p=1}^{N}\left(c^\dagger_{+,p}c_{+,p} - c^\dagger_{-,p}c_{-,p}\right) \qquad J_y = \frac{1}{2i}(J_+ - J_-)$$

$$J_+ = \sum_{p=1}^{N} c^\dagger_{+,p}c_{-,p}, \quad J_- = J_+^\dagger, \qquad J_x = \frac{1}{2}(J_+ + J_-)$$

N=40 particles

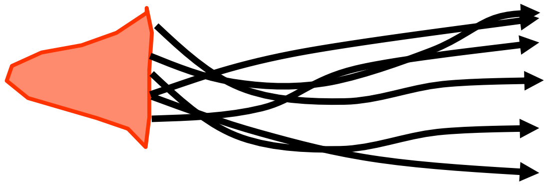


Exact dynamics

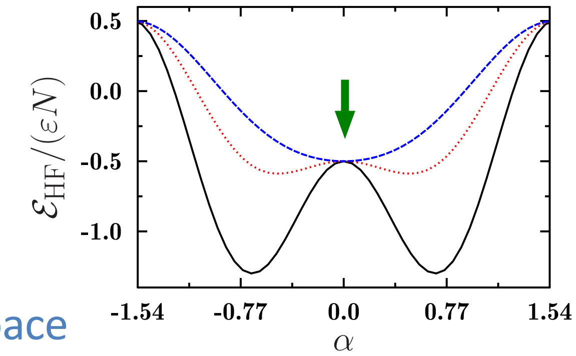


Mean-field is stationary

The stochastic mean-field solution



$\rho \rightarrow \rho^{\lambda}$



One-body observables

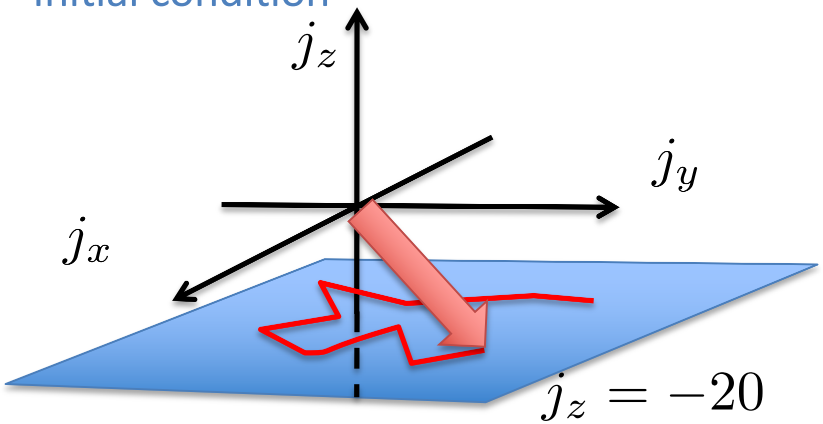
Formulation in quasi-spin space

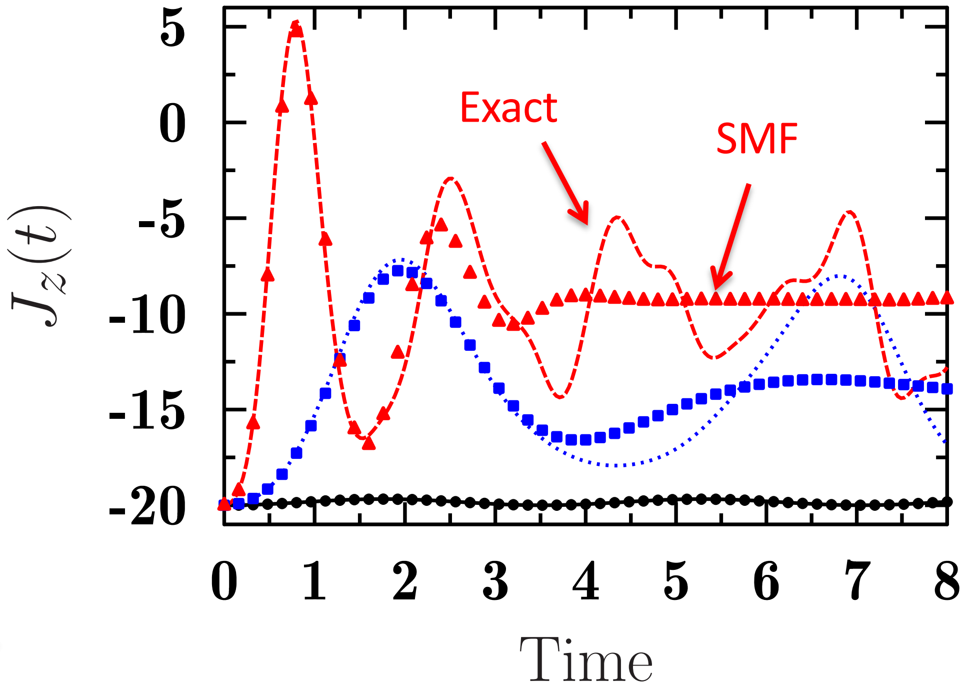
$j_i \equiv \langle J_i \rangle / N \rightarrow j_i^{\lambda}$

$$\overline{j_i^{\lambda}(t_0)} = 0$$

$$\overline{j_x^{\lambda}(t_0) j_x^{\lambda}(t_0)} = \overline{j_y^{\lambda}(t_0) j_y^{\lambda}(t_0)} = \frac{1}{4N}.$$

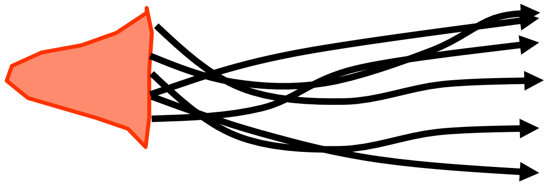
Initial condition



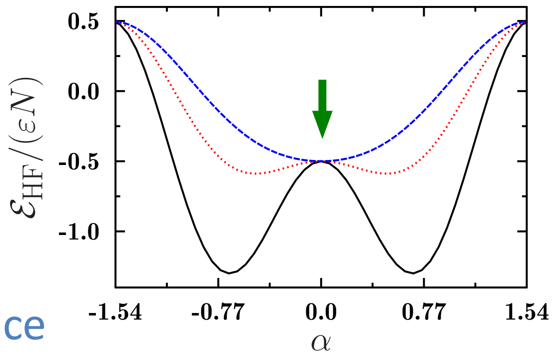


Lacroix, Ayik, Yilmaz, PRC 85 (2012)

The stochastic mean-field solution



$\rho \Rightarrow \rho^{\lambda}$



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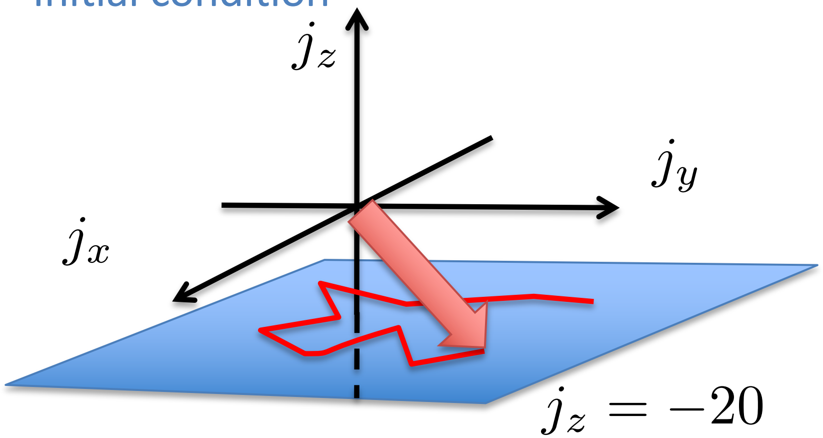
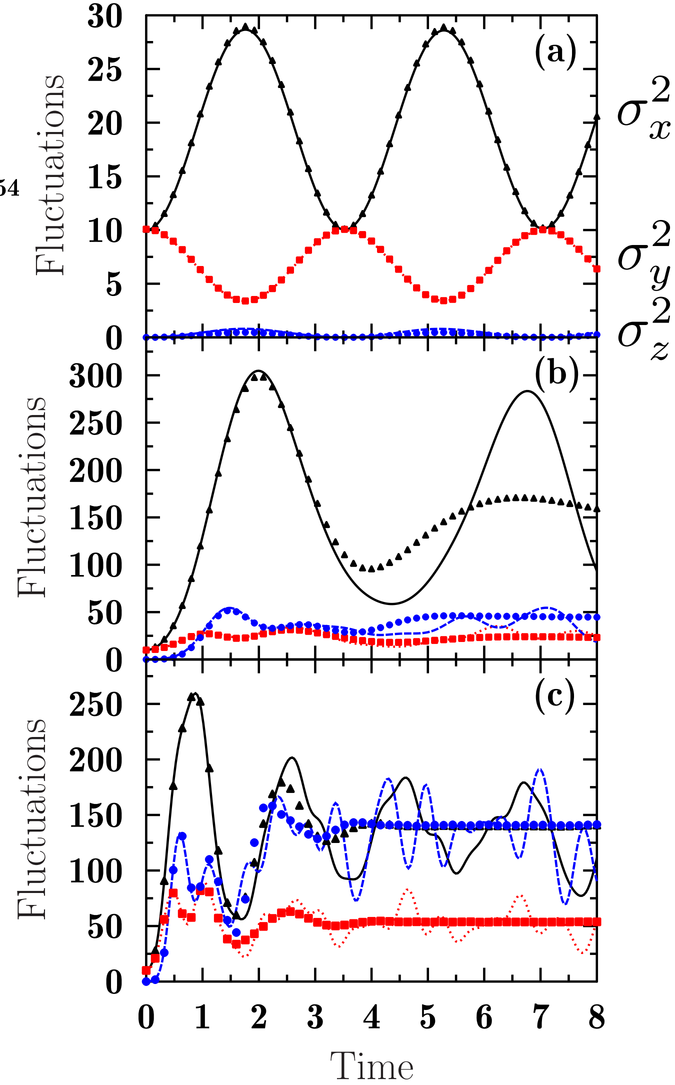
$$\overline{j_x^{\lambda}(t_0) j_x^{\lambda}(t_0)} = \overline{j_y^{\lambda}(t_0) j_y^{\lambda}(t_0)} = \frac{1}{4N}.$$

Initial condition



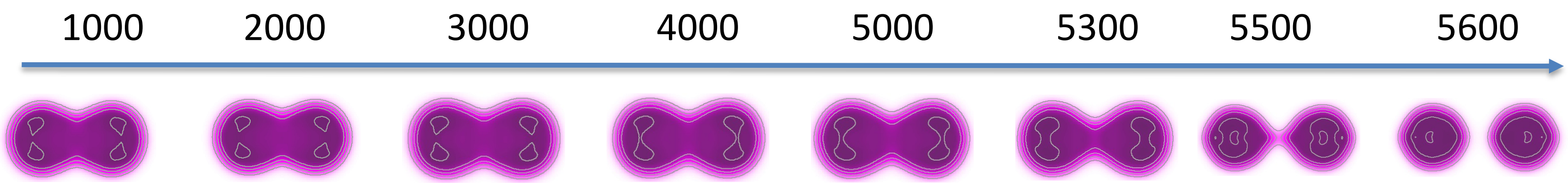
Lacroix, Ayik, Yilmaz, PRC 85 (2012)

Fluctuations

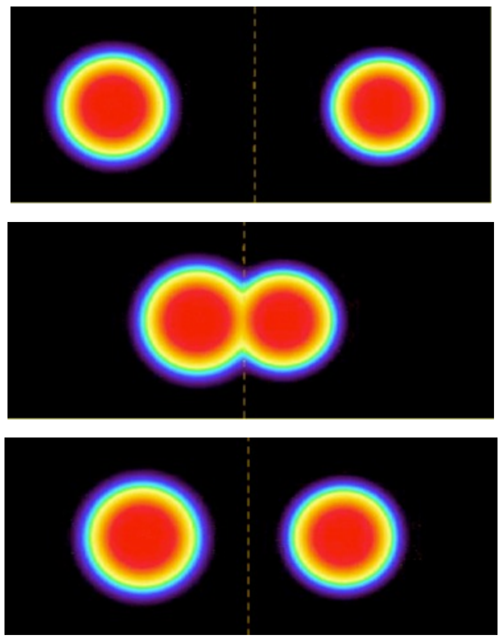


Phase-space method applied in the nuclear physics context

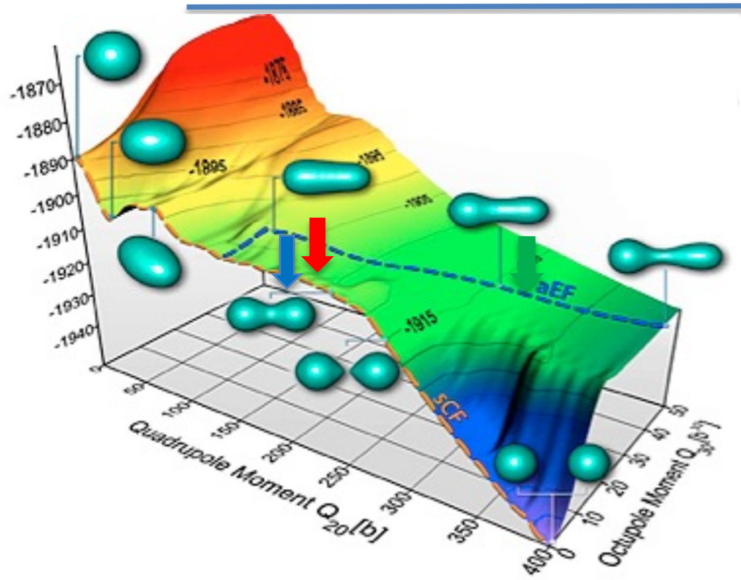
Nuclear Fission



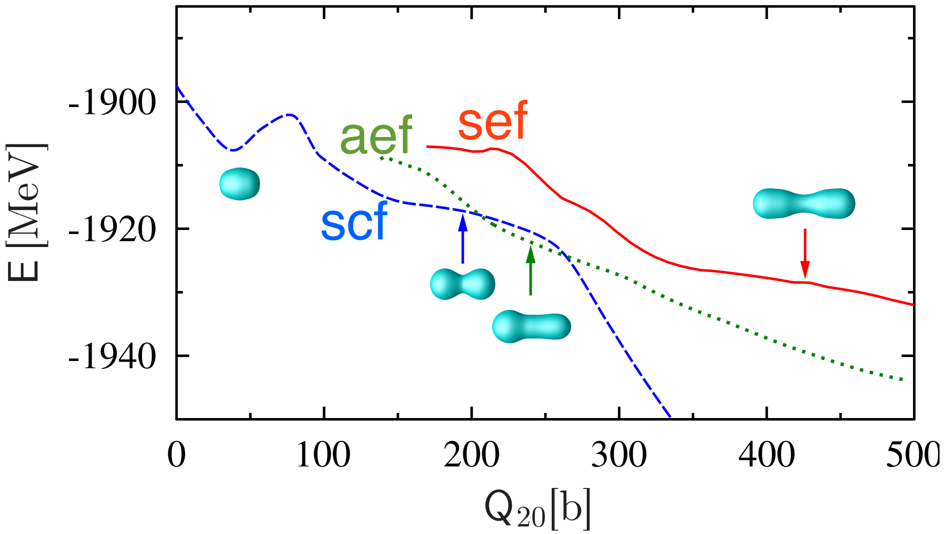
Transfer reactions



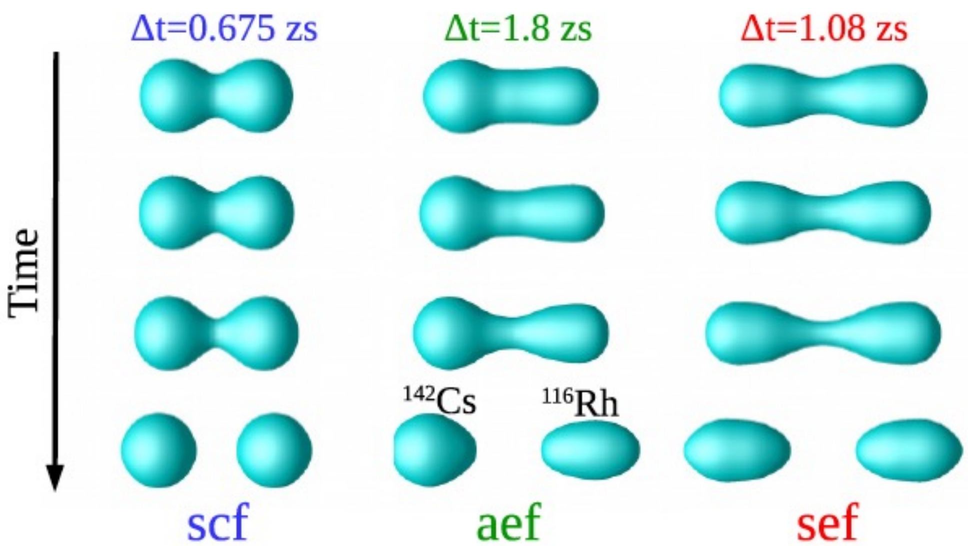
Fission of superfluid ^{258}Fm

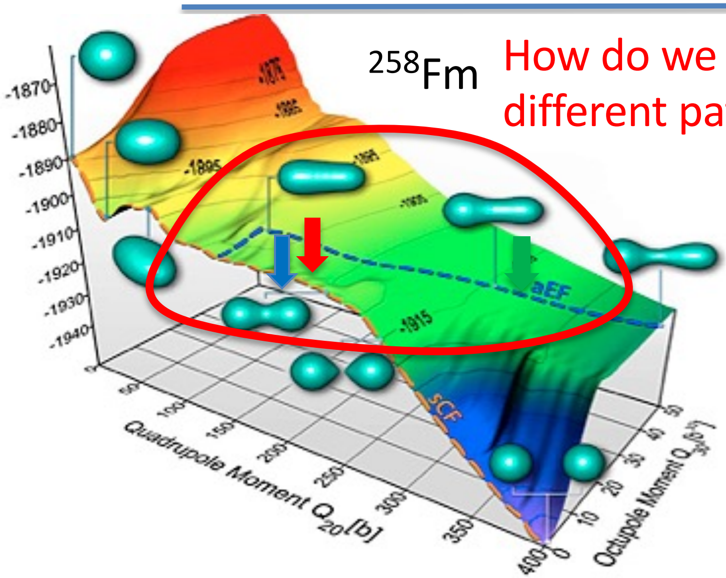


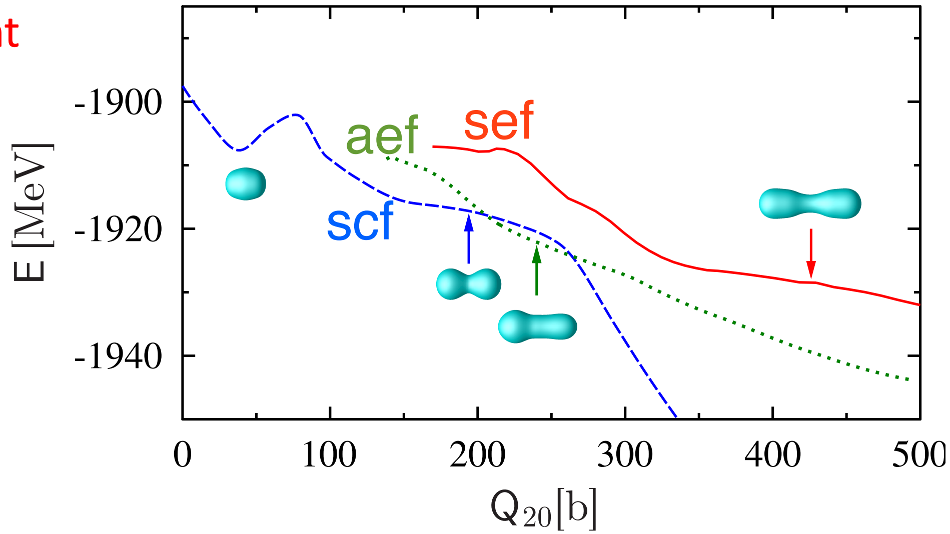
Identification of main fission paths



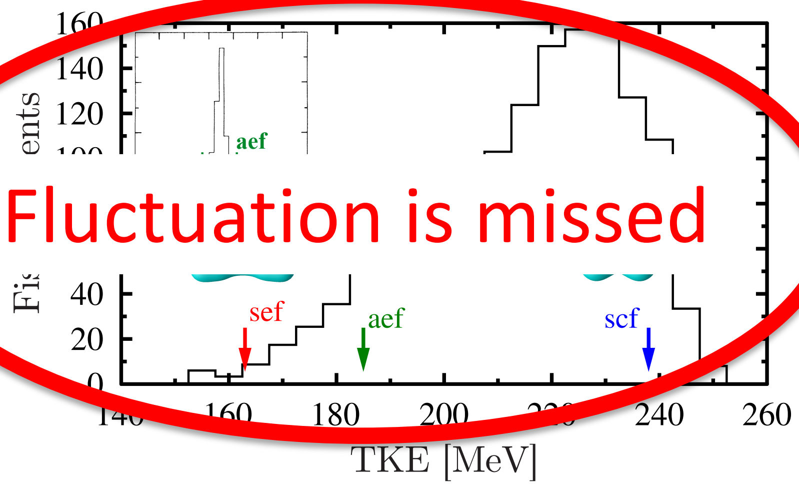
1 zs = 10^{-21} s







Total Kinetic Energy



Some conclusions

- TKE seems compatible with experiments
- Dynamic seems almost adiabatic up to scission point and then is Well describe by TDHF-BCS

Remaining problem

- Fluctuations are underestimated
- Weight of each paths?

Scamps, Simenel, DL, PRC 92 (2015)

Mean-field only will never be able to describe completely fission

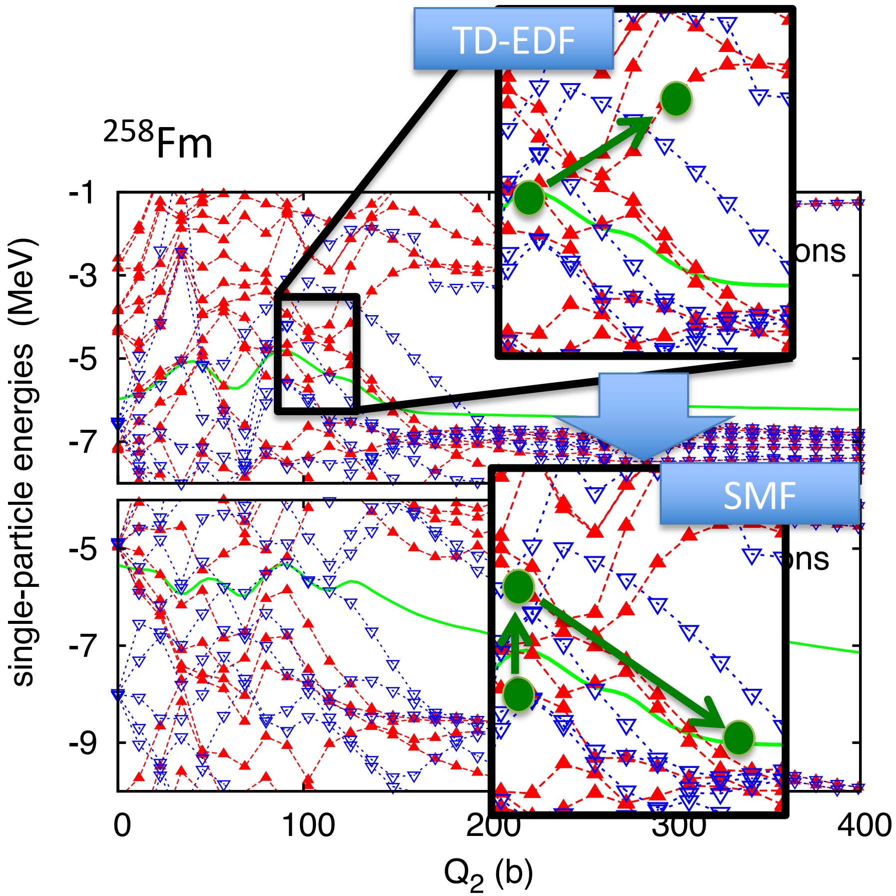
SMF in density matrix space

$$\rho(\mathbf{r},\mathbf{r}',t_0) = \sum_i \Phi_i^*(\mathbf{r},t_0) n_i \Phi_j(\mathbf{r}',t_0)$$

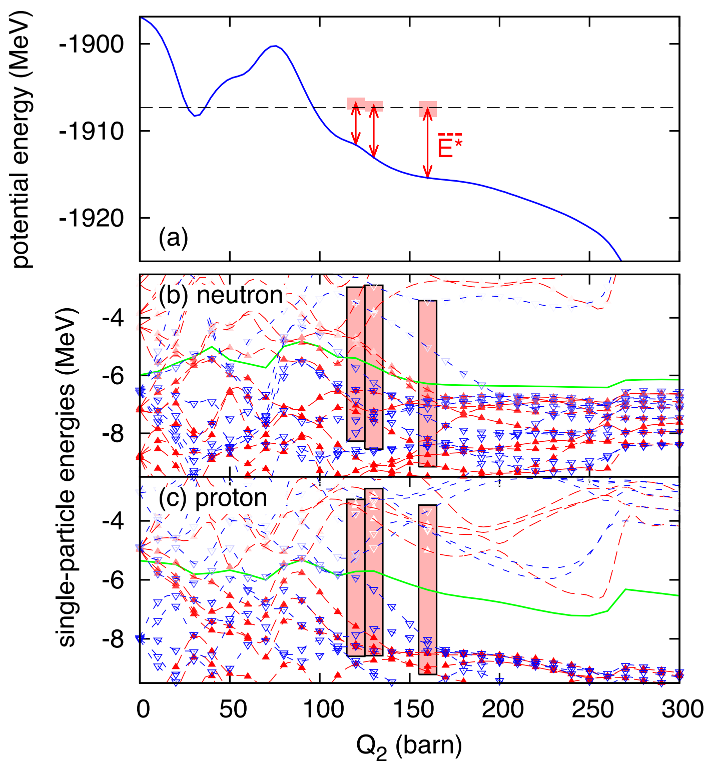
$$\rho^\lambda(\mathbf{r},\mathbf{r}',t_0) = \sum_{ij} \Phi_i^*(\mathbf{r},t_0) \rho_{ij}^\lambda \Phi_j(\mathbf{r}',t_0)$$

$$\overline{\rho_{ij}^\lambda} = \delta_{ij} n_i$$

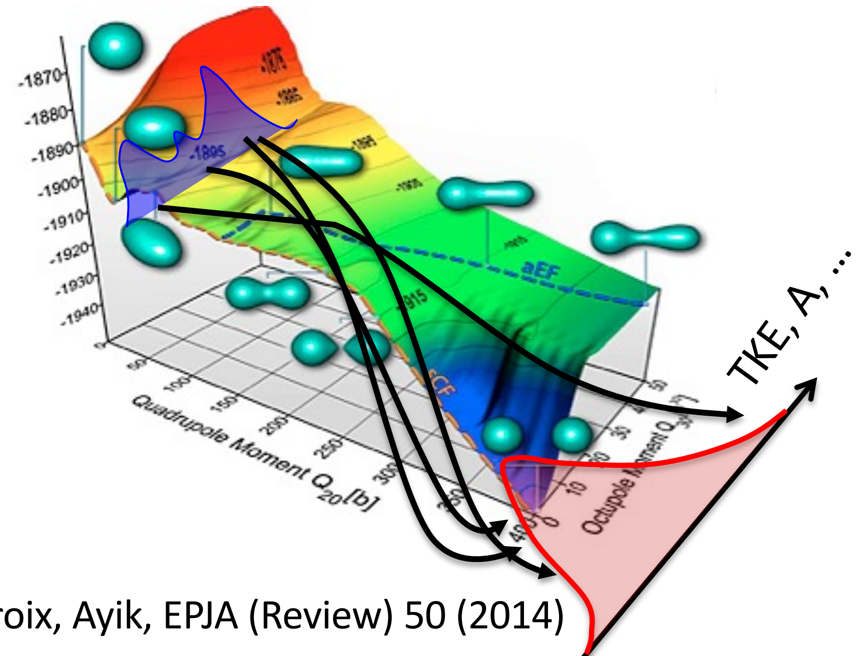
$$\overline{\delta\rho_{ij}^\lambda \delta\rho_{j'i'}^\lambda} = \frac{1}{2}\delta_{jj'}\delta_{ii'}\left[n_i(1-n_j)+n_j(1-n_i)\right].$$



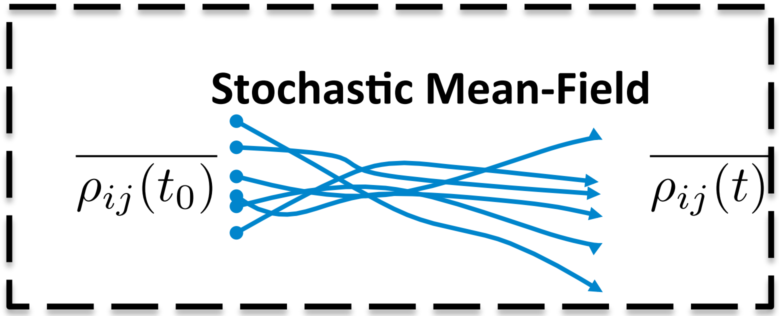
Range of fluctuation fixed by energy cons.



How to conceal microscopic deterministic approach and randomness ?

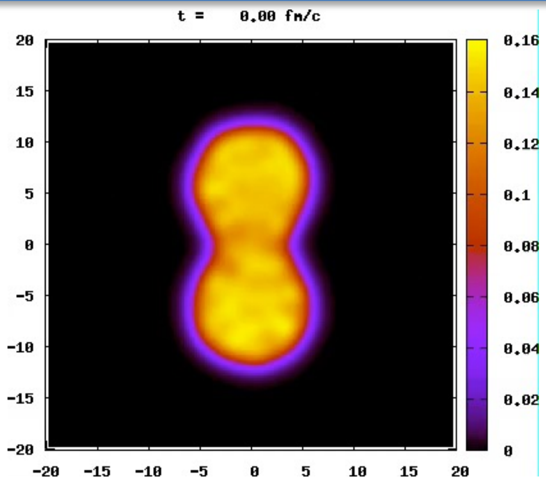


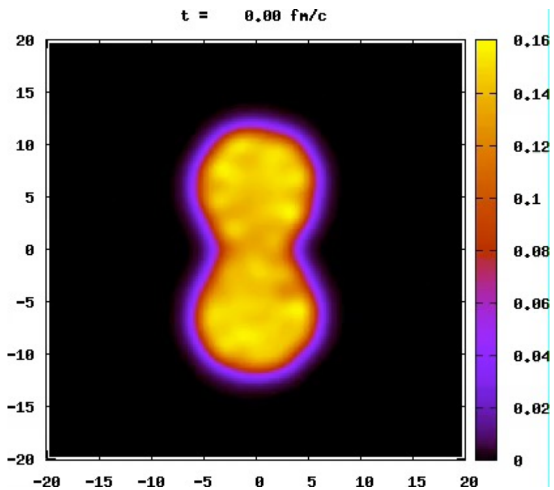
Lacroix, Ayik, EPJA (Review) 50 (2014)



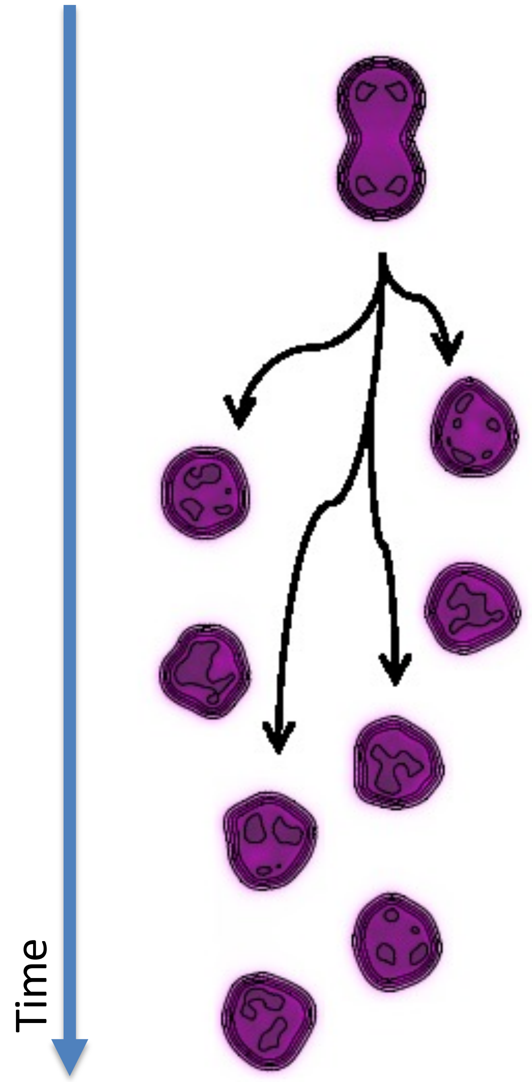
Constrains:
-Generates a sample of microscopic trajectories (typically 300)
-Each trajectory is 8-10 days CPU time

Some trajectories illustration





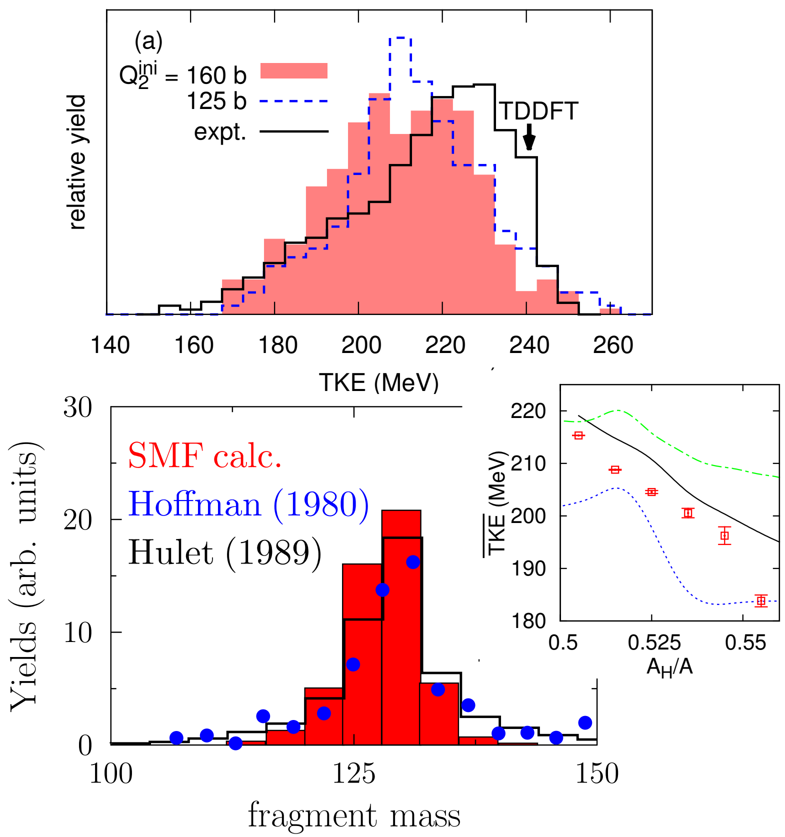
How to conceal microscopic deterministic approach and randomness ?



Tanimura, Lacroix, Ayik, PRL (2017)

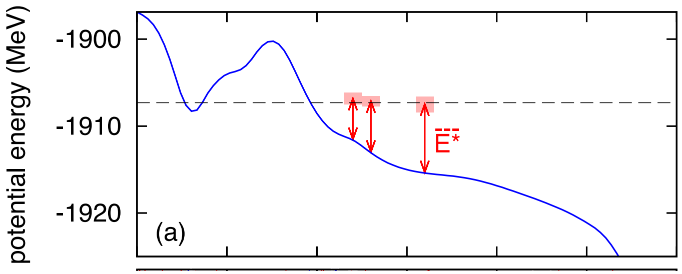
From deterministic to statistical approach

Theory vs experiment



Some informal discussion

Range of fluctuation fixed by energy cons.



An interesting "ongoing" discussions:
A. Bulgac, et al, Phys. Rev. C 100, 034615.
S. Ayik and D. Lacroix, arXiv:1909.13761.
A. Bulgac, arXiv:1910.07644.

- Actually, density fluctuations diverges in a small volume leading to no natural cutoff in momentum space

- The method works when the single-particle space is restricted.
  Is our E* criteria the correct one?

- Another issue is that the method (as often) is Hamiltonian based !
  It leads to numerical problem with ρ^{α} terms

- More generally, the method poses the problem of defining a trajectory in our ptoblems

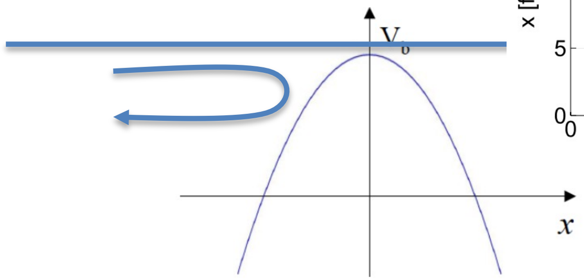
Here is an interesting ongoing discussion:

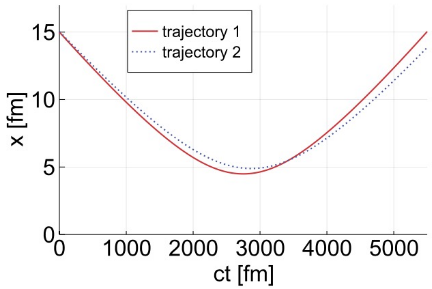
Mean-Field and GCM vision

Time-dependent generator coordinate method
for many-particle tunneling
Hasegawa, Hagino, Tanimura, PLB 808 (2020)

$$\delta \int dt \frac{\langle\Psi|i\hbar\frac{\partial}{\partial t}-H|\Psi\rangle}{\langle\Psi|\Psi\rangle}=0,$$

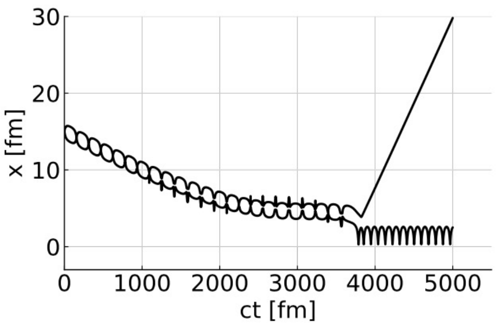
Pure mean-field

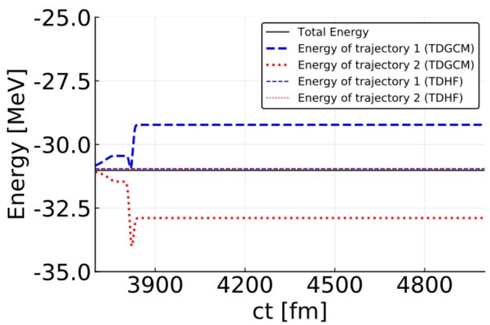




Time-Dependent GCM

$$\Psi(t)=\sum_a f_a(t)\Phi_a(t),$$





Phase-space vision

Phase-space consideration on barrier transmission in a time-dependent variational approach with superposed wave packets, A. Ono, PLB 808 (2020)

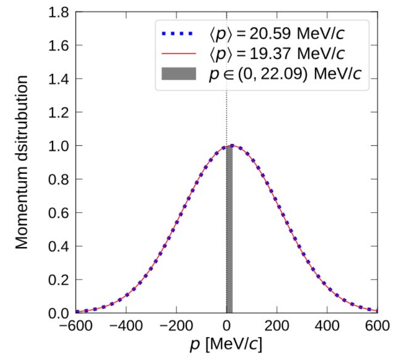
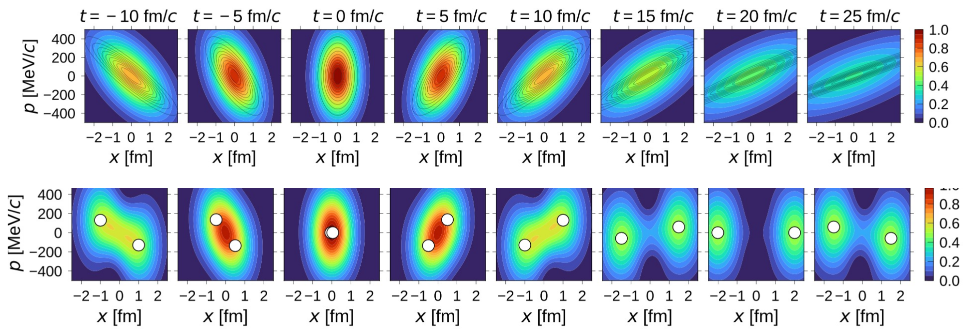
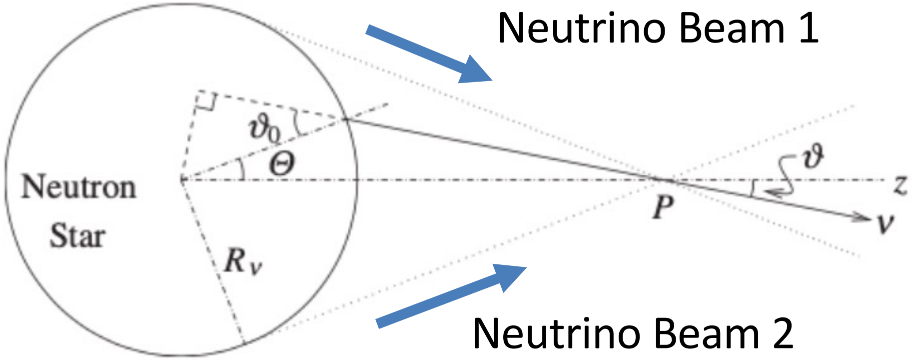


Figure 1: The momentum distributions for the two Gaussian wave packets which were used in the initial state in the calculation of Ref. [1]. The gray area indicates the region that is relevant to quantum tunneling ($E < 0.13$ MeV and $p > 0$).

Husimi quasi-probability distribution: exact and TDGCM



Phase-space characterization (neutrino systems)

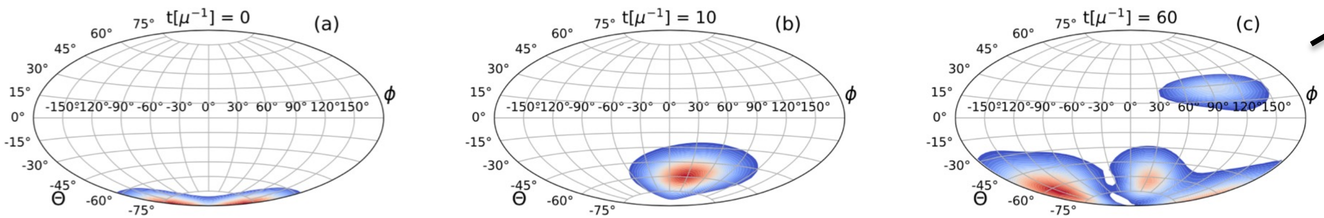


$$\frac{H}{\mu} = \frac{\Omega}{2}\vec{B}.\left(\vec{J}_A - \vec{J}_B\right) + \frac{2}{N}\vec{J}_A.\vec{J}_B$$

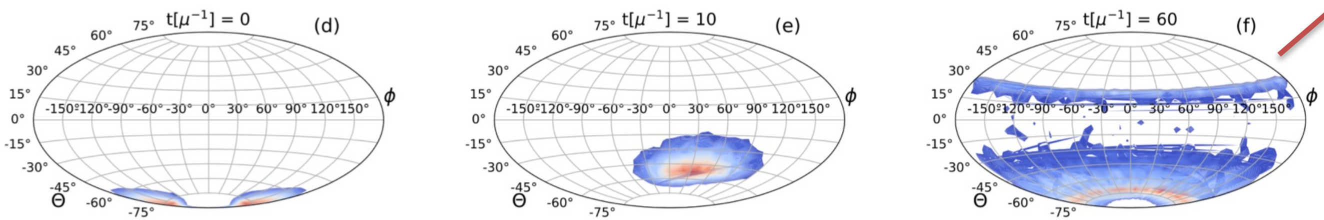
Equivalent to two coupled Lipkin models

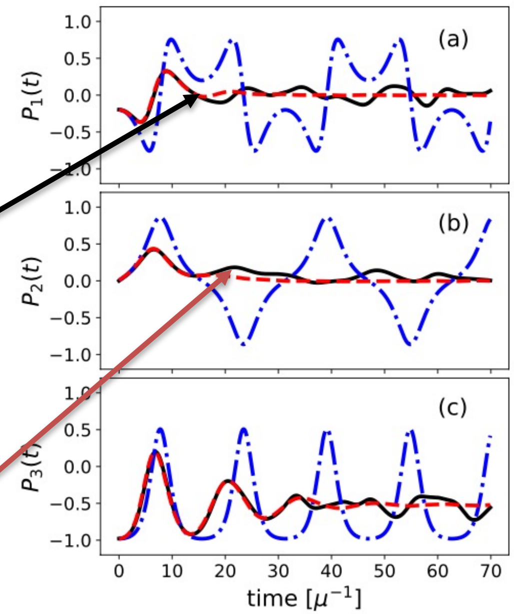
Full characterization of Phase-space

Exact Husimi distribution



Semiclassical equivalent Phase-space





"True" quantum effects are pretty small ?
What are true and fake quantum effect?

D. Lacroix et el, in preparation

Thank you