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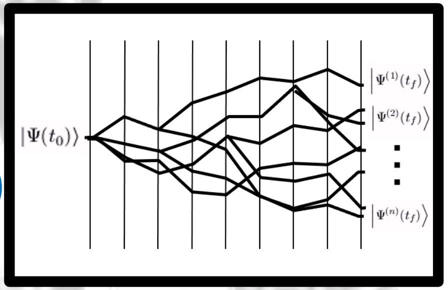
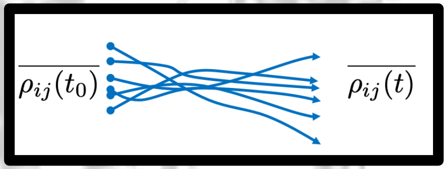
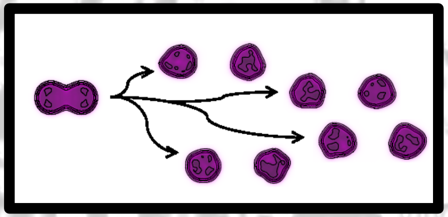
Quantum Stochastic methods for the N-body "Nuclear" problem (II)

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







A few more words on exact stochastic methods

Auxiliary field technic

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

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

Use the Hubbard Stratonovich transformation

$$\exp\left(-\tfrac{\Delta t}{i\hbar}O^2\right)|\Phi(t)\rangle \; = \int d\sigma G(\sigma)\exp(a\sigma O)|\Phi(t)\rangle$$

$$\rightarrow \quad |\Phi(t+\Delta t)\rangle \; = \int d\sigma G(\sigma)|\Phi_\sigma(t+\Delta t)\rangle$$

Interpretation of the integral in terms of stochastic Schrödinger equation

$$|\Phi_\sigma(t+\Delta t)\rangle = \exp\left(\frac{\Delta t}{i\hbar}H_1 + a\sigma O\right)|\Phi(t)\rangle$$

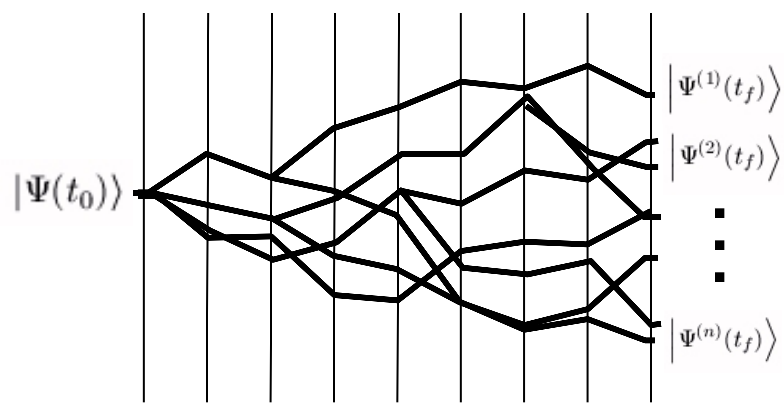
$$\rightarrow \quad \Delta|\Phi_\sigma\rangle = \left(\frac{\Delta t}{i\hbar}H + a\sigma O\right)|\Phi\rangle$$

The many-body problem

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

$$\downarrow \qquad \qquad \downarrow$$

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



More insight in mean-field dynamics:

Exact state → Trial states

$$|\Psi(t)\rangle \rightarrow \begin{cases} |Q(t)\rangle \\ |Q+\delta Q\rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha}|Q\rangle \end{cases}$$

The approximate evolution is obtained by minimizing the action:

$$S = \int_{t_0}^{t_1} ds \langle Q | i\hbar\partial_t - H | Q\rangle$$

Included part: average evolution

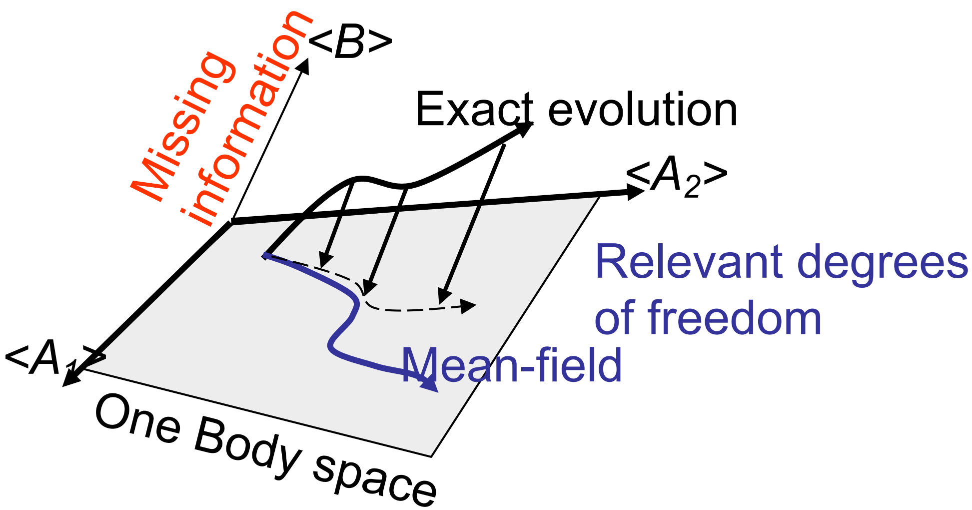
$$i\hbar \frac{d\langle A_\alpha\rangle}{dt} = \langle [A_\alpha, H]\rangle \rightarrow \text{exact Ehrenfest evolution}$$

$$H = \mathcal{P}_1 H + (1-\mathcal{P}_1) H$$

Missing part: correlations

$$|dQ\rangle = \sum_\alpha dq_\alpha A_\alpha \quad |dQ\rangle = \frac{dt}{i\hbar}\mathcal{P}_1(t) H |Q\rangle$$

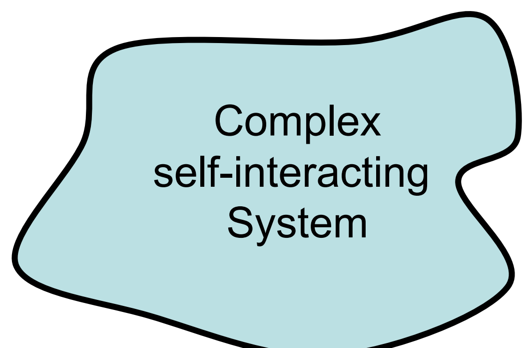
$$\rightarrow \quad i\hbar \frac{d\langle A_\alpha A_\beta\rangle}{dt} \neq \langle [A_\alpha A_\beta, H]\rangle$$



Hamiltonian splitting

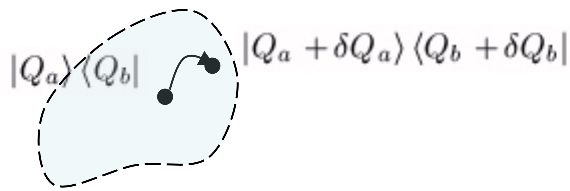
$$H = \underbrace{\mathcal{P}_1 H}_{\text{System}} + \underbrace{(1-\mathcal{P}_1) H}_{\text{Environment}}$$

System Environment



The idea is now to treat the missing information as the *Environment* for the Relevant part (*System*)

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



Theorem :
One can always find a stochastic process for trial states such that $\overline{\langle A_\alpha\rangle},\ \overline{\langle A_\alpha\, A_\beta\rangle},\cdots\overline{\langle A_{\alpha_1}\, A_{\alpha_2}\cdots A_{\alpha_k}\rangle}$
evolves exactly over a short time scale.

with
$$
\begin{aligned}
|Q_a+\delta Q_a\rangle &= e^{\sum_\alpha \delta q_\alpha^{[a]} A_\alpha}\,|Q_a\rangle \\
|Q_b+\delta Q_b\rangle &= e^{\sum_\alpha \delta q_\alpha^{[b]} A_\alpha}\,|Q_b\rangle
\end{aligned}
$$

Valid for $D=|Q_a\rangle\langle Q_b|$

or $D=\dfrac{|Q_a\rangle\langle Q_b|}{\langle Q_b\,|\,Q_a\rangle}$

In practice

Mean-field level

$$
\begin{cases}
\delta q_\alpha^{[a]} = \delta q_\alpha^{a} \\
\delta q_\alpha^{[b]*} = \delta q_\alpha^{b\,*}
\end{cases}
\qquad
i\hbar\frac{d}{dt}\langle A_\alpha\rangle = \langle[A_\alpha,H]\rangle
$$

Mean-field + noise

$$
\begin{cases}
\delta q_\alpha^{[a]} = \delta q_\alpha^{a} + \delta\xi_\alpha^{[2]} \\
\delta q_\alpha^{[b]*} = \delta q_\alpha^{b\,*} + \delta\eta_\alpha^{[2]}
\end{cases}
\qquad
\begin{aligned}
i\hbar\frac{d\overline{\langle A_\alpha\rangle}}{dt} &= \overline{\langle[A_\alpha,H]\rangle} \\
i\hbar\frac{d\overline{\langle A_\alpha A_\beta\rangle}}{dt} &= \overline{\langle[A_\alpha A_\beta,H]\rangle}
\end{aligned}
$$

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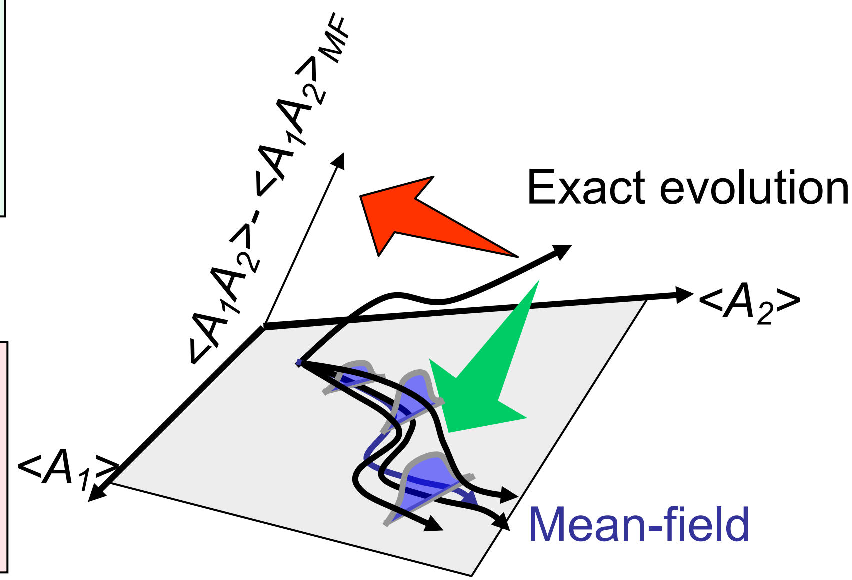
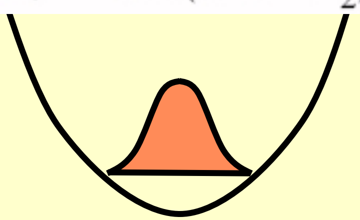


$$H_0 = \hbar\omega(a^+a + \tfrac{1}{2})$$

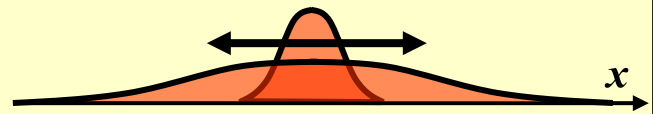
$t=0$



$\langle x^2 \rangle = \frac{1}{2\eta}$ with $\eta = \frac{m\omega}{\hbar}$

$t>0$

$$H = \frac{p^2}{2m} = -\frac{\hbar\omega}{4}(a^+ - a)^2$$

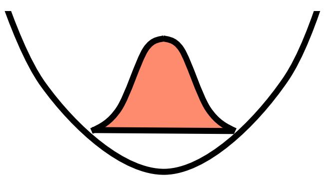


$$\langle x^2 \rangle = \frac{1}{2\eta} + \frac{\hbar^2\eta}{2m^2}t^2$$

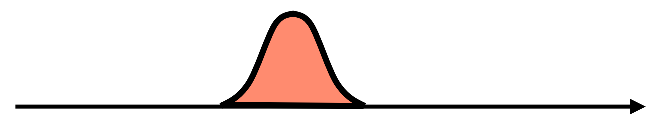
Reduction of the information:

I want to simulate the expansion with Gaussian wave-function having fixed widths. $\langle x^2 \rangle = cte, \quad \langle p^2 \rangle = cte$

“Mean-field” evolution:



$t>0$



Relevant/Missing information:

Relevant degrees of freedom

$\langle x \rangle, \quad \langle p \rangle$

$\langle a^+ \rangle, \quad \langle a \rangle$

Missing information

$\langle x^2 \rangle, \quad \langle p^2 \rangle, \quad \langle xp \rangle$

$\langle {a^+}^2 \rangle, \quad \langle a^2 \rangle, \quad \langle a^+a \rangle$

Trial states

$$|Q + \delta Q\rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha}|Q\rangle$$

Coherent states

$$|\alpha + d\alpha\rangle = e^{d\alpha a^+}|\alpha\rangle$$

Densities

$$D = \frac{|\alpha\rangle\langle\beta|}{\langle\beta|\alpha\rangle} \quad \text{with} \quad \begin{aligned} \langle\beta + \mathrm{d}\beta| &= \langle\beta|e^{\mathrm{d}\beta^* a} \\ |\alpha + \mathrm{d}\alpha\rangle &= e^{\mathrm{d}\alpha a^+}|\alpha\rangle \end{aligned}$$

Stochastic c-number evolution from Ehrenfest theorem

$$\begin{cases} \mathrm{d}\alpha = \overline{\mathrm{d}\alpha} + \mathrm{d}\xi^{[2]}, \\ \mathrm{d}\beta^* = \overline{\mathrm{d}\beta^*} + \mathrm{d}\eta^{[2]} \end{cases}$$

mean values

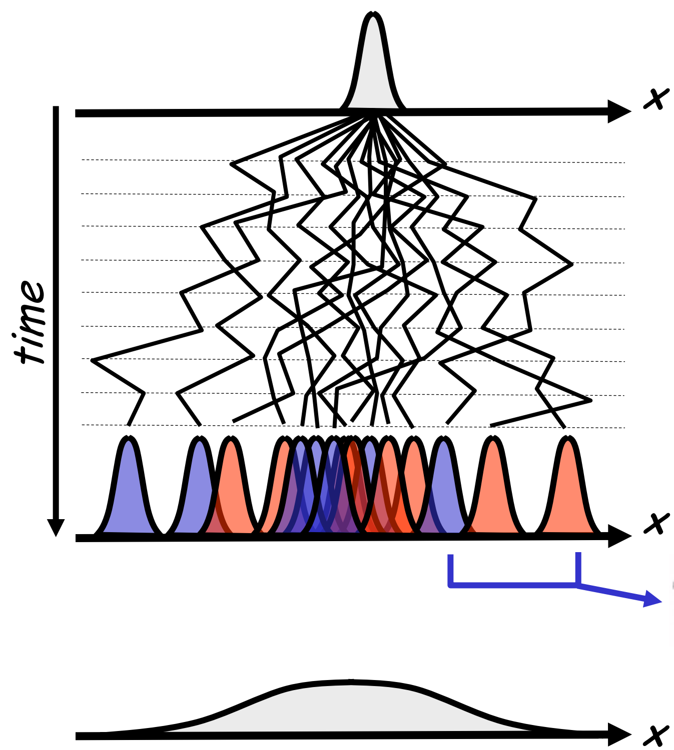
$$\overline{d\langle a\rangle} = \overline{d\alpha}$$

$$\overline{d\langle a^+\rangle} = \overline{d\beta^*}$$

fluctuations

$$\overline{d\langle a^2\rangle} = 2\alpha\overline{d\alpha} + \overline{d\xi^{[2]}d\xi^{[2]}}$$

$$\overline{d\langle a^{+2}\rangle} = 2\beta^*\overline{d\beta^*} + \overline{d\eta^{[2]}d\eta^{[2]}}$$



$$\mathrm{Tr}(Dx^2) = \frac{1}{2\eta} + X^2$$

$$\overline{\mathrm{Tr}(Dx^2)} = \frac{1}{2\eta} + \frac{\hbar^2\eta}{2m^2}t^2$$

Nature of the stochastic mechanics

$$\begin{cases} X = \frac{1}{\sqrt{2\eta}}(\alpha + \beta^*), \\ P = i\hbar\sqrt{\frac{\eta}{2}}(\beta^* - \alpha) \end{cases} \Rightarrow \begin{cases} \mathrm{d}X = \frac{P}{m}\mathrm{d}t + \mathrm{d}\chi_1 \\ \mathrm{d}P = \mathrm{d}\chi_2, \end{cases}$$

with $\overline{\mathrm{d}\chi_1\,\mathrm{d}\chi_2} = \frac{\hbar^2\eta}{2m}\mathrm{d}t$

the quantum wave spreading can be simulated by a classical brownian motion in the complex plane

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

Starting point: $H = \sum_{ii} \langle i|T|j\rangle a_i^+ a_j + \frac{1}{2}\sum_{ijkl} \langle ij|v_{12}|lk\rangle a_i^+ a_j^+ a_l a_k$

$D_{ab} = |\Phi_a\rangle\langle\Phi_b|$ with $\langle\Phi_b \mid \Phi_a\rangle = 1$

$\rho_1 = \sum |\alpha_i\rangle\langle\beta_i|$

Observables $\langle j|\rho_1|i\rangle = \langle a_i^+ a_j\rangle$

Fluctuations $\langle ij|\rho_{12}|kl\rangle = \langle a_k^+ a_l^+ a_j a_i\rangle$

Ehrenfest theorem ➡ BBGKY hierarchy

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho_1 = [h_{\mathrm{MF}}, \rho_1],$$

$$v_{12} = \sum_\lambda O_\lambda(1) O_\lambda(2)$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho_{12} = [h_{\mathrm{MF}}(1) + h_{\mathrm{MF}}(2), \rho_{12}] + (1-\rho_1)(1-\rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2 v_{12}(1-\rho_1)(1-\rho_2)$$

Stochastic one-body evolution

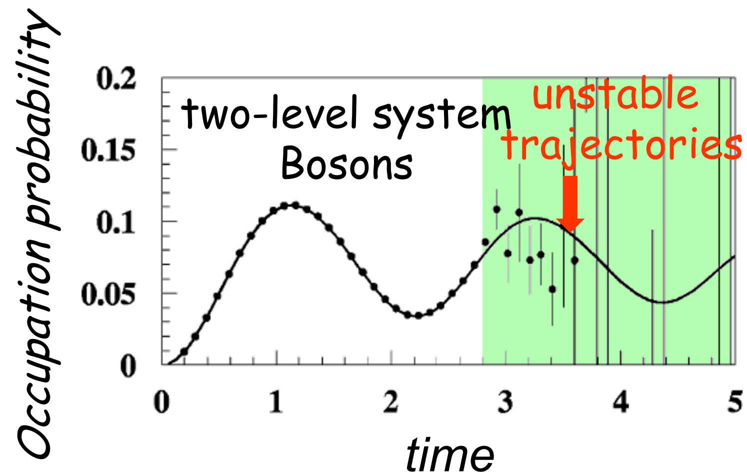
$$\begin{aligned} d\rho_1 &= [h_{MF}, \rho_1] \\ &+ \sum_\lambda d\xi_\lambda^{[2]}(1-\rho_1)O_\lambda\rho_1 + \sum_\lambda d\eta_\lambda^{[2]}(1-\rho_1)O_\lambda\rho_1 \end{aligned}$$

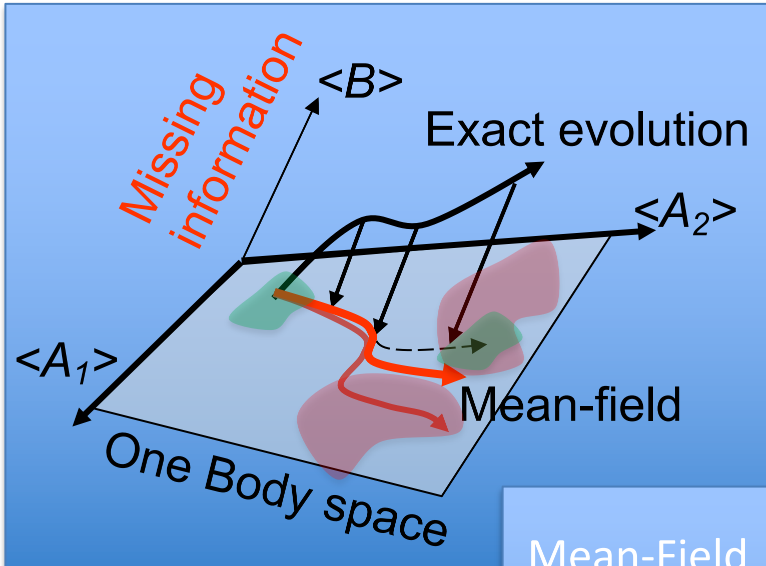
with $\overline{d\xi_\lambda^{[2]} d\xi_{\lambda'}^{[2]}} = -\overline{d\eta_\lambda^{[2]} d\eta_{\lambda'}^{[2]}} = \delta_{\lambda\lambda'} \frac{dt}{i\hbar}$

- 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…





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

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

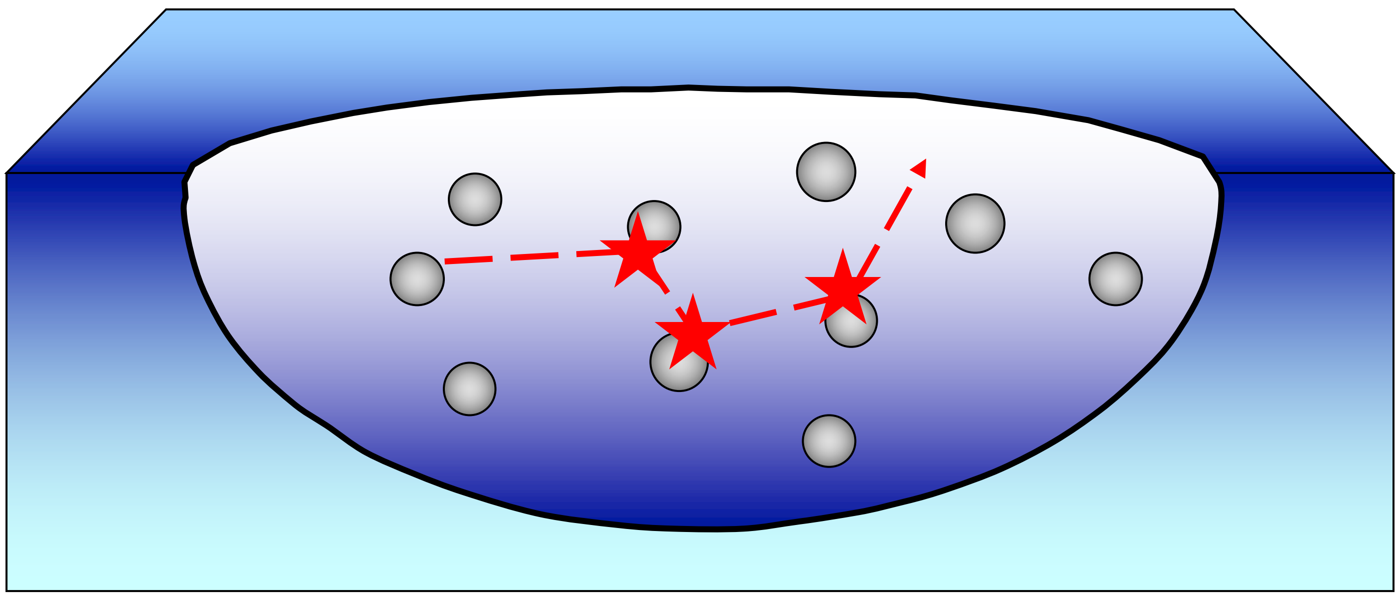
Correlation that built up in time

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

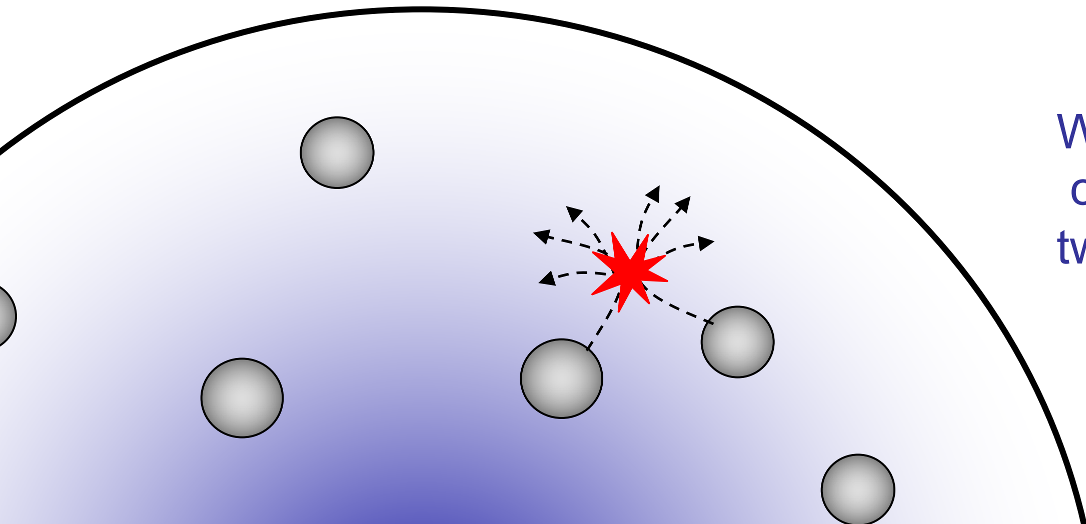
Weak coupling approximation : perturbative treatment

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

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

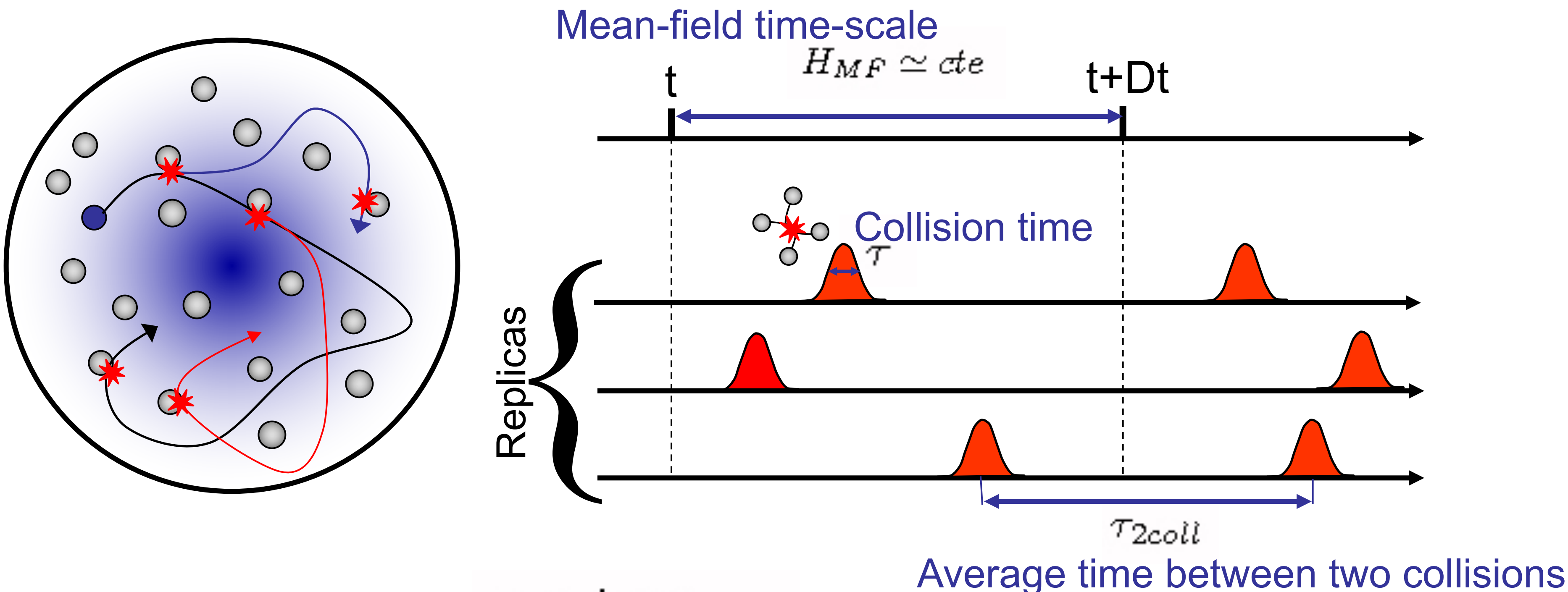
Residual interaction in the mean-field interaction picture

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:

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

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

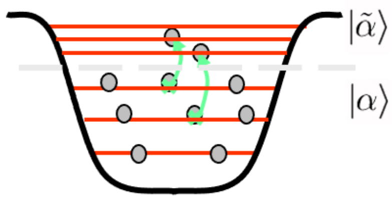
$$D = |\Phi\rangle\langle\Phi|$$

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

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

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

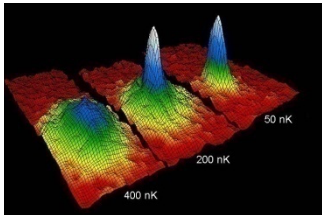
Separability of the interaction $v_{12} = \sum_\lambda O_\lambda(1)O_\lambda(2)$

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

- 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

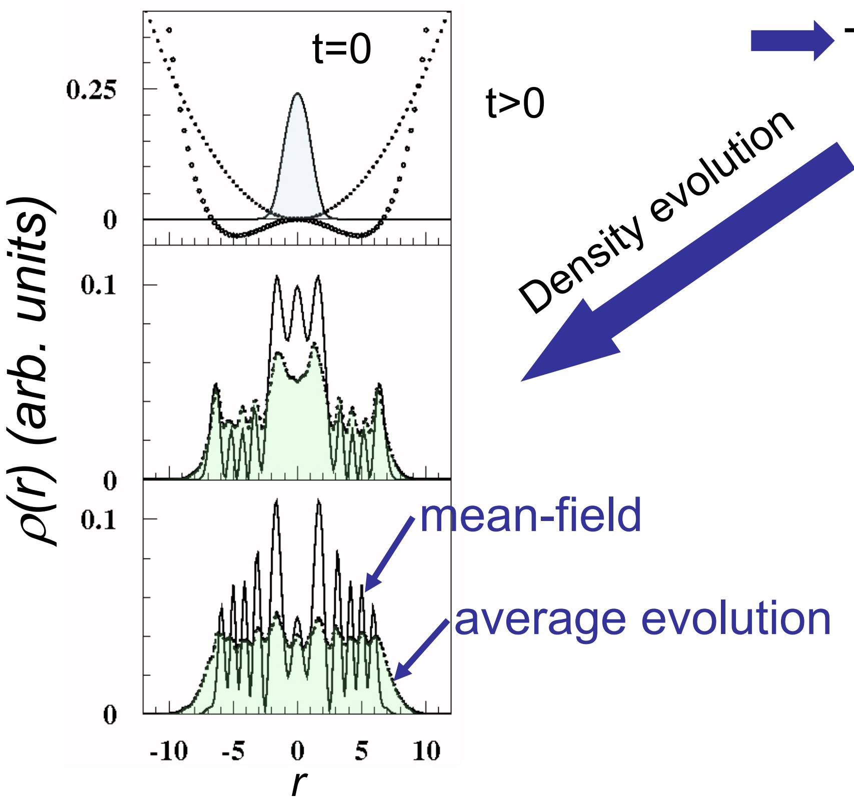
N-body density: $D = |N : \alpha\rangle \langle N : \alpha|$

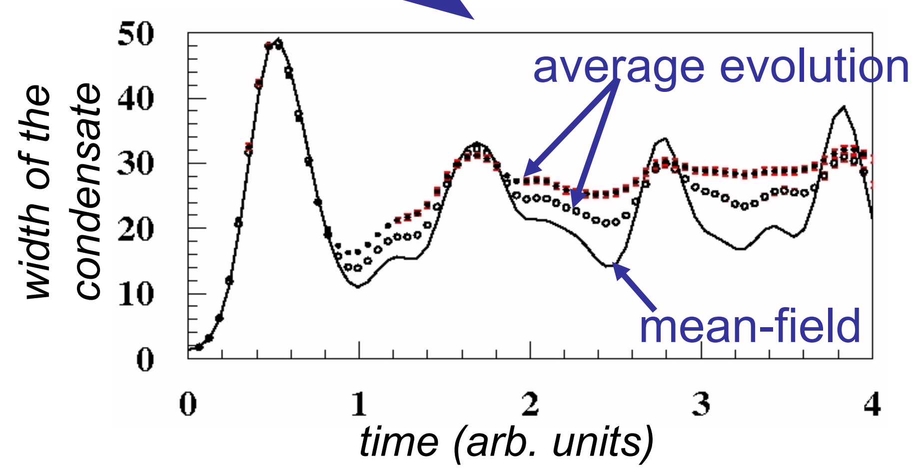
SSE on single-particle state :

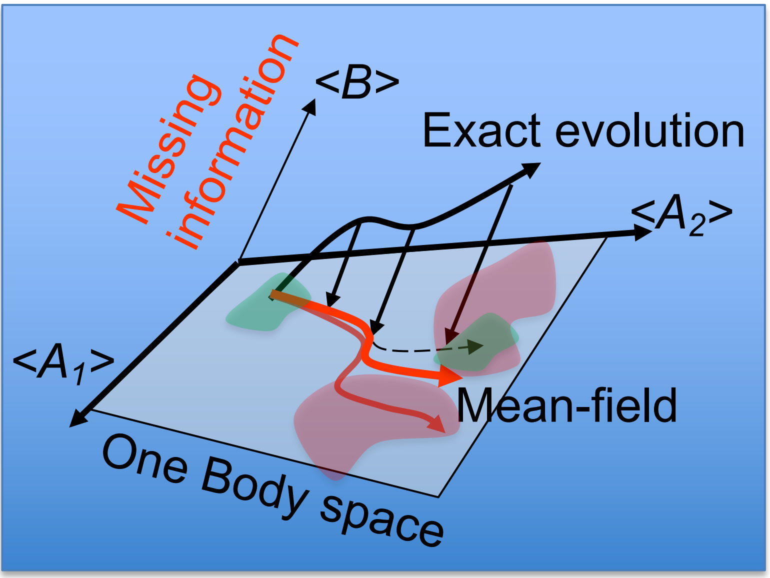
$$d\,|\alpha\rangle = \left\{ \frac{dt}{i\hbar} h_{MF}(\rho) + \sum_k dW_k (1-\rho) A_k - \frac{dt\tau}{2\hbar^2} \sum_k \gamma_k \left[A_k^2 \rho + \rho A_k \rho A_k - 2 A_k \rho A_k \right] \right\} |\alpha\rangle$$

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

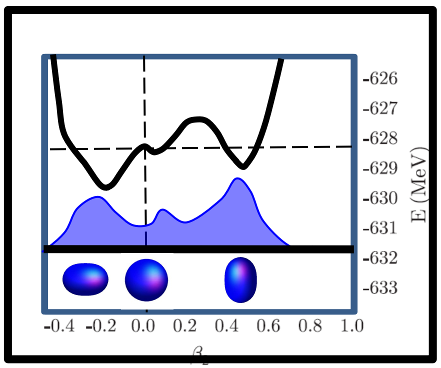






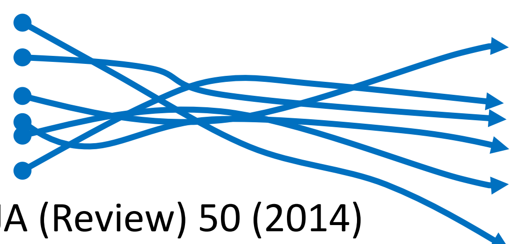
Correlations that are here initially and propagates can play a major role

A typical example in nuclear physics: deformation



Phase-space approach for Fermi systems

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

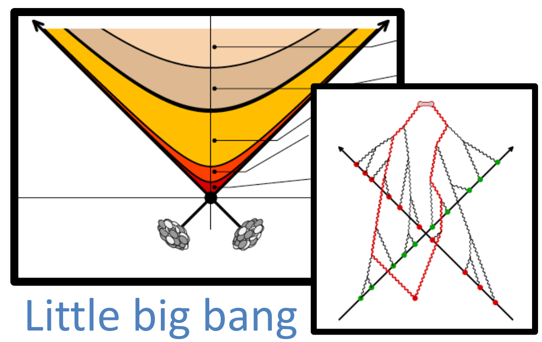


$$\overline{\rho_{ij}(t)}$$

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

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

Particle physics



Little big bang

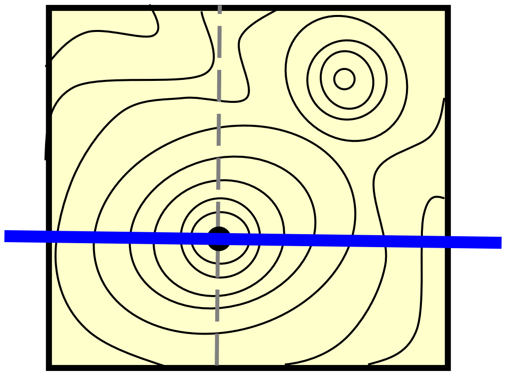
Gelis, Schenke, arxiv 2016

Cold atoms: the truncated Wigner approach

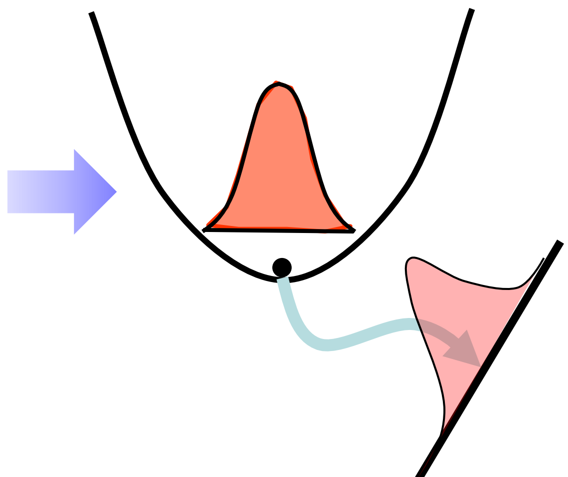
Sinatra, Lobo, Castin, J. Phys. B 35 (2002)

What is the idea behind phase-space methods?

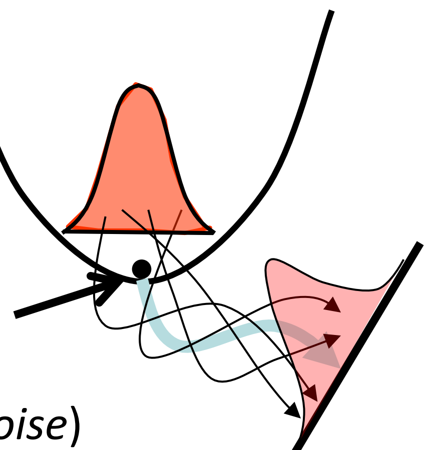
Collective energy landscape



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

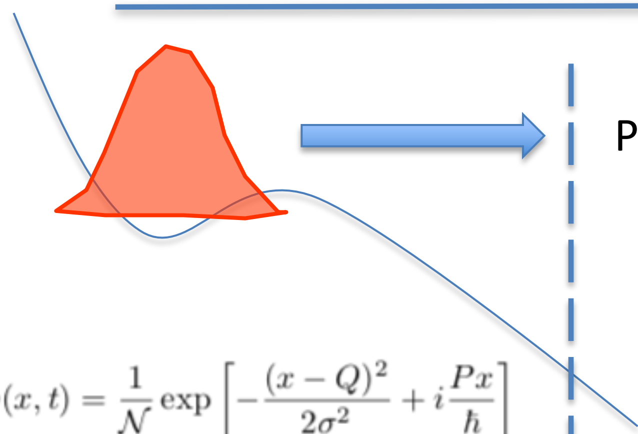
$$f(r,p,t)$$

+ dynamical evolution

Classical mechanics With random initial fluctuations

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

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

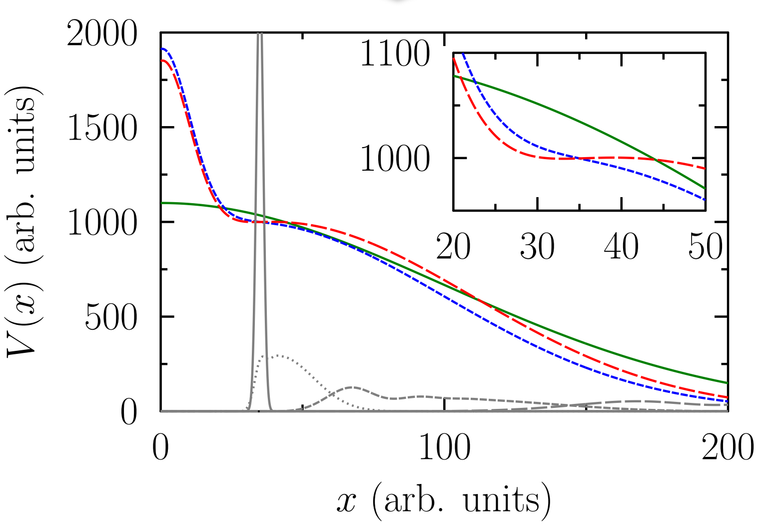


$$\varphi(x,t) = \frac{1}{\mathcal{N}} \exp\left[-\frac{(x-Q)^2}{2\sigma^2} + i\frac{Px}{\hbar}\right]$$

Probability to decay?

Quantum mechanics

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



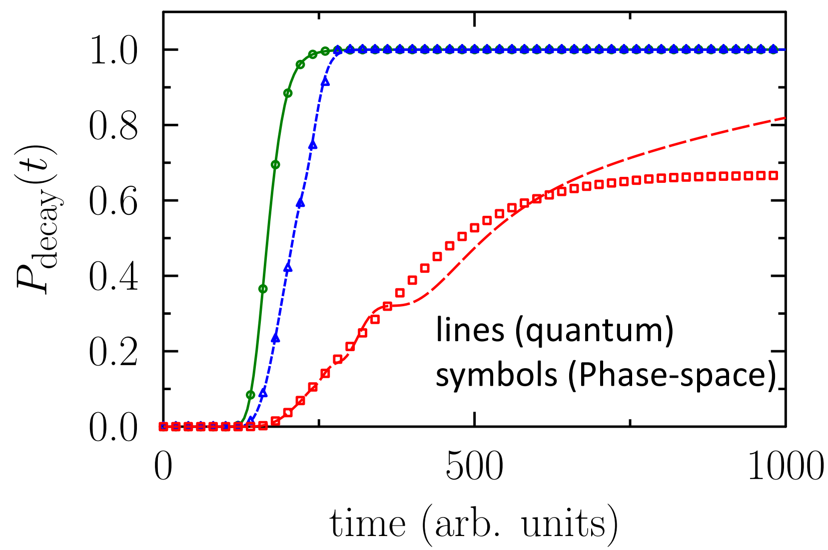
Phase-space equivalent

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

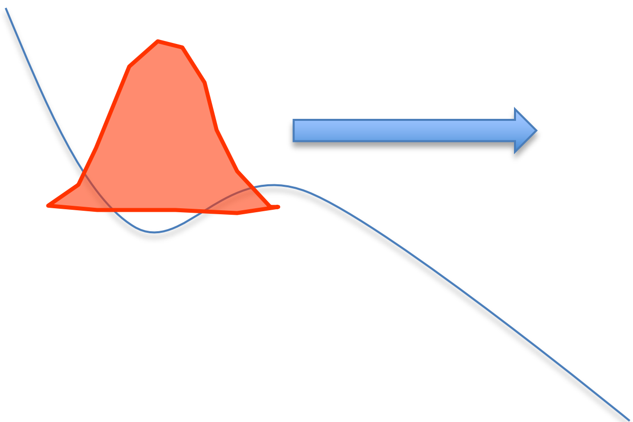
$$\begin{cases} \dot{Q}^{(n)} = P^{(n)}(t)/m \\ \dot{P}^{(n)}(t) = F(P^{(n)}(t), Q^{(n)}(t)) \end{cases}$$



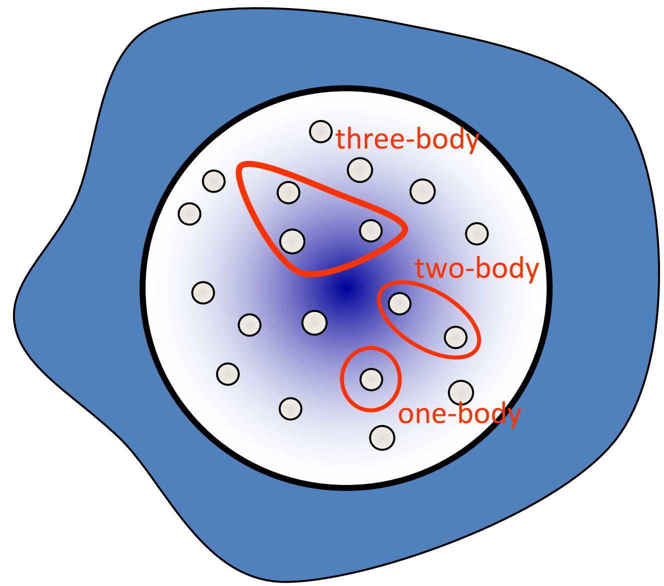
This works surprisingly well
if "true" quantum effects have a weak effect !

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 ?

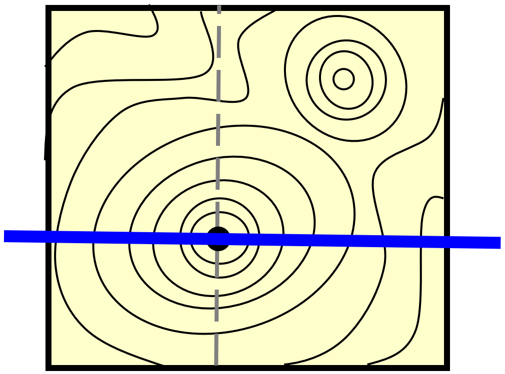
Initial fluctuations should reproduce in average quantum fluctuations.

What is the equivalent to classical mechanics ?

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

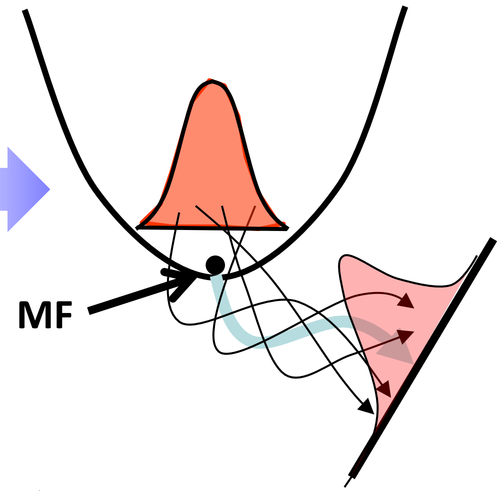
What do we call classical for Fermi systems?

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

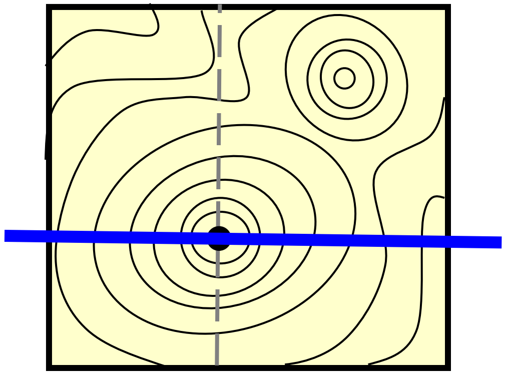
$$\frac{dA_\alpha^{(n)}}{dt} = \mathcal{F}\left(\{A_\beta^{(n)}\}\right)$$

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

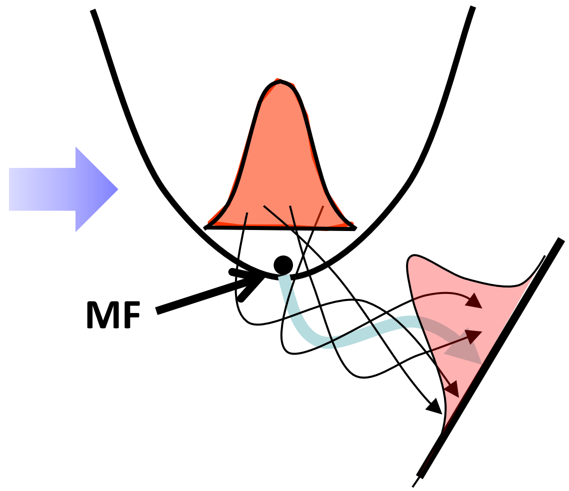
at all time $\Sigma_C^2 = \overline{A^{(n)} A^{(n)}} - \overline{A^{(n)}}^2$

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

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



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



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

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

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

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

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

SMF in collective space

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

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

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

TDHF level

$$\rho(t_i) \xrightarrow{\; i\hbar\dot{\rho} = [h(\rho), \rho] \;} \rho(t_f)$$

holes

Part.

$$\rho = \begin{pmatrix} \begin{matrix}1&&&\\&1&&\\&&1&\\&&&1\end{matrix} & \mathbf{0} \\ \mathbf{0} & \begin{matrix}0&&&&\\&0&&&\\&&0&&\\&&&0&\\&&&&0\end{matrix}\end{pmatrix}$$

TDHF with initial fluctuations

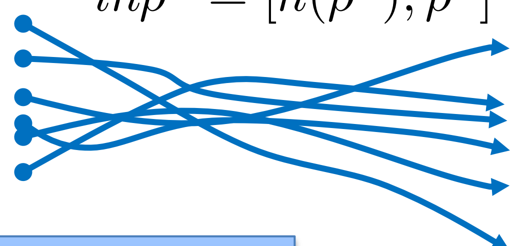
$$\overline{\delta\rho^{\lambda}_{ij}\delta\rho^{\lambda}_{j'i'}} \quad = \quad \frac{1}{2}\delta_{jj'}\delta_{ii'}\left[n_i(1-n_j) + n_j(1-n_i)\right].$$

$$\rho = \begin{pmatrix} \begin{matrix}1&&&\\&1&&\\&&1&\\&&&1\end{matrix} & \boxed{\neq 0} \\ \boxed{\neq 0} & \begin{matrix}0&&&&\\&0&&&\\&&0&&\\&&&0&\\&&&&0\end{matrix}\end{pmatrix}$$

Stochastic Mean-Field

$$i\hbar\dot{\rho}^{\lambda} = [h(\rho^{\lambda}), \rho^{\lambda}]$$

$\rho^{\lambda}(t_i)$



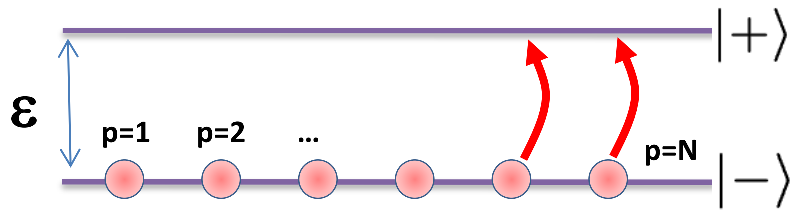
$\rho^{\lambda}(t_f)$

Some advantages

-Just N independent times something we know how to solve.
-Fluctuations can spontaneously break some symmetries.
-Can be applied with initial thermal equilibrium too.
-predicting power is remarkably good (see below)

The case of spontaneous symmetry breaking

Lipkin Model



See for instance : Ring and Schuck book

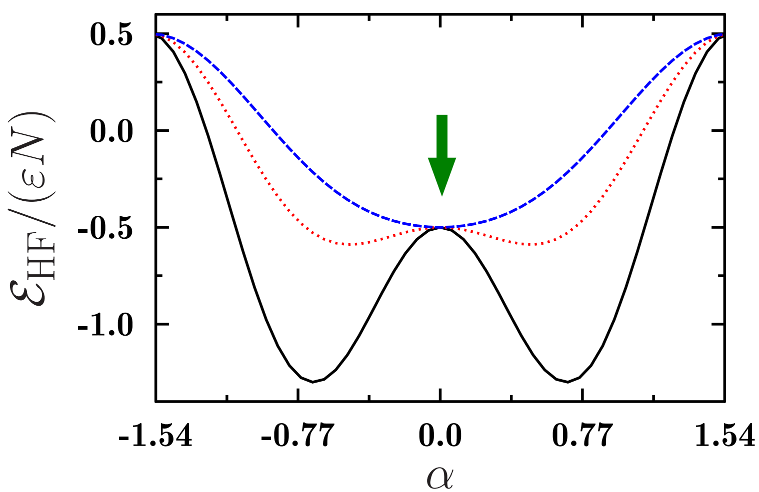
Severyukhin, Bender, Heenen, PRC74 (2006)

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

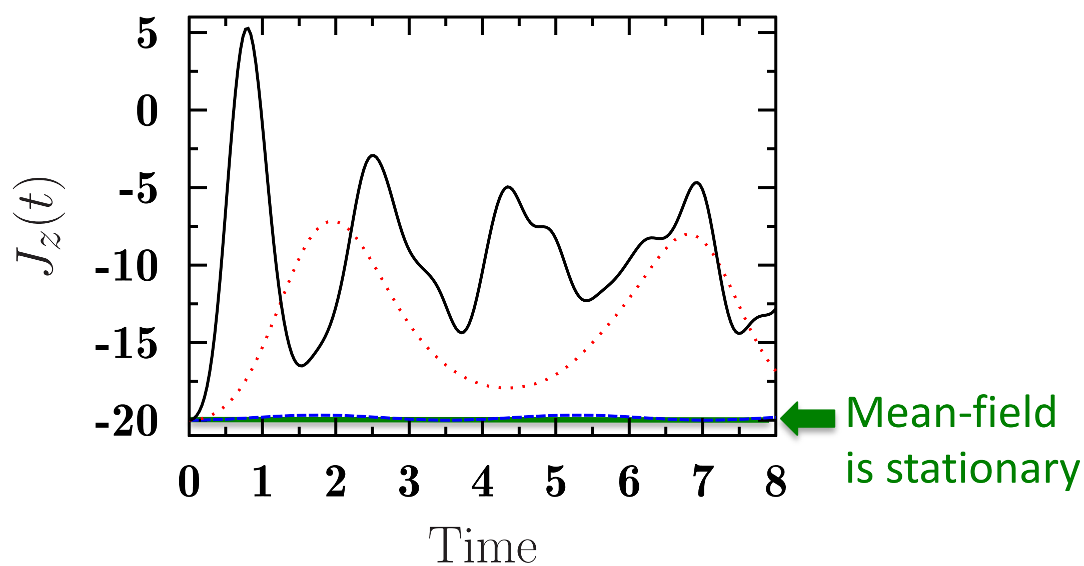
$$J_0 = \frac{1}{2}\sum_{p=1}^{N}\left(c^\dagger_{+,p}c_{+,p} - c^\dagger_{-,p}c_{-,p}\right) \qquad J_y = \frac{1}{2i}(J_+ - J_-)$$

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

N=40 particles

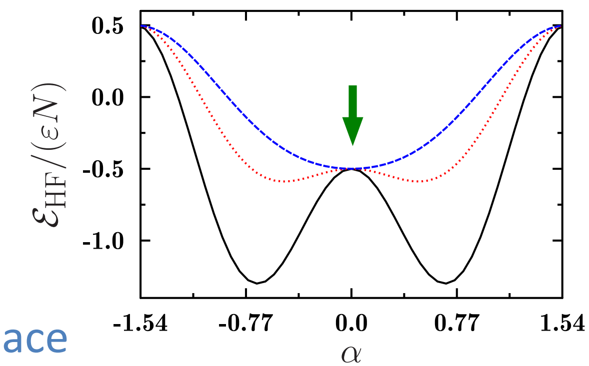


Exact dynamics



The stochastic mean-field solution

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



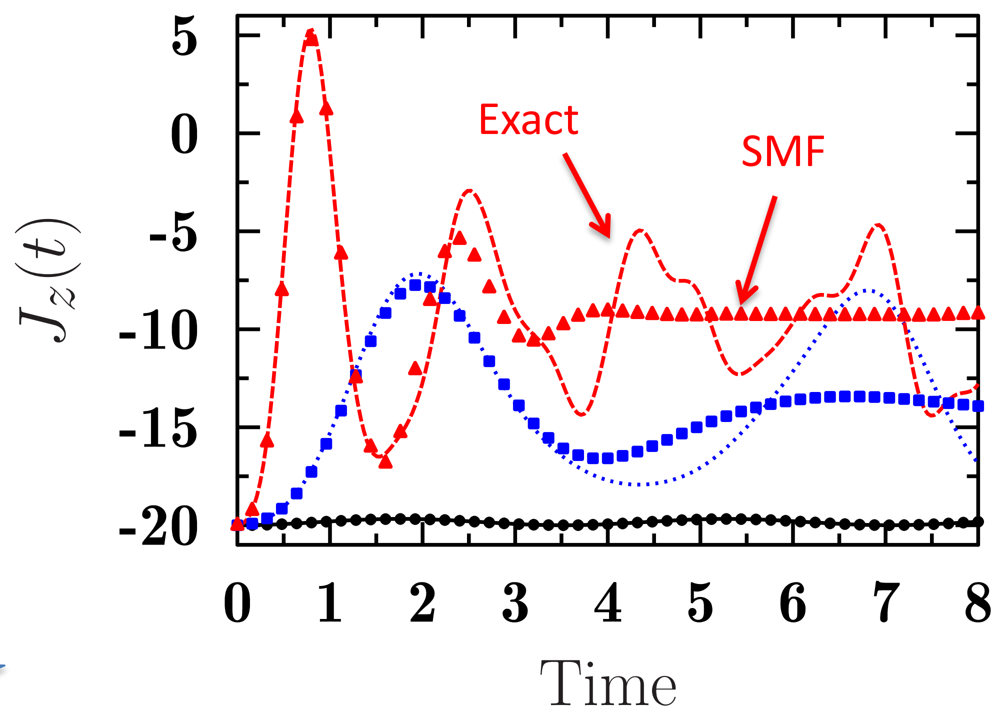
One-body observables

Formulation in quasi-spin space

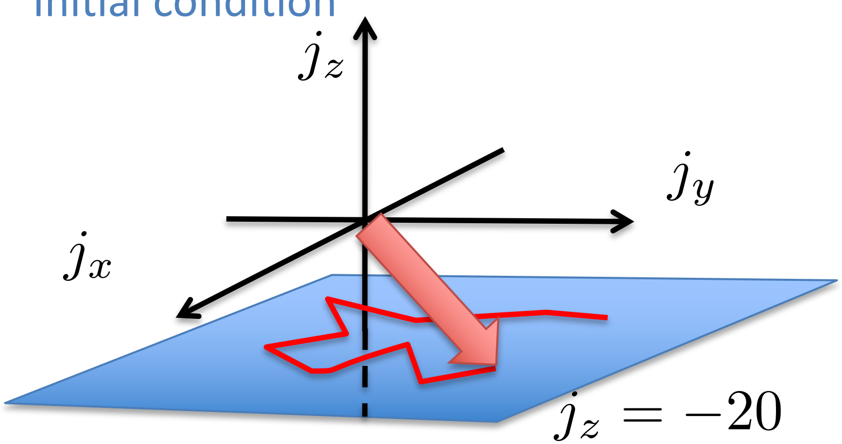
$j_i \equiv \langle J_i \rangle / N \Rightarrow j_i^{\lambda}$

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

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



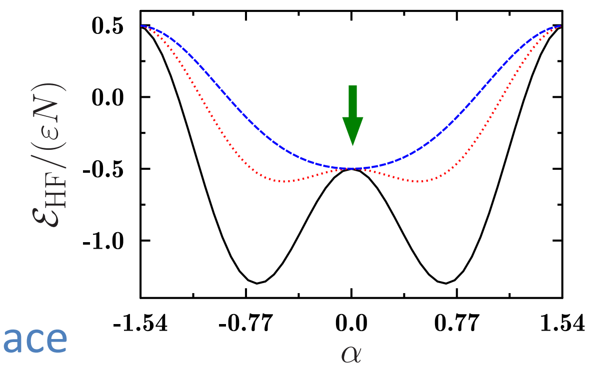
Initial condition



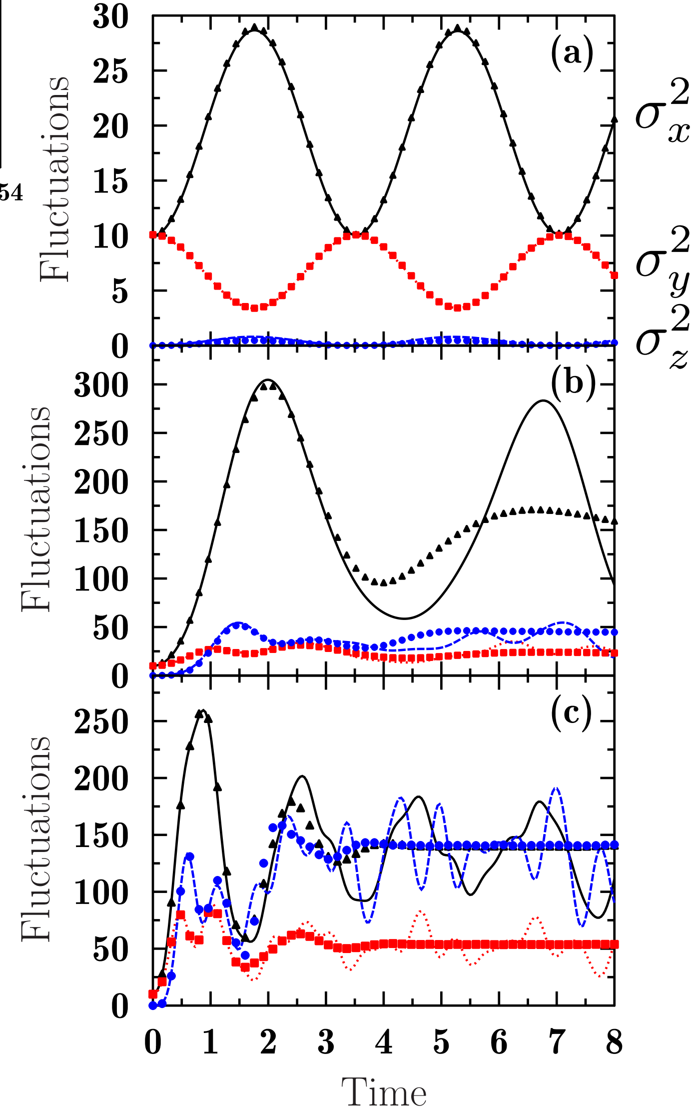
Lacroix, Ayik, Yilmaz, PRC 85 (2012)

The stochastic mean-field solution

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



Fluctuations



Formulation in quasi-spin space

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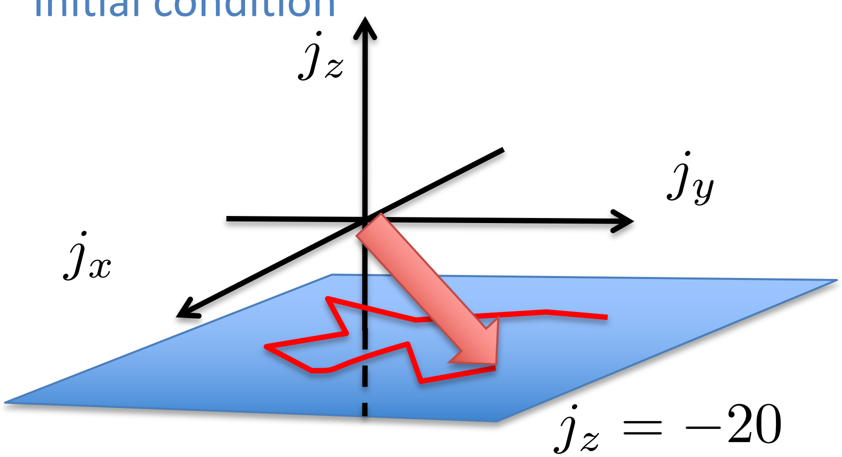
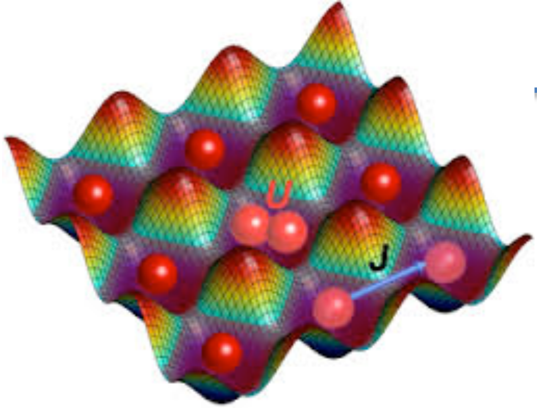
Initial condition



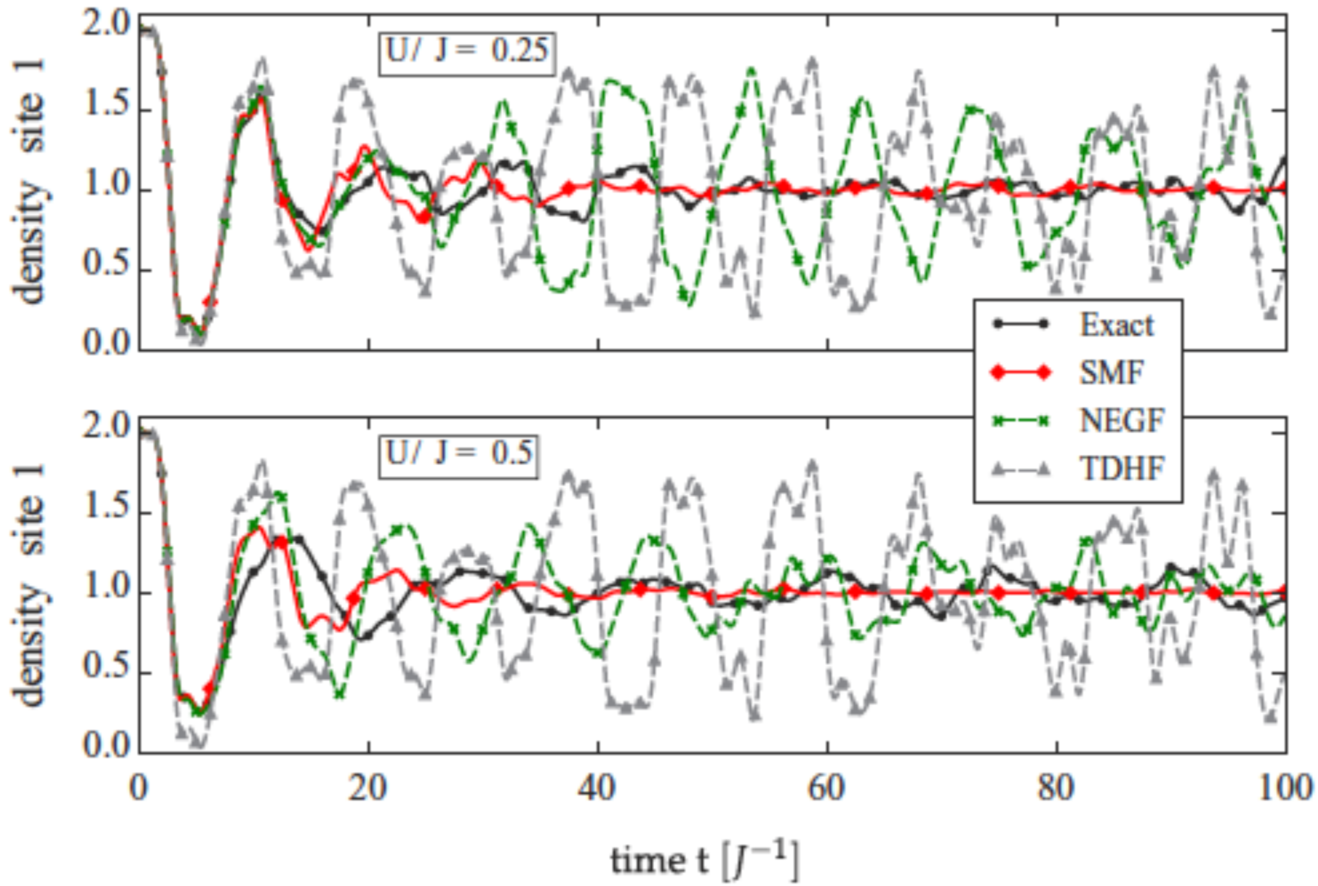
Lacroix, Ayik, Yilmaz, PRC 85 (2012)

Another example: application to systems on lattice



Lacroix, Hermanns, Hinz, Bonitz, PRB90 (2014)

$$H = -J \sum_{i,j}^{N_s} \sum_{\sigma} \delta_{\langle i,j \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i}^{N_s} c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow},$$



Link with a non-truncated simplified BBGKY hierarchy

Lacroix, Tanimura, Lacroix and Yimaz, EPJA (2016)

From $$i\hbar\frac{\mathrm{d}\rho^{(n)}}{\mathrm{d}t} = \left[h(\rho^{(n)}), \rho^{(n)}\right]$$

One can obtain a set of coupled equations for: $C_{1\dots k} = \overline{\delta\rho_1^{(n)} \dots \delta\rho_k^{(n)}}$.

The first two equations are:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\overline{\rho}(t) = [h(\overline{\rho}(t)), \overline{\rho}(t)] + \mathrm{Tr}_2\left[\tilde{v}_{12}, C_{12}\right]$$

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}C_{12} &= [h_1[\overline{\rho}] + h_2[\overline{\rho}], C_{12}] \\ &+ \mathrm{Tr}_3\left[\tilde{v}_{13} + \tilde{v}_{23}, C_{13}\overline{\rho}_2 + C_{23}\overline{\rho}_1\right] \\ &+ \mathrm{Tr}_3\left[\tilde{v}_{13} + \tilde{v}_{23}, C_{123}\right], \end{aligned}$$

Here starts the approximation.

And more generally:

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}C_{1\dots k} = &\left[\sum_{\alpha\leq k} t_\alpha, C_{1\dots k}\right] \\ &+ \sum_{\alpha=1}^{k} \mathrm{Tr}_{k+1}[\tilde{v}_{\alpha k+1}, C_{1\dots k}\overline{\rho_{k+1}}] \\ &+ \sum_{\alpha=1}^{k} \mathrm{Tr}_{k+1}\left[\tilde{v}_{\alpha k+1}, C_{1\dots(\alpha-1)(\alpha+1)\dots(k+1)}\overline{\rho_\alpha}\right] \\ &+ \sum_{\alpha=1}^{k} \mathrm{Tr}_{k+1}\left[\tilde{v}_{\alpha k+1}, C_{1\dots(\alpha-1)(\alpha+1)\dots k}C_{\alpha k+1}\right] \\ &+ \sum_{\alpha=1}^{k} \mathrm{Tr}_{k+1}\left[\tilde{v}_{\alpha k+1}, C_{1\dots(k+1)}\right]. \qquad (6) \end{aligned}$$

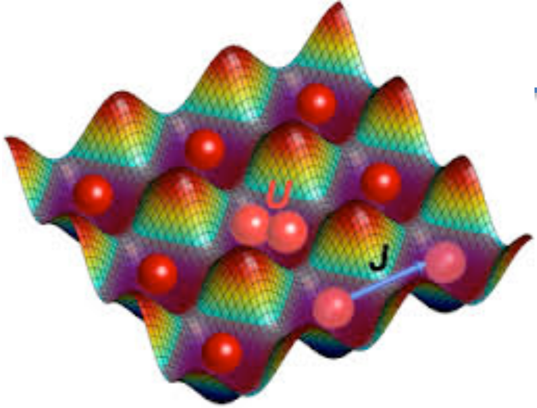
+ Independent MF trajectories

Non-truncated BBGKY like hierarchy

– Some terms are not correct
Starting at second order

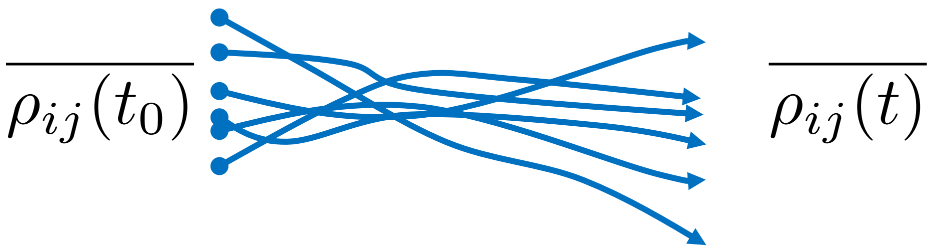
Can we use this to improve the approach ?

Hybrid approach: merging SMF and BBGKY

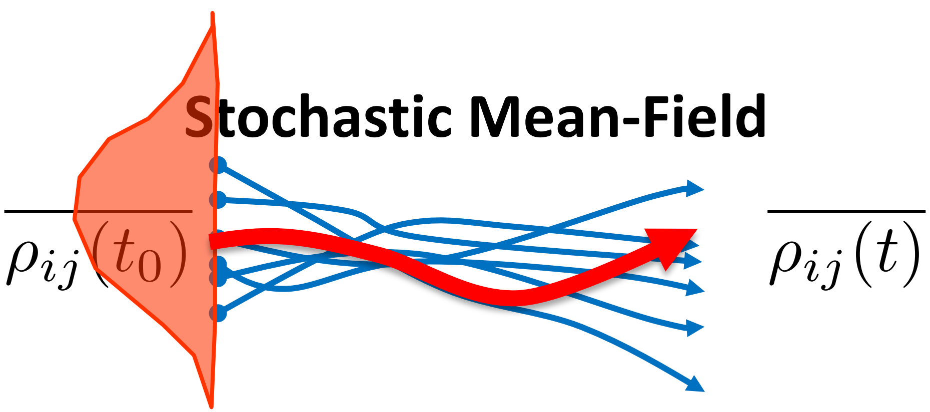


Czuba, Lacroix, Regnier, Ulgen, Yilmaz, EPJA 56 (2020)

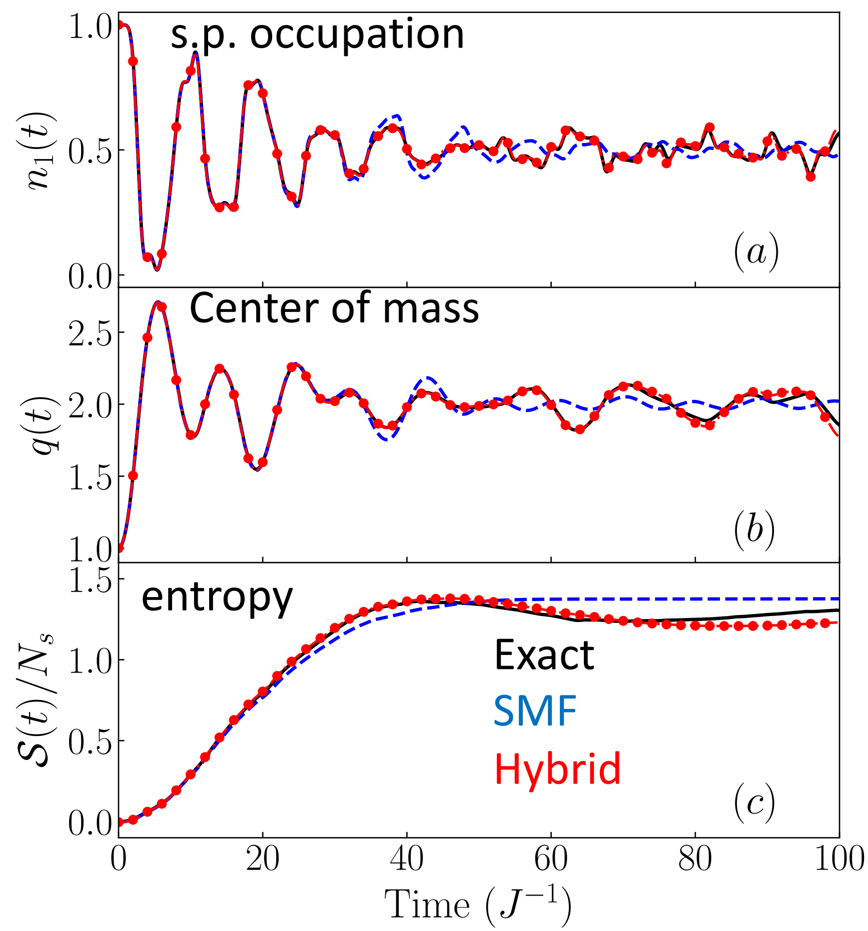
Stochastic Mean-Field



Stochastic Mean-Field



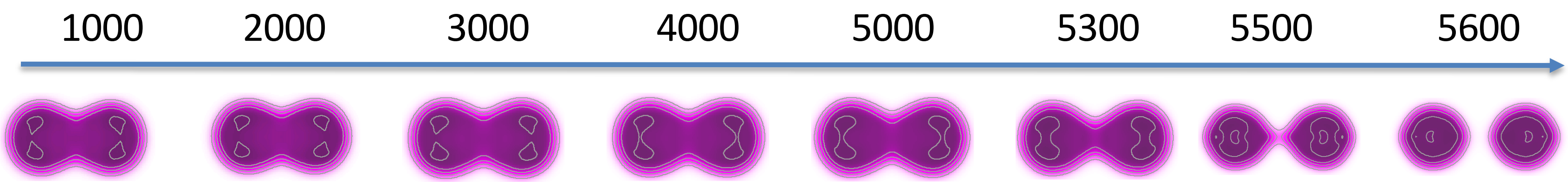
8 fermions on a 1D lattice



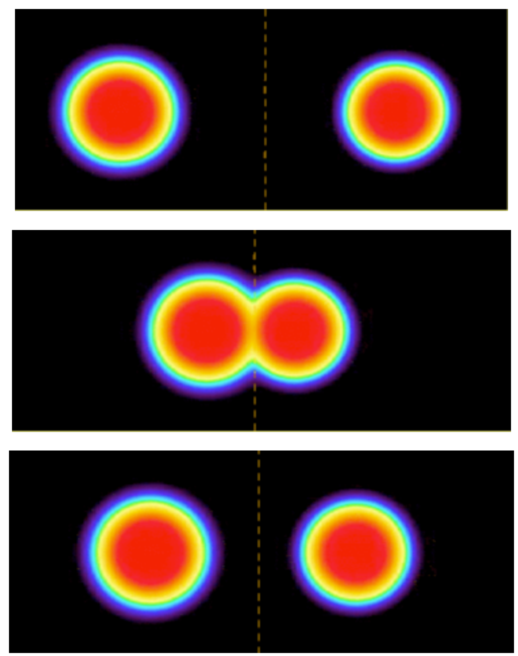
Mean-Field: stochastic + average correlation effect

Phase-space method applied in the nuclear physics context

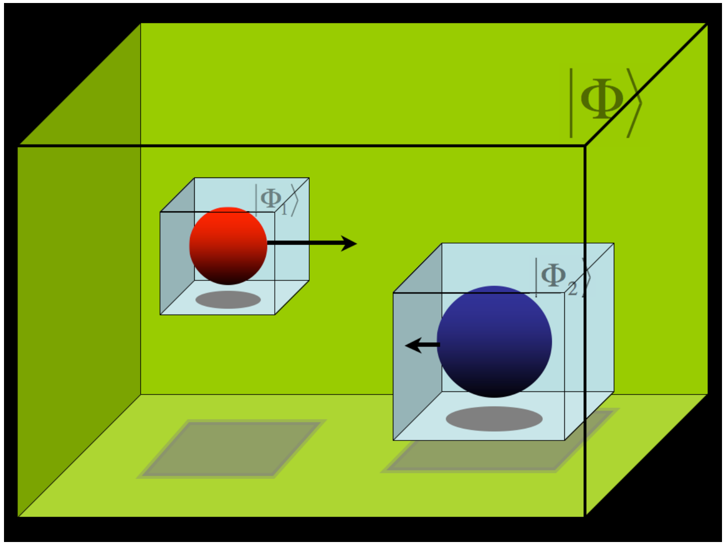
Nuclear Fission



Transfer reactions



Nuclear reaction with normal/superfluid nuclei on a mesh



TDHF is a standard tool $|\Phi_i\rangle$: Slater

$$i\hbar\frac{d\rho}{dt} = [h(\rho), \rho]$$ ⇒ Single-particle evolution

Simenel, Lacroix, Avez, arXiv:0806.2714v2

Introduction of pairing: TDHFB

$$i\hbar\frac{d}{dt}\mathcal{R} = [\mathcal{H}(\mathcal{R}), \mathcal{R}] \qquad \mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho \end{pmatrix}$$

⇒ Quasi-particle evolution

(Active Groups: France, US, Japan…)

TDHFB = 1000 * (TDHF)

⇒ Full TDHFB (Skyrme-spherical symmetry) Avez, Simenel, Chomaz, PRC 78 (2008).

Full TDHFB (Skyrme-symmetry unrestricted) Stetcu, Bulgac, Magierski, and Roche, PRC 84 (2011)

(Gogny-axial symmetry) Hashimoto, PRC 88 (2013).

⇒ Symmetry unrestricted TDBCS limit of TDHFB (also called Canonical basis TDHFB)

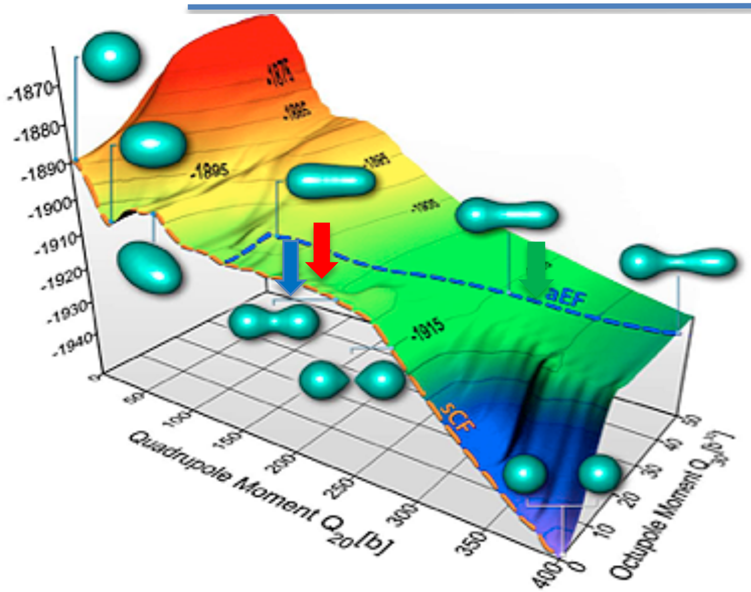
Neglect Δ_{ij} ⇒ $|\Phi(t)\rangle = \prod_{k>0}\left(u_k(t) + v_k(t)a_k^\dagger(t)a_{\bar{k}}^\dagger(t)\right)|-\rangle.$

TDBCS = 2-3 * (TDHF)

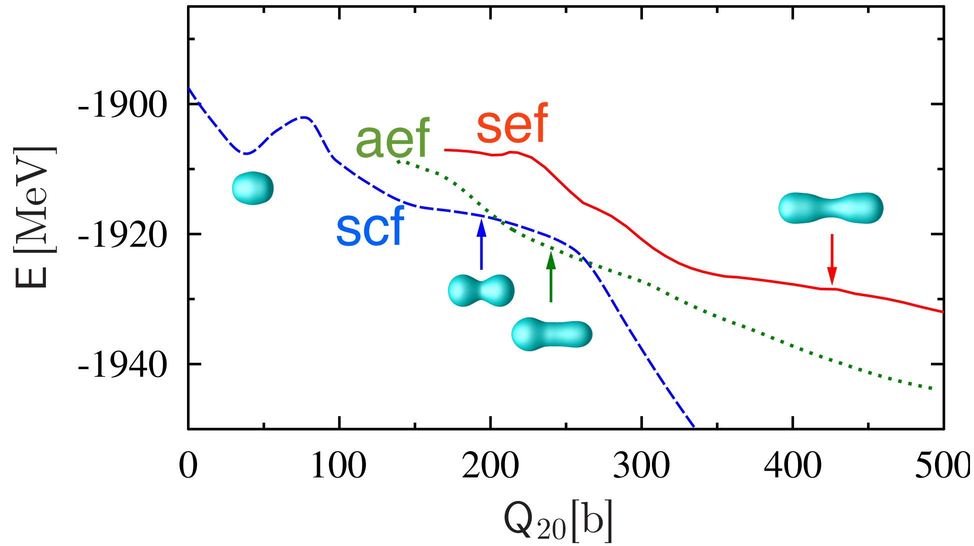
Ebata, Nakatsukasa et al, PRC82 (2010)
Scamps, Lacroix, PRC88 (2013).

⇒ Very good predictive power

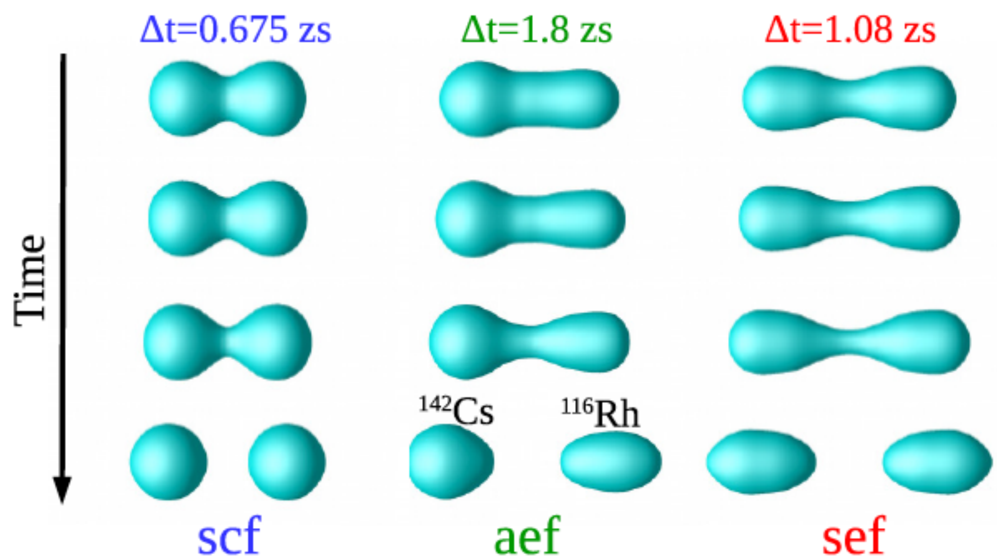
Fission of superfluid ^{258}Fm

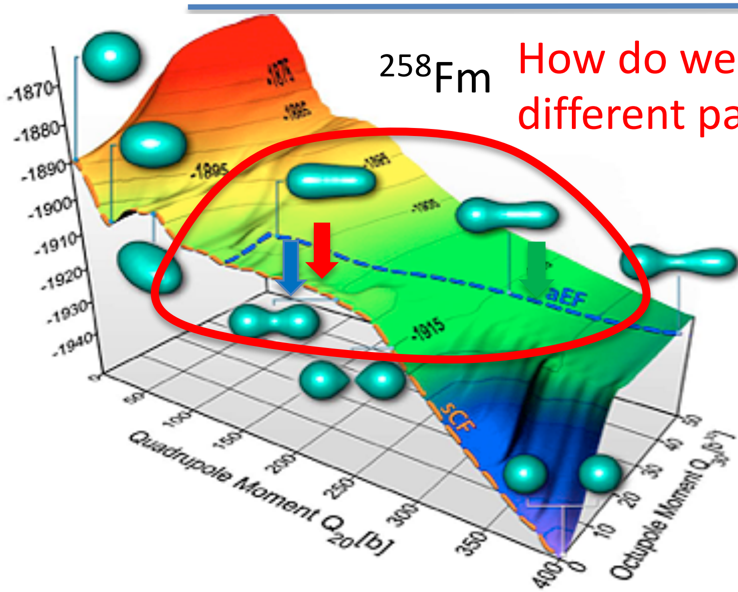


Identification of main fission paths

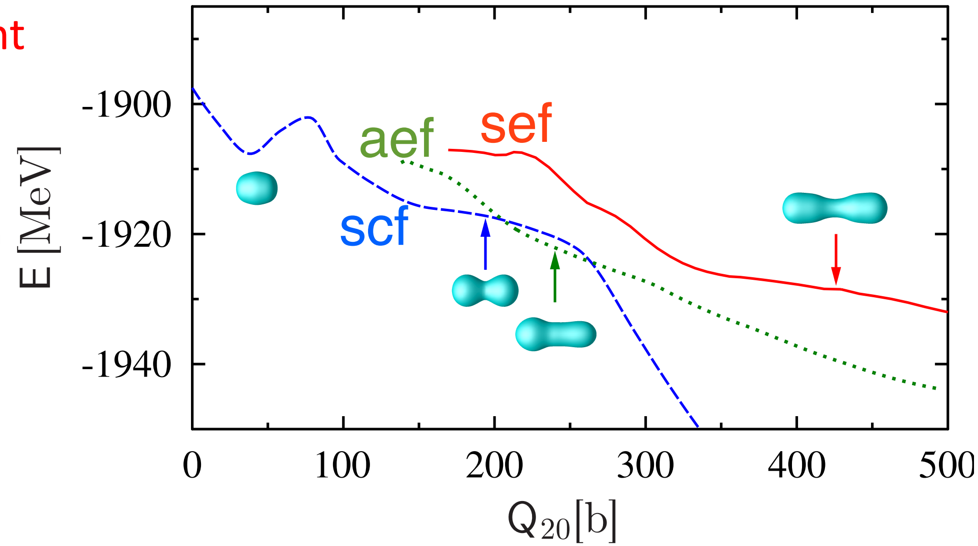


1 zs = 10^{-21} s

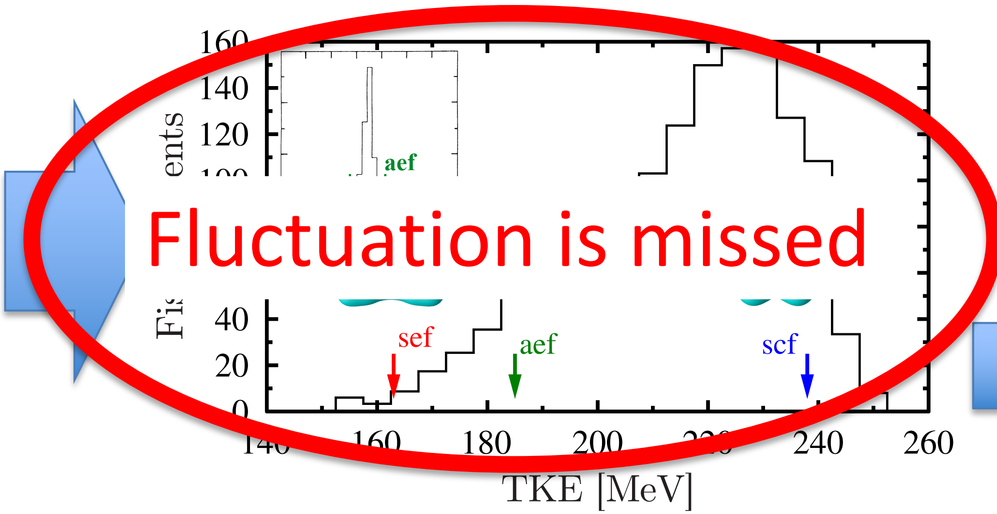




How do we weight different paths?



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

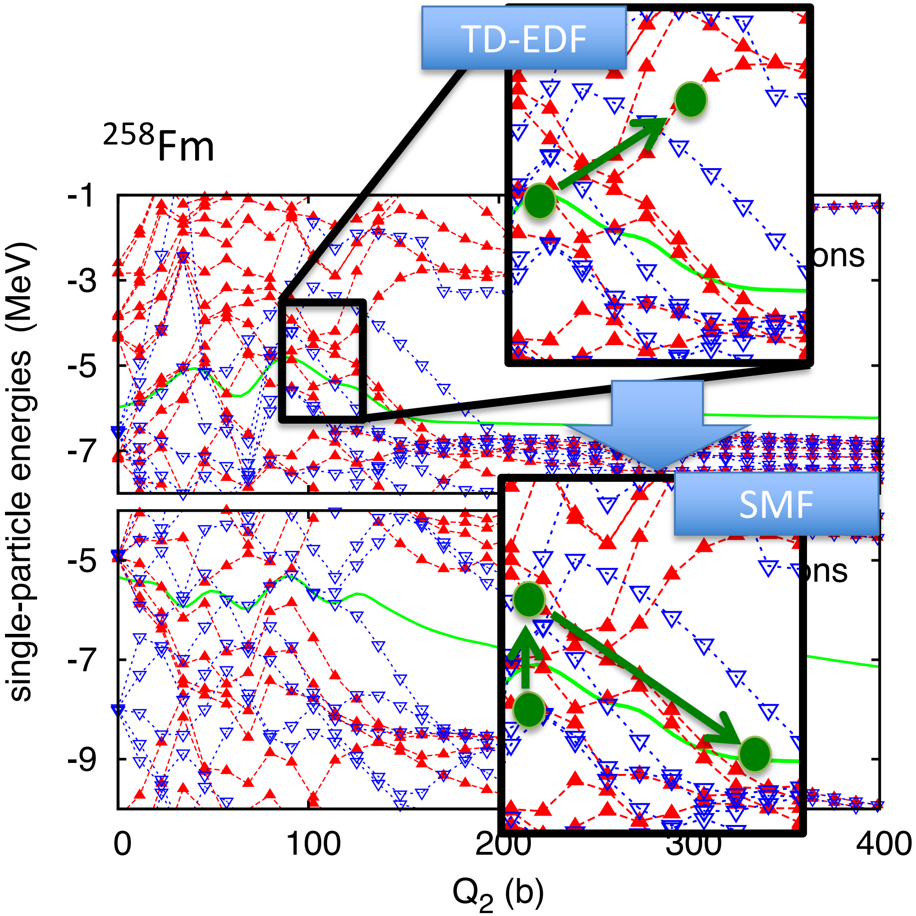
SMF in density matrix space

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

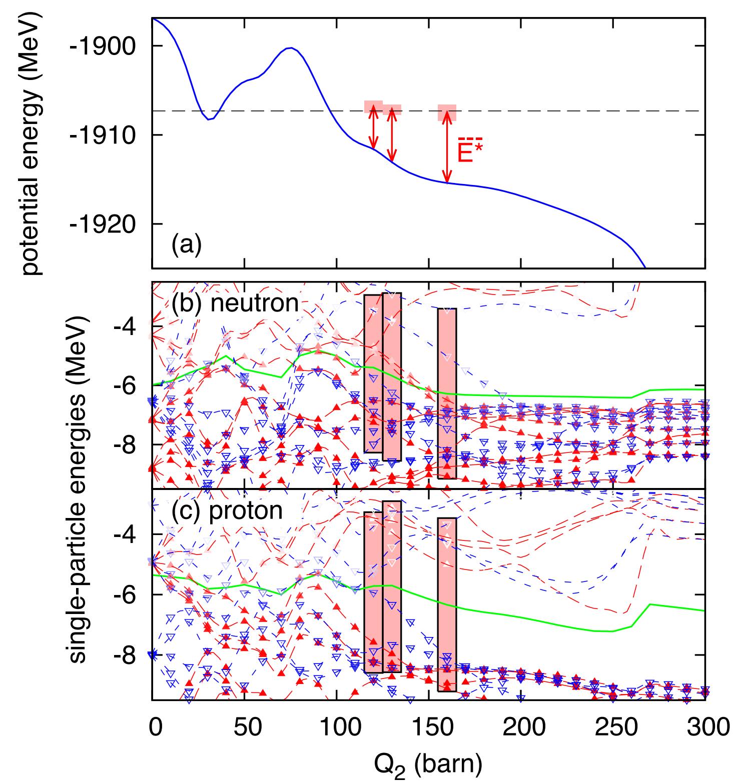
$$\rho^\lambda(\mathbf{r},\mathbf{r}',t_0) = \sum_{ij} \Phi_i^*(\mathbf{r},t_0) \rho^\lambda_{ij} \Phi_j(\mathbf{r}',t_0)$$

$$\overline{\rho^\lambda_{ij}} = \delta_{ij} n_i$$

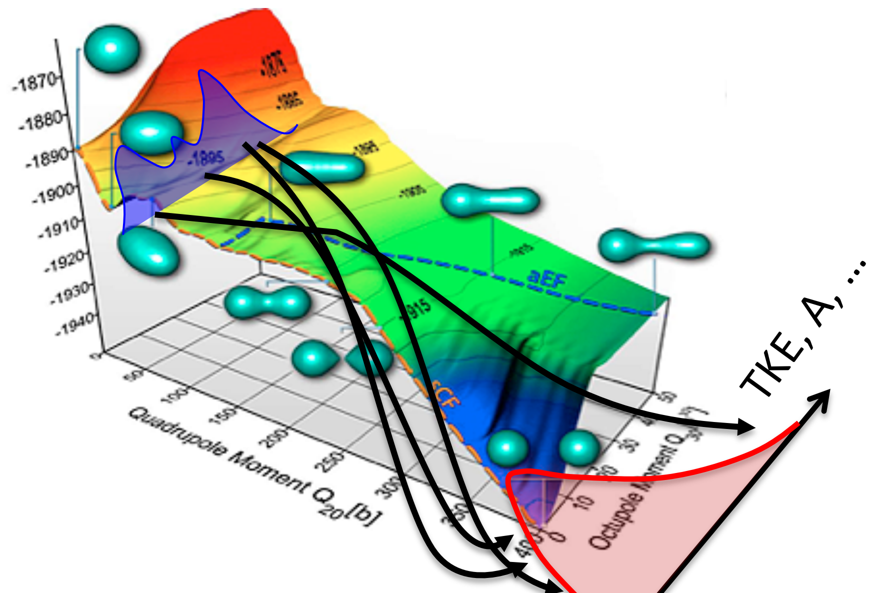
$$\overline{\delta\rho^\lambda_{ij}\delta\rho^\lambda_{j'i'}} = \frac{1}{2}\delta_{jj'}\delta_{ii'}\left[n_i(1-n_j)+n_j(1-n_i)\right].$$



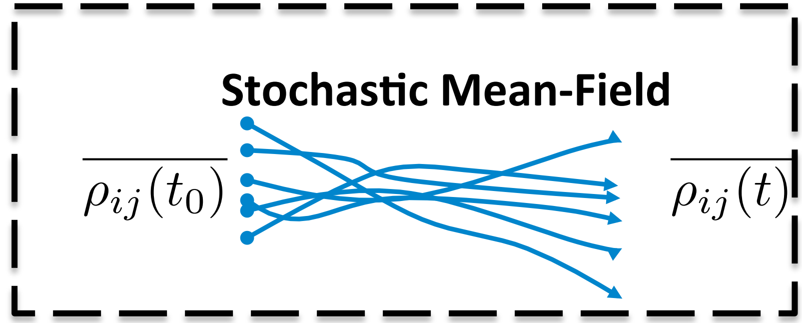
Range of fluctuation fixed by energy cons.



How to conceal microscopic deterministic approach and randomness ?



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

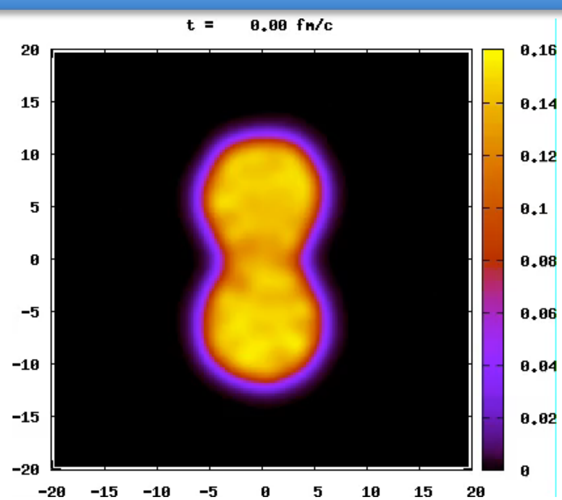


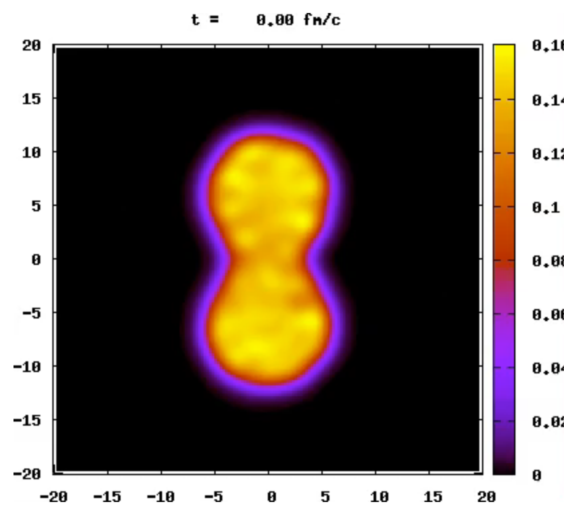
Constrains:

-Generates a sample of microscopic trajectories (typically 300)

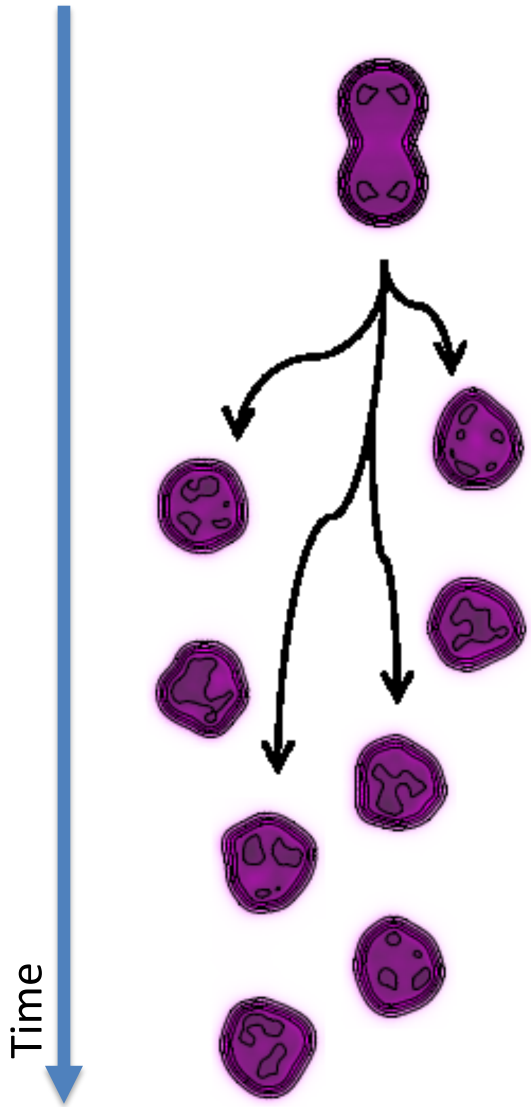
-Each trajectory is 8-10 days CPU time

Some trajectories illustration



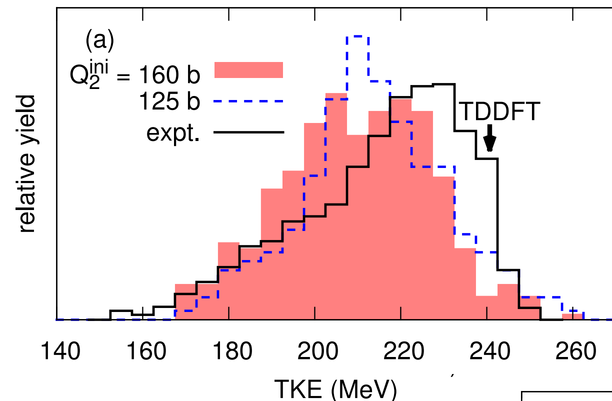


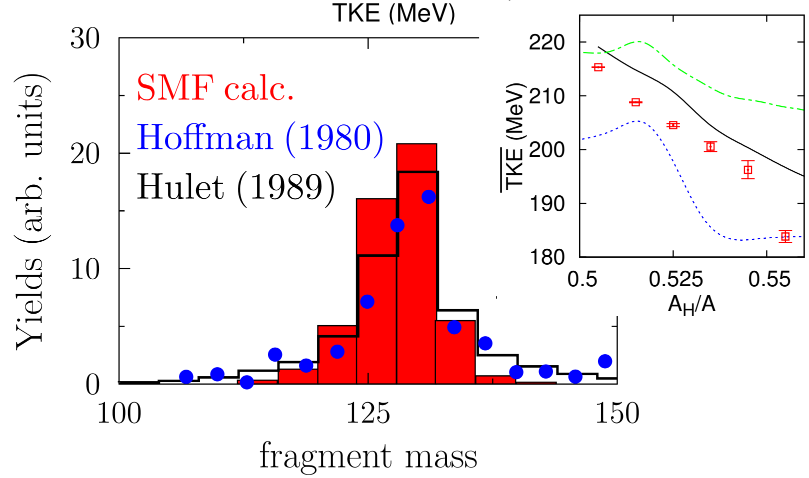
How to conceal microscopic deterministic approach and randomness ?



From deterministic to statistical approach

Theory vs experiment





Tanimura, Lacroix, Ayik, PRL (2017)

Summary and outlook

Part 1 : Lorenzo

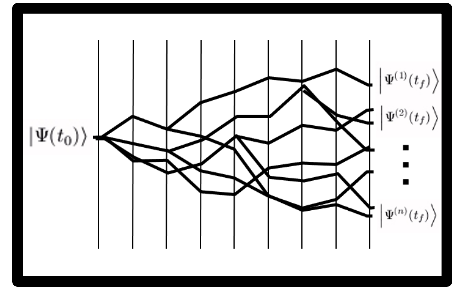
Exact stochastic methods

Quantum Monte Carlo can solve high dimensional quantum problems.

Variational QMC is fast and precise, but relays on a good parametrization of the wavefunction

Green function QMC allows to extract the groundstate of the system using a diffusion in imaginary time

Auxiliary field QMC permits to find the groundstate energy of many-fermions

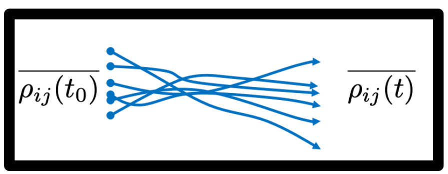


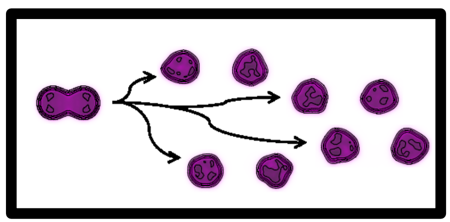
Extension to real-time evolution

Part 2

For perturbative systems, there are alternative jump theories - STDHF

Phase-space approaches for Fermi systems (powerful and versatile)





Open for discussion: how can we use these approximate approach for static properties ?