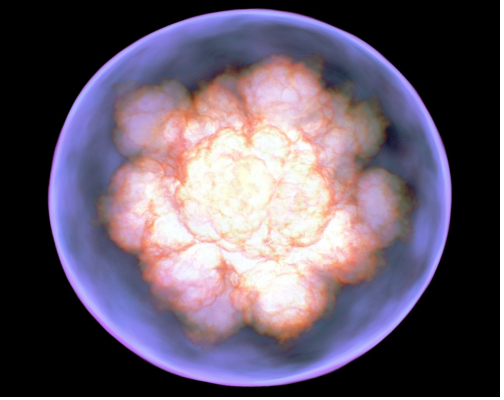
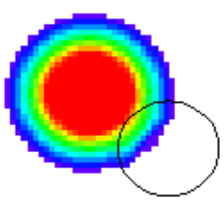


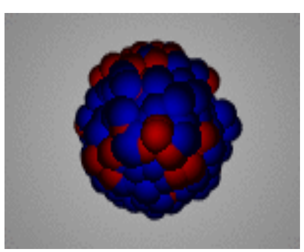
International Summer School "Nuclear Theory and Astrophysical Applications" (NTAA17), Dubna, -10 - 22, 2017.

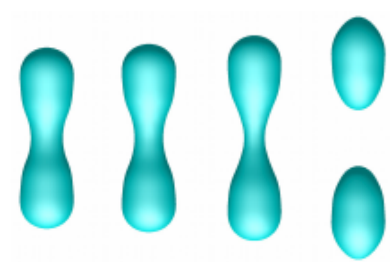
Mean-field and beyond mean-field dynamical theories for nuclei

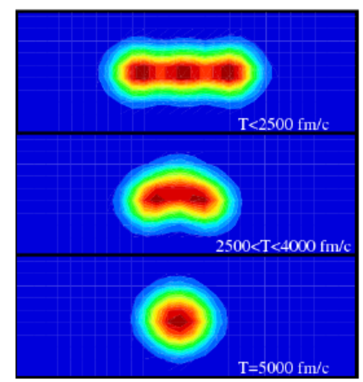
Denis Lacroix

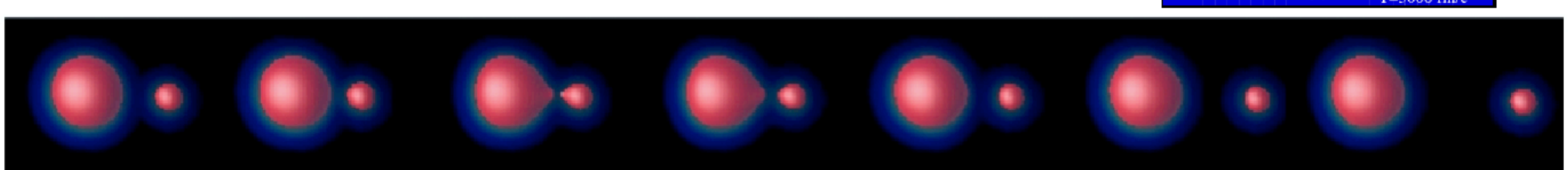
INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY









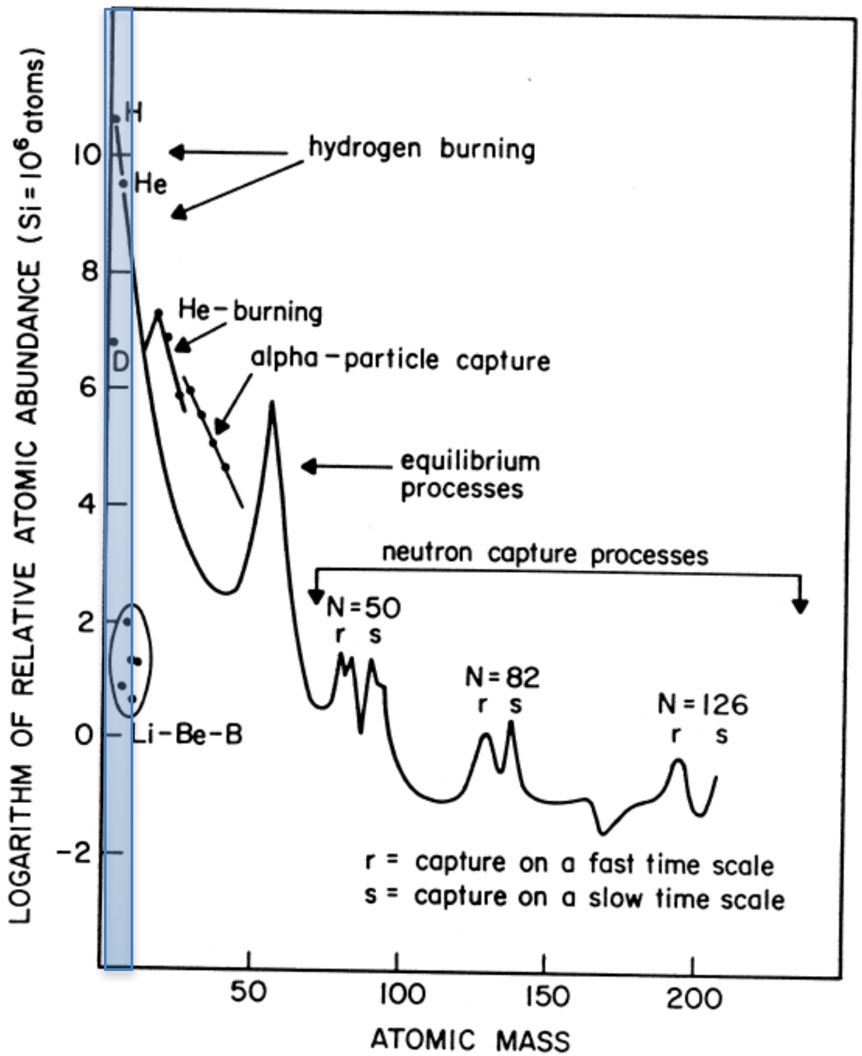


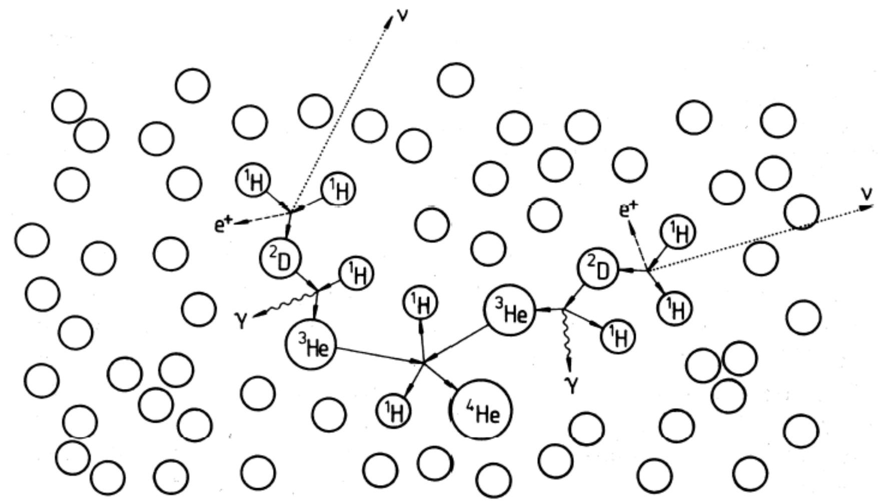
Some astrophysical motivations for the microscopic description of large amplitude collective motion

Interest of the lecture from an astrophysics perpsective

Observation of today's abundancy

Solar abundancy





Light nuclei formation

$p + p \rightarrow d + e^+ + \nu_e$ $Q = 0.42$ MeV

$p + e^- + p \rightarrow d + \nu_e$ $Q = 1.42$ MeV

$d + p \rightarrow {}^3He + \gamma$ $Q = 5.49$ MeV

${}^3He + {}^3He \rightarrow {}^4He + 2p$ $Q = 12.96$ MeV

ppI chain

91 % sun energy

${}^3He + {}^4He \rightarrow {}^7Be + \nu_e$

$e^- + {}^7Be \rightarrow {}^7Li + \nu_e$ $Q = 0.86$ MeV

$p + {}^7Li \rightarrow 2\,{}^4He$

${}^7Be + p \rightarrow {}^8B + \gamma$

${}^8B \rightarrow {}^8Be^* + e^+ + \nu_e$

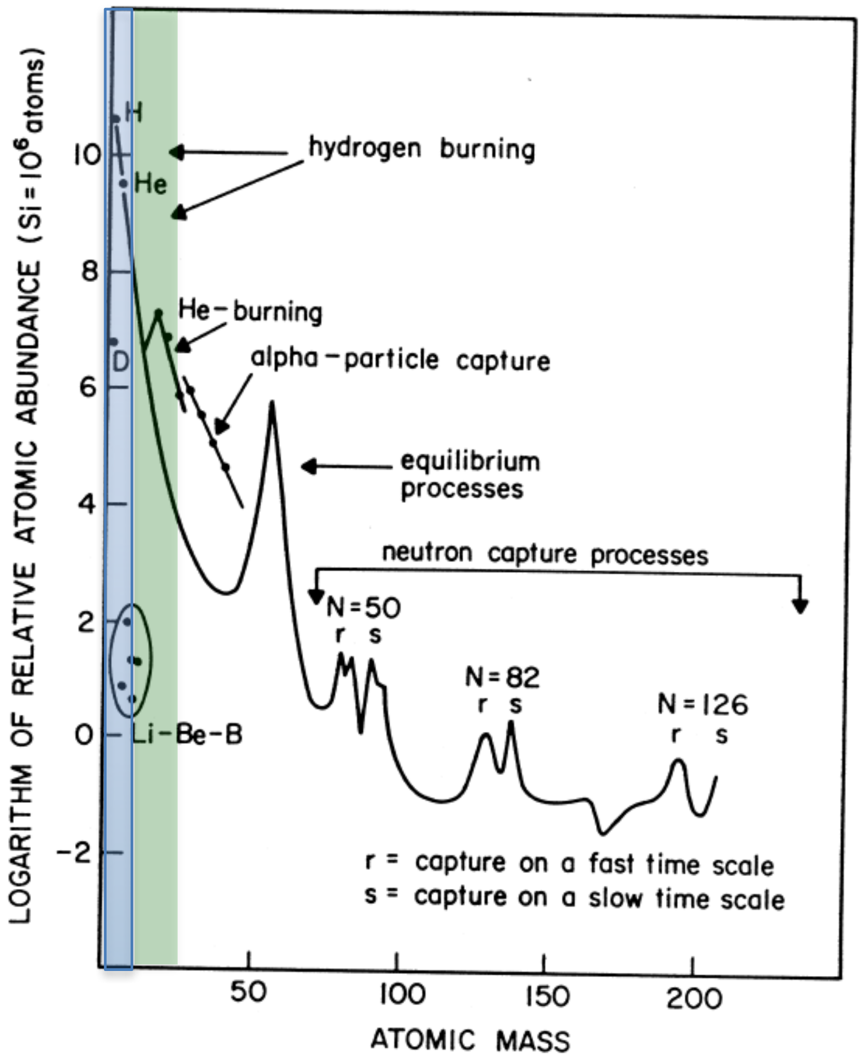
${}^8Be^* \rightarrow 2\,{}^4He$

…

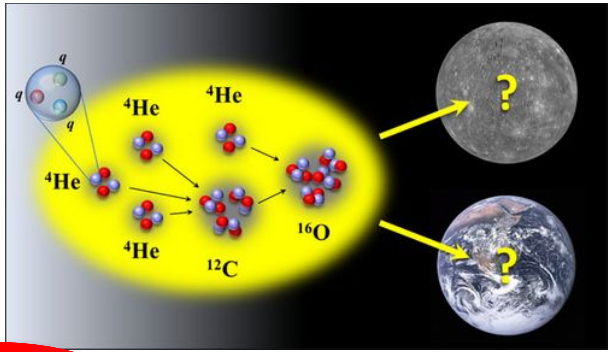
Problem:
How to have heavier systems?

Observation of today's abundancy

Solar abundancy



Alpha burning $\alpha + \alpha + \alpha \rightarrow {}^{12}\mathrm{C}$



Ternary Fusion

$$^{4}He + {}^{12}C \rightarrow {}^{16}O + \gamma \quad Q = 7.16\ MeV$$

$$^{4}He + {}^{16}O \rightarrow {}^{20}Ne + \gamma \quad Q = 4.73\ MeV$$

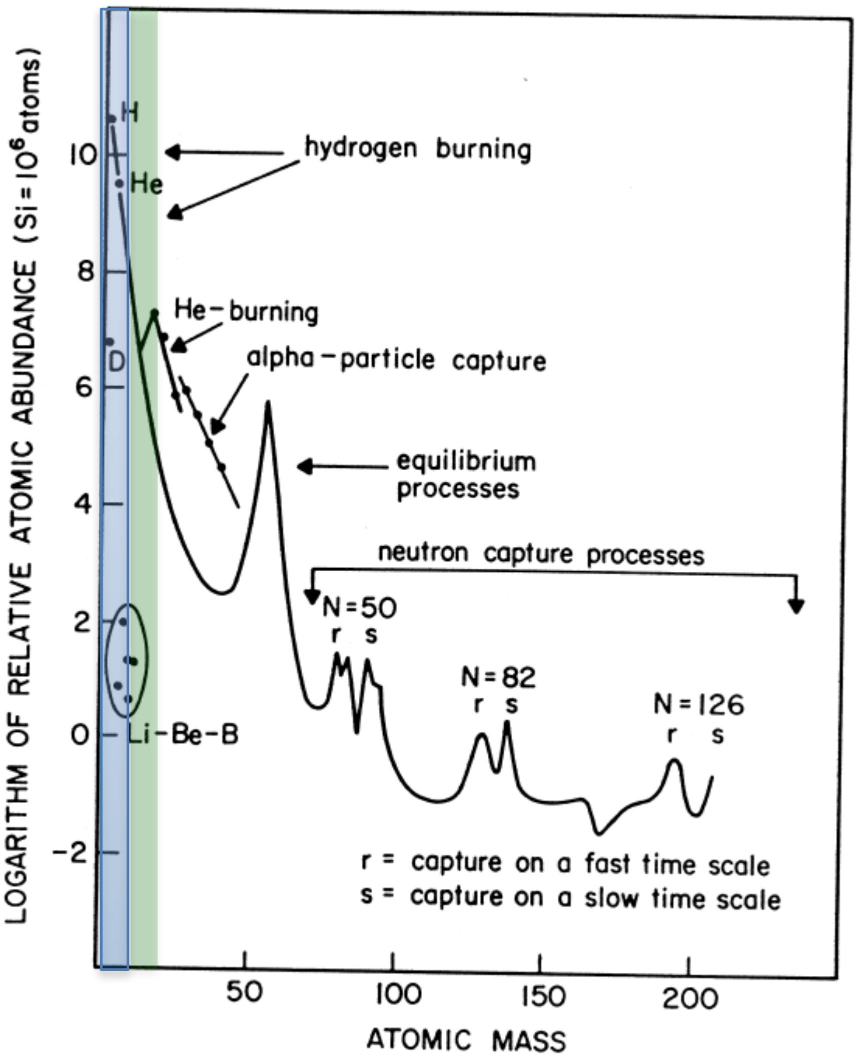
$$^{20}Ne + \gamma \rightarrow {}^{4}He + {}^{16}O$$

$$^{4}He + {}^{20}Ne \rightarrow {}^{24}Mg + \gamma$$

Interest of the lecture from an astrophysics perpsective

Observation of today’s abundancy

Solar abundancy



CNO cycle

$$^{12}C + p \rightarrow {}^{13}N + \gamma$$

$$^{13}N \rightarrow {}^{13}C + e^{+} + \nu_e$$

$$^{13}C + p \rightarrow {}^{14}N + \gamma$$

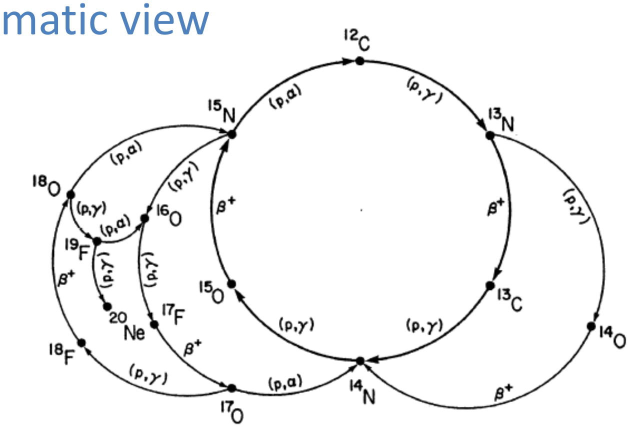
$$^{14}N + p \rightarrow {}^{15}O + \gamma$$

$$^{15}O \rightarrow {}^{15}N + e^{+} + \nu_e$$

$$^{15}N + p \rightarrow {}^{12}C + {}^{4}He$$

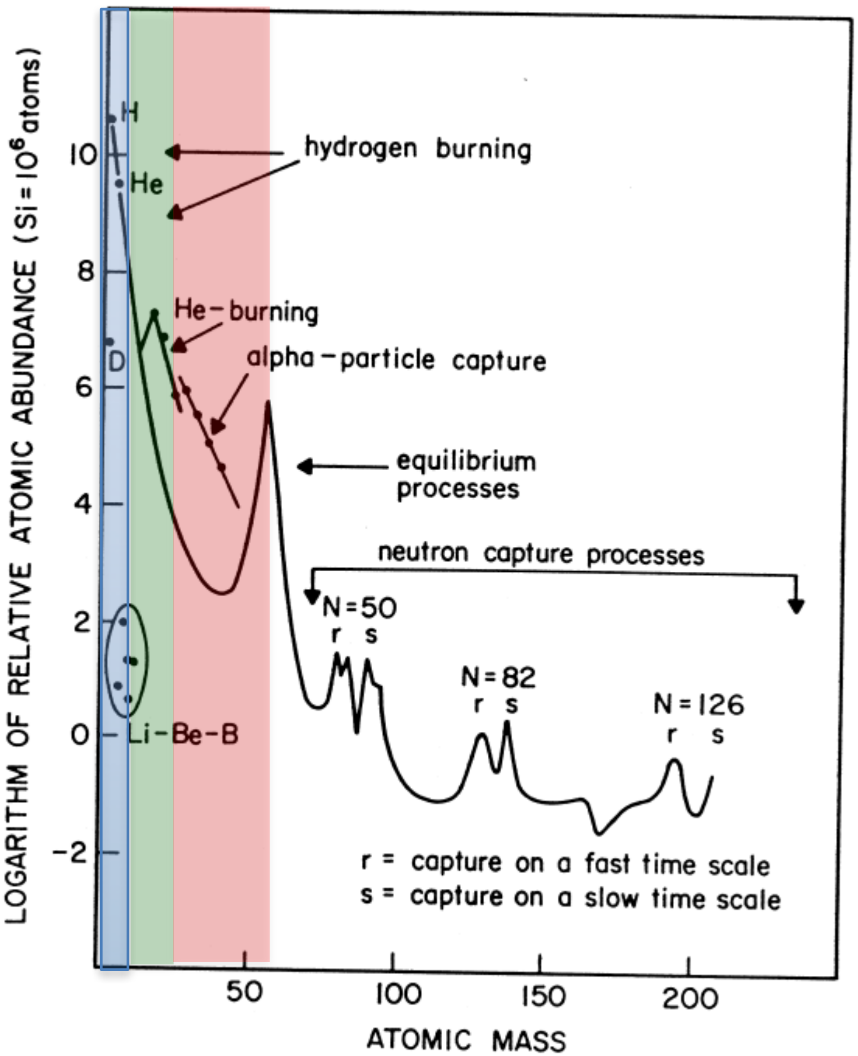
2 % sun energy

Schematic view



Observation of today's abundancy

Solar abundancy



Synthesis of Nuclei with A < 60

$^{12}C + ^{12}C \rightarrow ^{20}Ne + ^{4}He$

$^{12}C + ^{12}C \rightarrow ^{23}Na + p$

$^{12}C + ^{12}C \rightarrow ^{23}Mg + n$

$^{12}C + ^{12}C \rightarrow ^{24}Mg + \gamma$

$^{16}O + ^{16}O \rightarrow ^{24}Mg + 2\,^{4}He$

$^{16}O + ^{16}O \rightarrow ^{28}Si + ^{4}He$

$^{16}O + ^{16}O \rightarrow ^{31}P + p$

$^{16}O + ^{16}O \rightarrow ^{31}S + n$

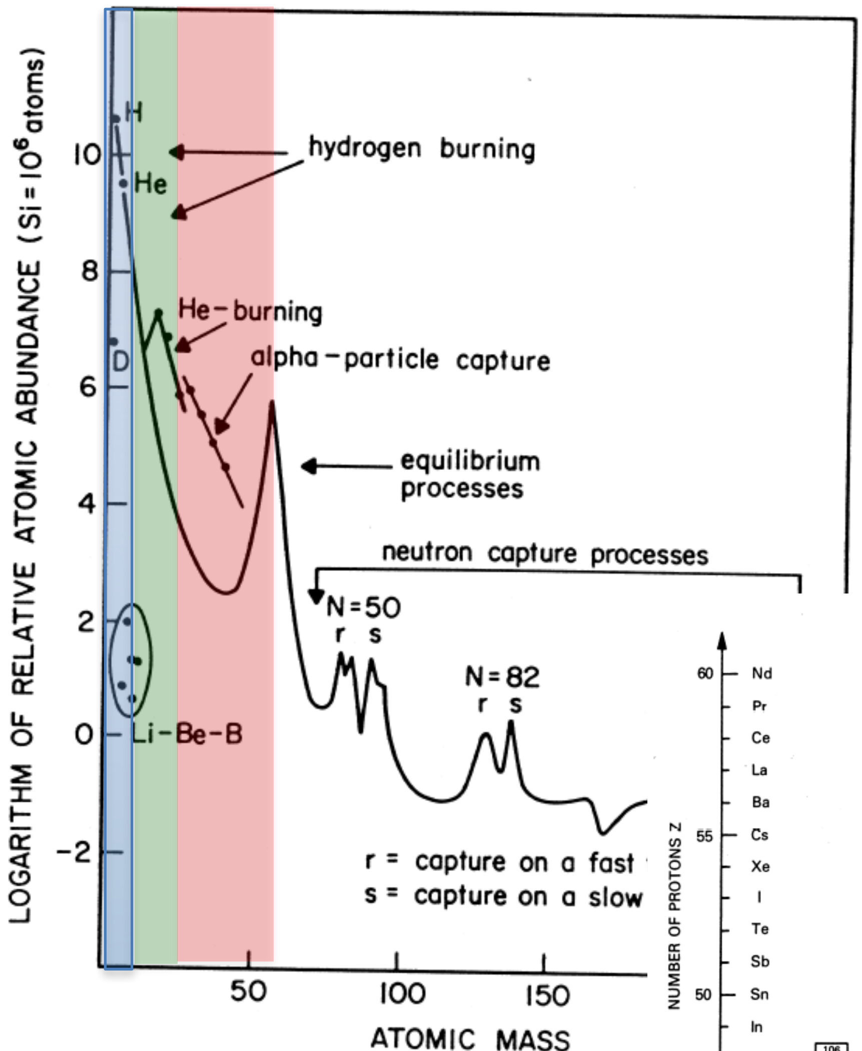
$^{16}O + ^{16}O \rightarrow ^{32}S + \gamma$

Light Ion fusion or incomplete fusion

Interest of the lecture from an astrophysics perpsective

Observation of today's abundancy

Solar abundancy



Synthesis of nuclei with A > 60

s-process: competition between neutron capture and beta decay

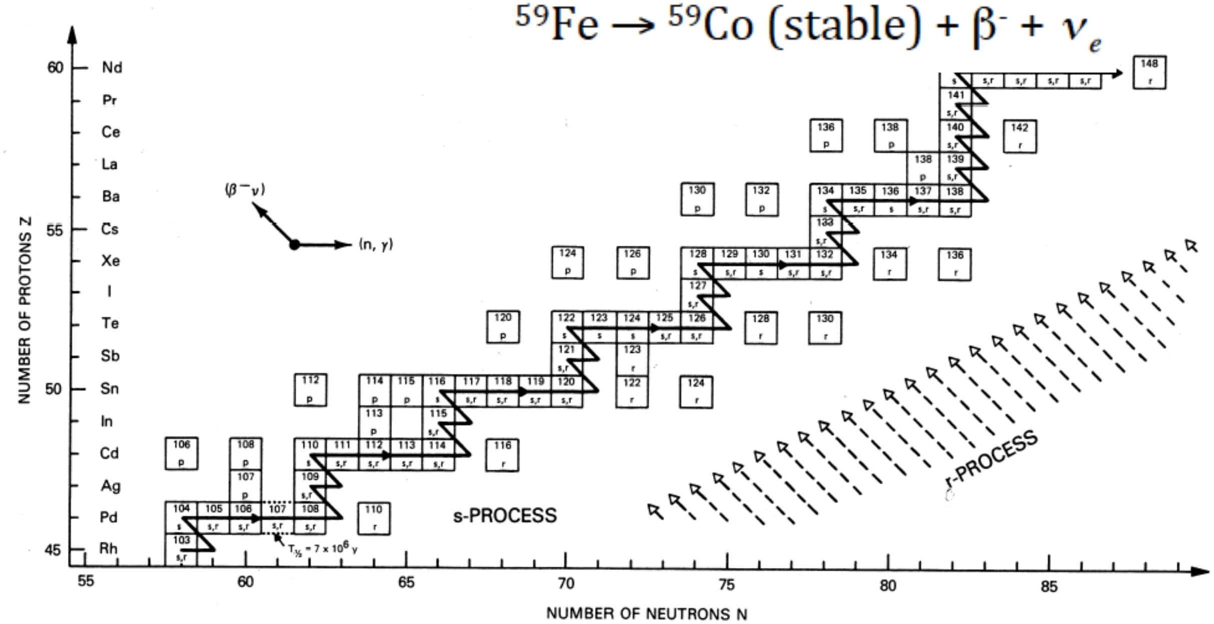
Example

$$^{56}\mathrm{Fe} + n \rightarrow {}^{57}\mathrm{Fe}\ (\mathrm{stable}) + \gamma$$

$$^{57}\mathrm{Fe} + n \rightarrow {}^{58}\mathrm{Fe}\ (\mathrm{stable}) + \gamma$$

$$^{58}\mathrm{Fe} + n \rightarrow {}^{59}\mathrm{Fe}\ (t_{1/2} = 44.5\ \mathrm{d}) + \gamma$$

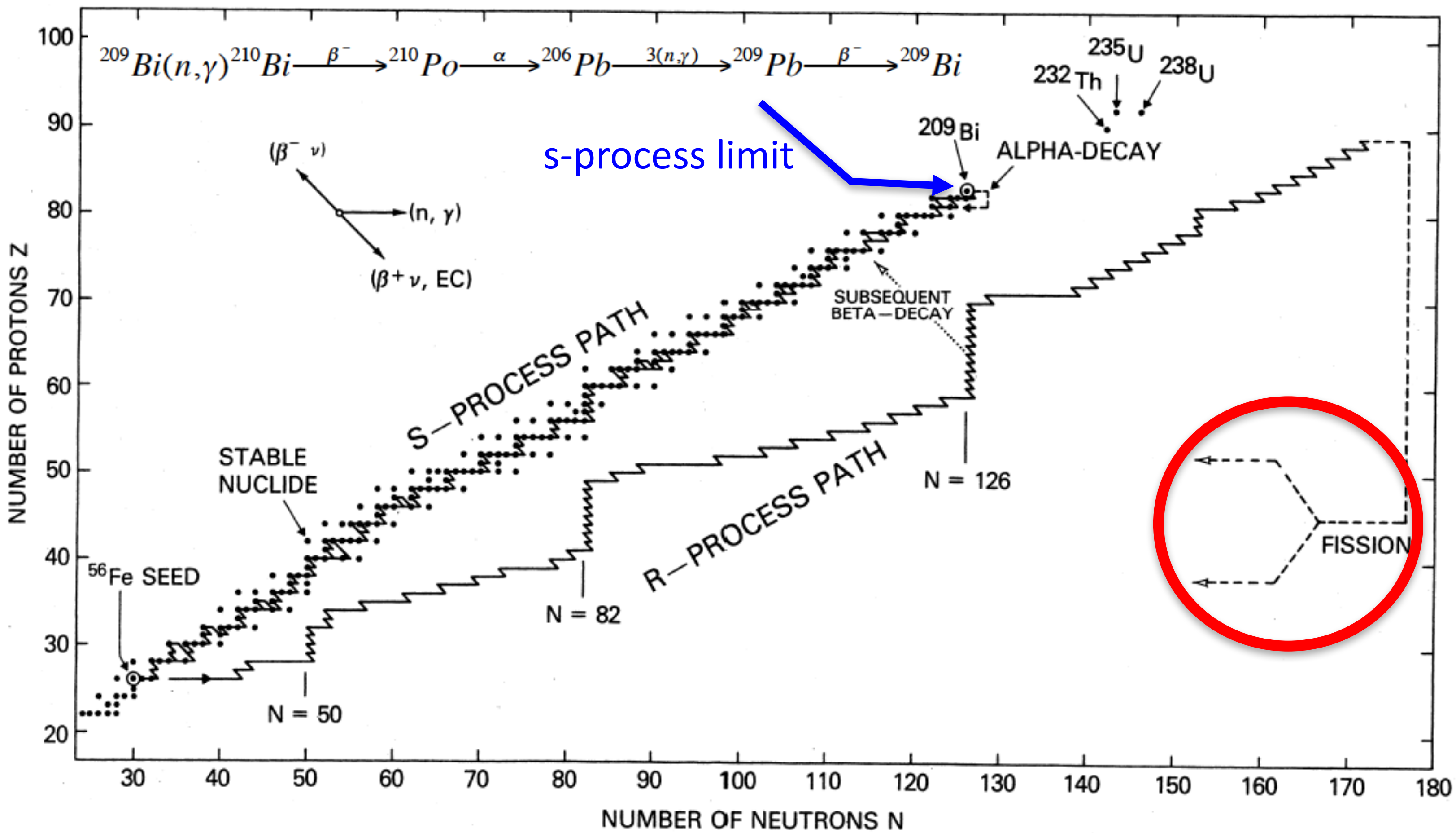
$$^{59}\mathrm{Fe} \rightarrow {}^{59}\mathrm{Co}\ (\mathrm{stable}) + \beta^{-} + \overline{\nu_e}$$



Interest of the lecture from an astrophysics perpsective

Observation of today's abundancy

The s-process compete with the r-process (rapid neutron capture)
If neutron density is high



Scope of the lecture :

large amplitude collective motion described with microscopic theory

Basic aspects of quantum dynamics (Schroedinger, Liouville, Ehrenfest picture)

Information theory and selection of relevant degrees of freedom

Illustration on simple quantum mechanics models and many-body theory

Time dependent mean-field theory in nuclear physics

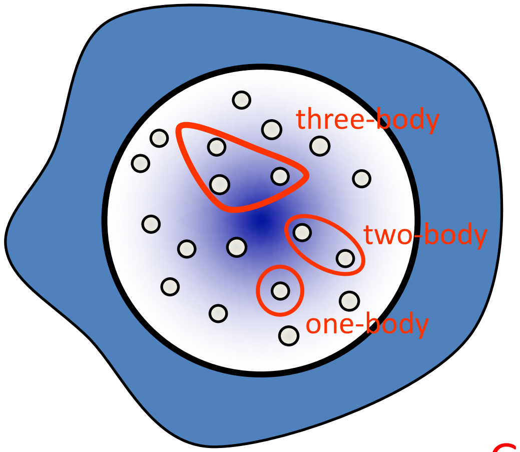
Illustration on collective motion, fusion, deep inelastic collisions

The dynamics of superfluid nuclei

Limitation of mean-field theory (complexity in nuclei)

Stochastic methods (phase-space approach, Stochastic TDHF, Auxiliary field, …)

Illustrations

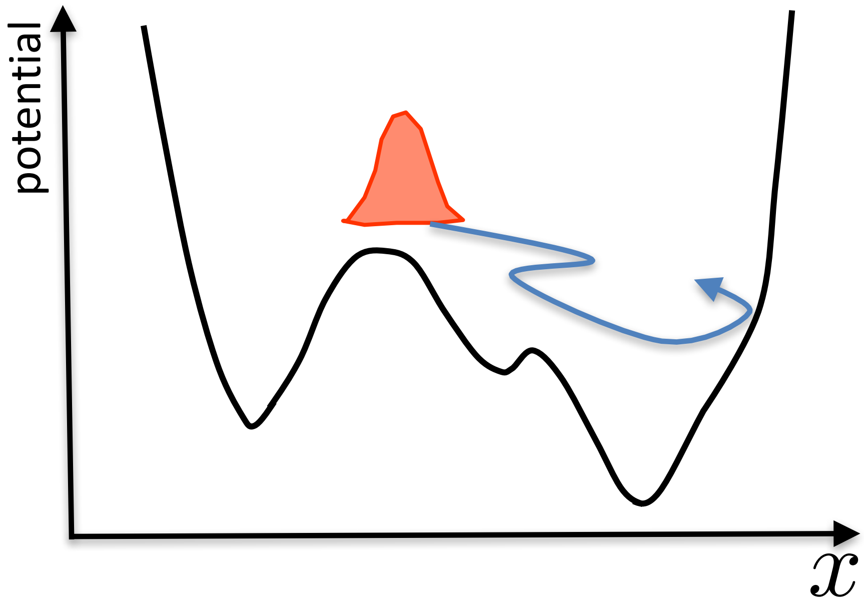


Nuclei are complex
quantum
many-body systems

Goal: Be able to describe in a unified way static and dynamical properties of these systems

Dynamics of quantum systems

Schrödinger picture



Given a Hamiltonian: H

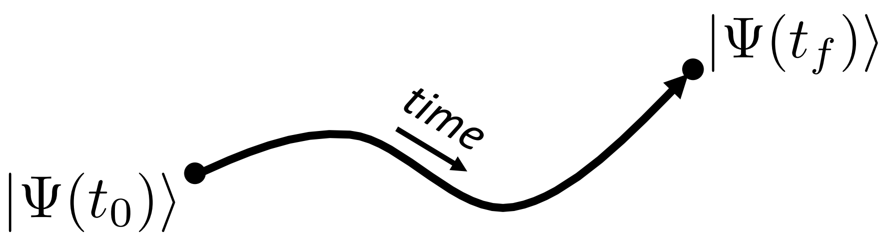
and an initial condition: $|\Psi(t_0)\rangle$

The Goal is to know the state of
The system for $t > t_0$

Schrödinger equation

Formal solution

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \quad \Rightarrow \quad |\Psi(t)\rangle = e^{\frac{1}{i\hbar}(t-t_0)H}|\Psi(t_0)\rangle$$



When is the formal solution useful?

For eigenstates of the Hamiltonian

$$|\Psi(t_0)\rangle = |\Phi_i\rangle. \qquad H|\Phi_i\rangle = E_i|\Phi_i\rangle$$

$$\Rightarrow \quad |\Psi(t)\rangle = e^{\frac{1}{i\hbar}(t-t_0)H}|\Psi_i\rangle = e^{\frac{1}{i\hbar}(t-t_0)E_i}|\Phi_i\rangle$$

If the initial state can be decomposed on eigenstates

$$|\Psi(t_0)\rangle = \sum_i c_i|\Phi_i\rangle. \quad \Rightarrow \quad |\Psi(t)\rangle = \sum_i c_i e^{\frac{1}{i\hbar}(t-t_0)E_i}|\Phi_i\rangle.$$

Difficulty

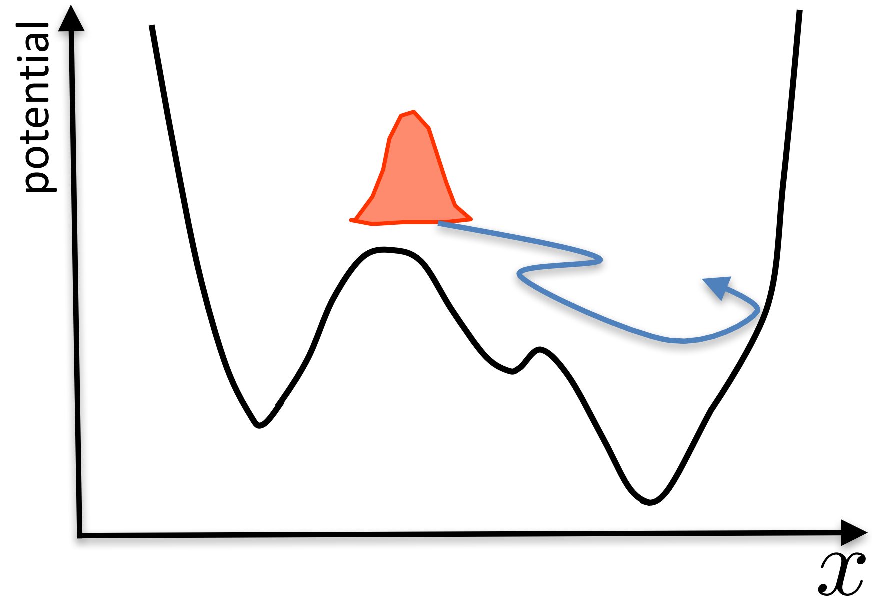
- In complex systems this method can rarely be used

⇒ Numerical methods for direct Schrödinger Eq. integration

⇒ Approximation should be made.

Simple Example: One Dimensional case

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \left\{\frac{\hat{p}^2}{2m} + V(\hat{x})\right\}|\Psi\rangle$$



Step 1 Representation → Step 2 Discretization → Step 3 Integration

Partial Differential Equation (PDE) in x representation:

$$\langle x|\Psi(t)\rangle = \Psi(x,t)$$

$$\langle x|\hat{p}|\Psi(t)\rangle = -i\hbar\frac{\partial}{\partial x}\Psi(x,t)$$

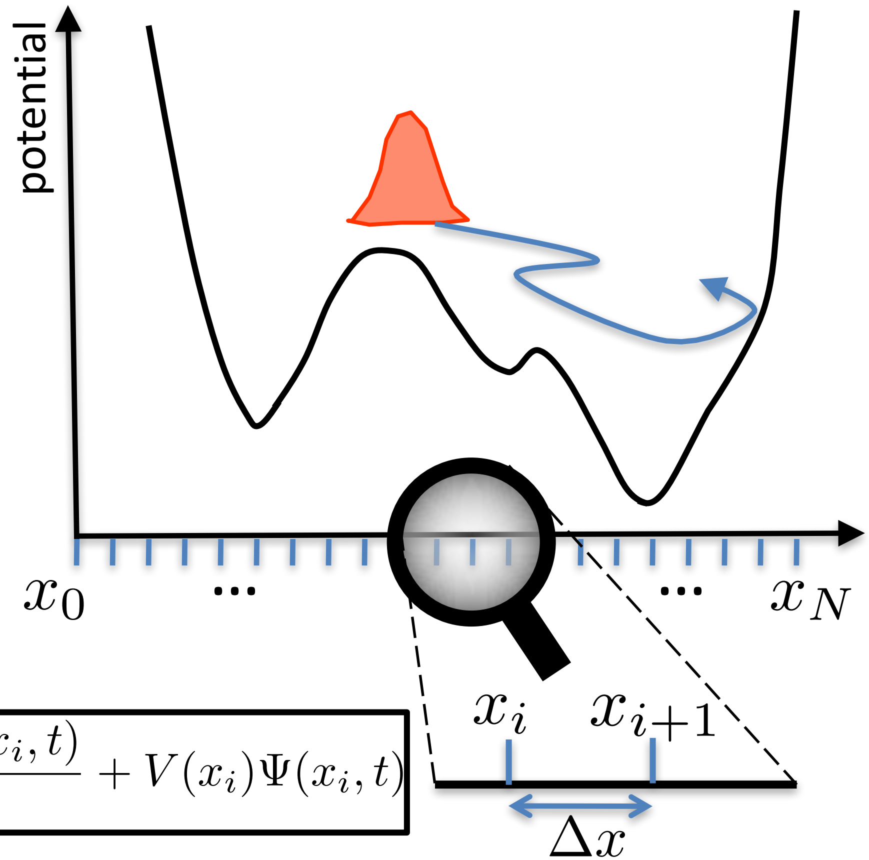
$$\langle x|V(\hat{x})|\Psi(t)\rangle = V(x)\Psi(x,t)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V(x)\right\}\Psi(x,t)$$

Numerical Method for quantum dynamics

Quantum mechanics on a mesh

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \Big\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V(x)\Big\}\Psi(x,t)$$



Discretization:

x-space: $\{x_i\}$ x-step: Δx

$$i\hbar\frac{\partial}{\partial t}\Psi(x_i,t) = -\frac{\hbar^2}{2m}\frac{\Psi(x_{i+1},t)+\Psi(x_{i-1},t)-2\Psi(x_i,t)}{2(\Delta x)^2} + V(x_i)\Psi(x_i,t)$$

$$i\hbar\dot{\mathbf{F}}(t) = \mathbf{H}\times\mathbf{F}(t)$$

$\mathbf{F}_i(t) = \Psi(x_i,t)$

$\mathbf{H}$ tridiagonal

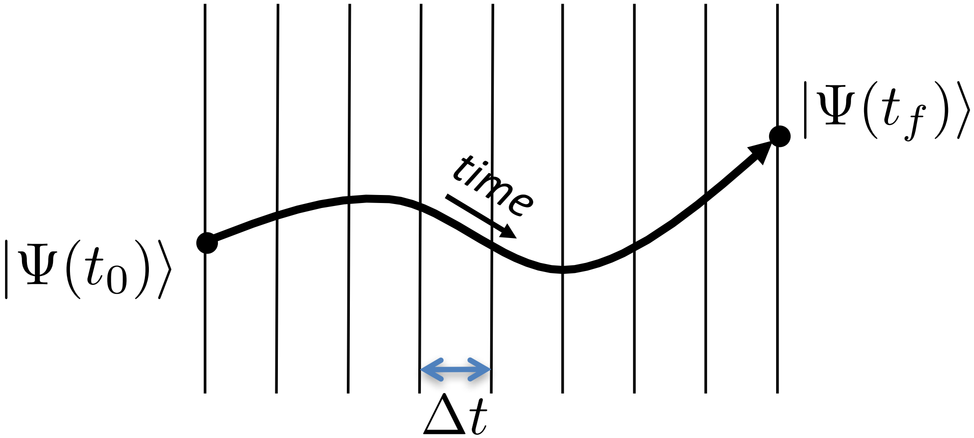
$$\mathbf{H}_{ii} = \frac{\hbar^2}{2m(\Delta x)^2} + V(x_i)$$

$$\mathbf{H}_{ii+1} = H_{i-1i} = -\frac{\hbar^2}{4m(\Delta x)^2}$$

Methods for time integration

$$i\hbar\dot{\mathbf{F}}(t) = \mathbf{H} \times \mathbf{F}(t)$$

$$\mathbf{F}(t+\Delta t) = \exp\left(\frac{\Delta t}{i\hbar}\mathbf{H}\right) \times \mathbf{F}(t)$$



Time discretization

time: $\{t_i\}$ time-step: Δt

Time integration:

Direct

$$\exp\left(-\frac{\Delta t}{i\hbar}\mathbf{H}\right) \simeq 1 + \frac{\Delta t}{i\hbar}\mathbf{H} + \frac{1}{2!}\left(\frac{\Delta t}{i\hbar}\mathbf{H}\right)^2 + \cdots$$

$(\Delta t)^n$, non-unitary, any dim.

Crank-Nicholson

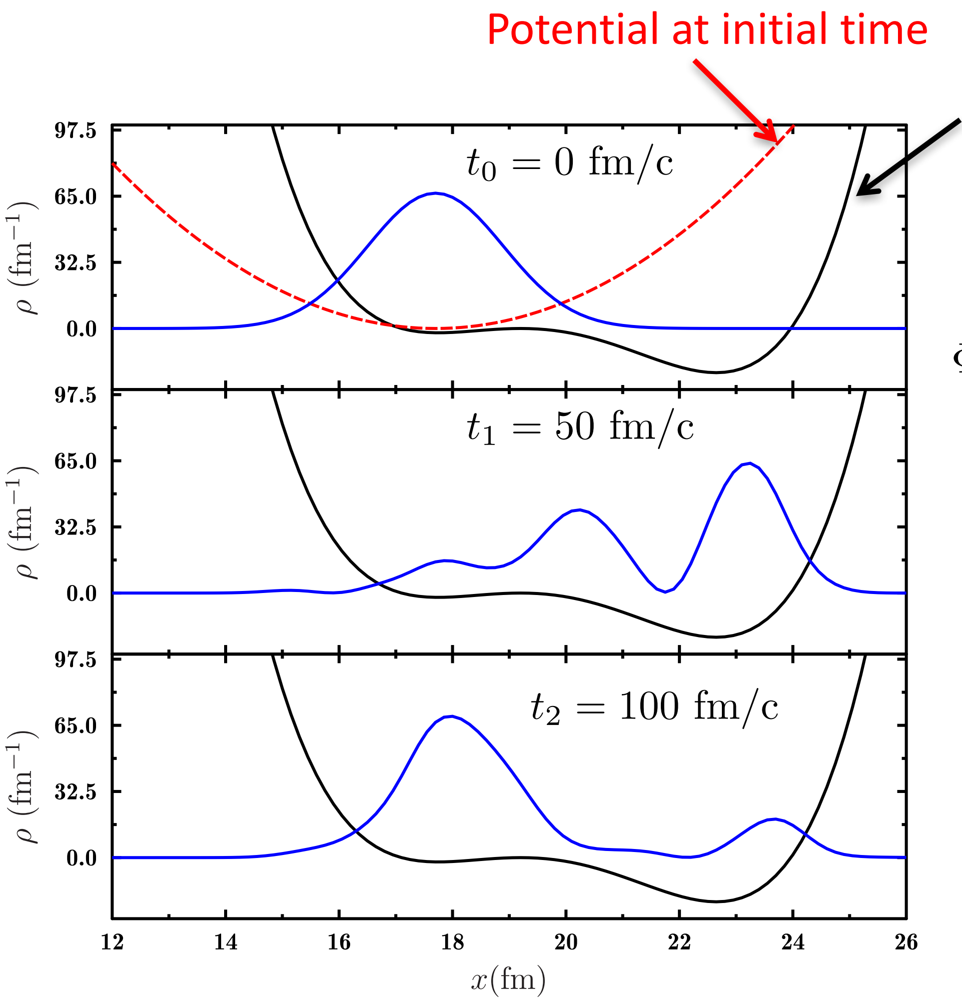
$$\mathbf{F}(t+\Delta t) = \frac{1 - \frac{\Delta t}{2i\hbar}\mathbf{H}}{1 + \frac{\Delta t}{2i\hbar}\mathbf{H}}\mathbf{F}(t)$$

$(\Delta t)^2$, unitary, 1D only

Split-Operator

$$\mathbf{F}(t+\Delta t) \simeq e^{-i\Delta t\frac{\mathbf{P}^2}{4\hbar m}} e^{-\frac{i}{\hbar}\Delta t\mathbf{V}} e^{-i\Delta t\frac{\mathbf{P}^2}{4\hbar m}} \times \mathbf{F}(t)$$

$(\Delta t)^2$, unitary, any dim.



Initial state (Coherent state)

$$\Phi(x) = \left(\frac{\eta}{\pi}\right)^{1/4} \exp\left(-\frac{\eta}{2}(x-q_0)^2 + i\frac{p_0 x}{\hbar} - i\frac{p_0 q_0}{2\hbar}\right)$$

with $p_0 = 0$

At t>0

$$H = \frac{p^2}{2m} + \frac{1}{2}ax^2 + \frac{1}{3}bx^3 + \frac{1}{4}cx^4$$

Numerical method:

-Split operator

- $\Delta x = 0.15$ fm - $\Delta t = 0.05$ fm/c

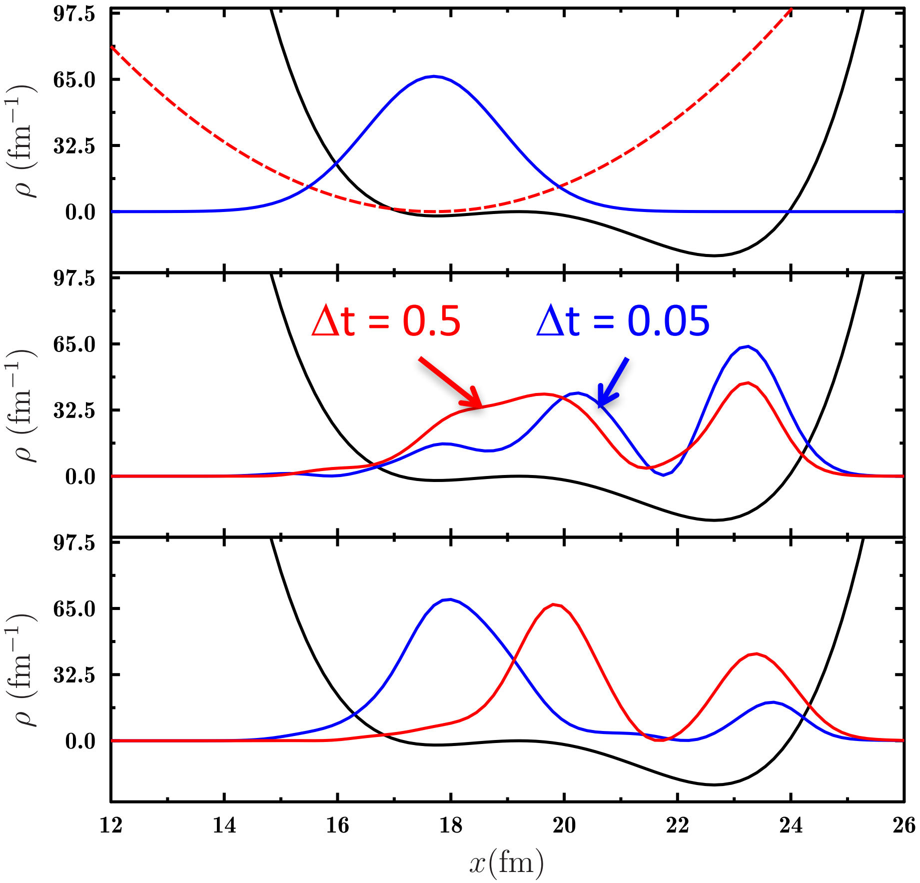
Density profile

$$\rho(x) = |\Phi(x,t)|^2$$

Same initial condition and Hamiltonian

-same $\Delta x = 0.15$ fm

-different Δt



How to know the correct values of parameters?

Simple estimate

$$\Delta x.\Delta p \simeq 2\pi\hbar \qquad \Delta t.\Delta E \simeq 2\pi\hbar$$

$$\Delta x.p_{\max} \simeq 2\pi\hbar \qquad \Delta t.E_{max} \simeq 2\pi\hbar$$

$$E_{\max} \simeq p_{\max}^2/2m$$

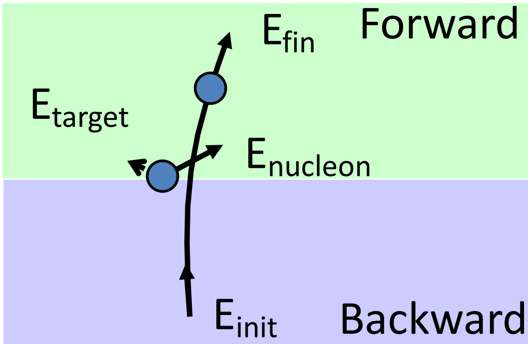
$$\frac{\Delta t}{(\Delta r)^2} \simeq \frac{m}{\pi\hbar}$$

Here:
$$\frac{\Delta t}{(\Delta r)^2} \simeq \frac{1000}{3 \times 200} = 1.7$$

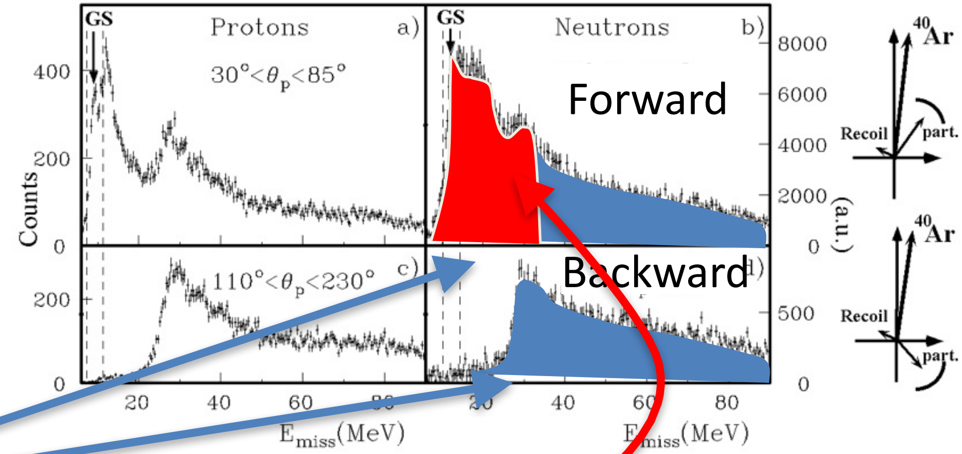
$\Delta x = 0.15$ fm ⇒ $\Delta t \simeq 0.04$ fm/c

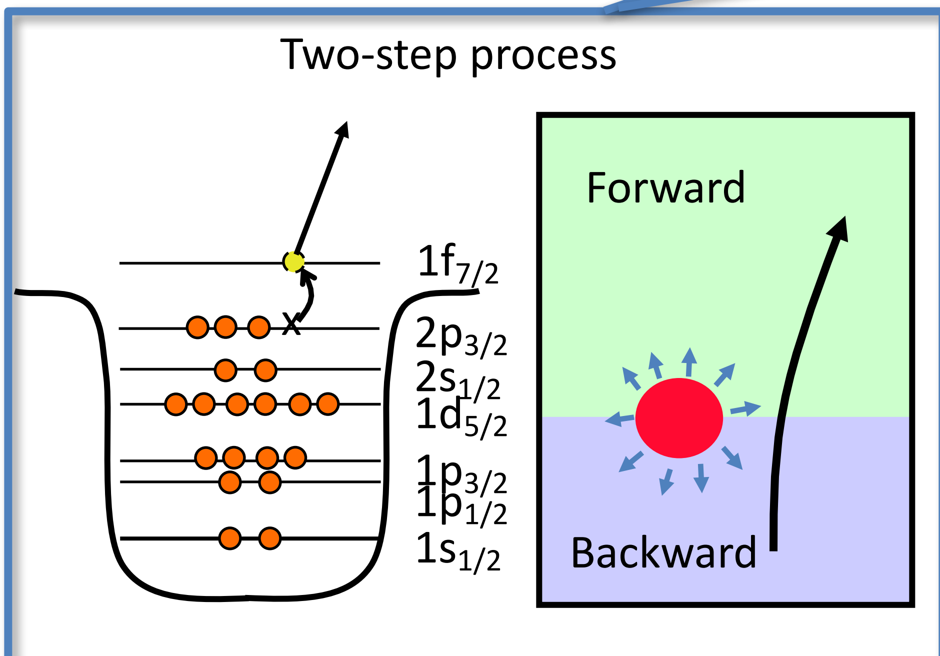
Example of realistic 3D application

Experimental motivation



J.A.Scarpaci et al., Phys. Lett. B428 (1998) 241





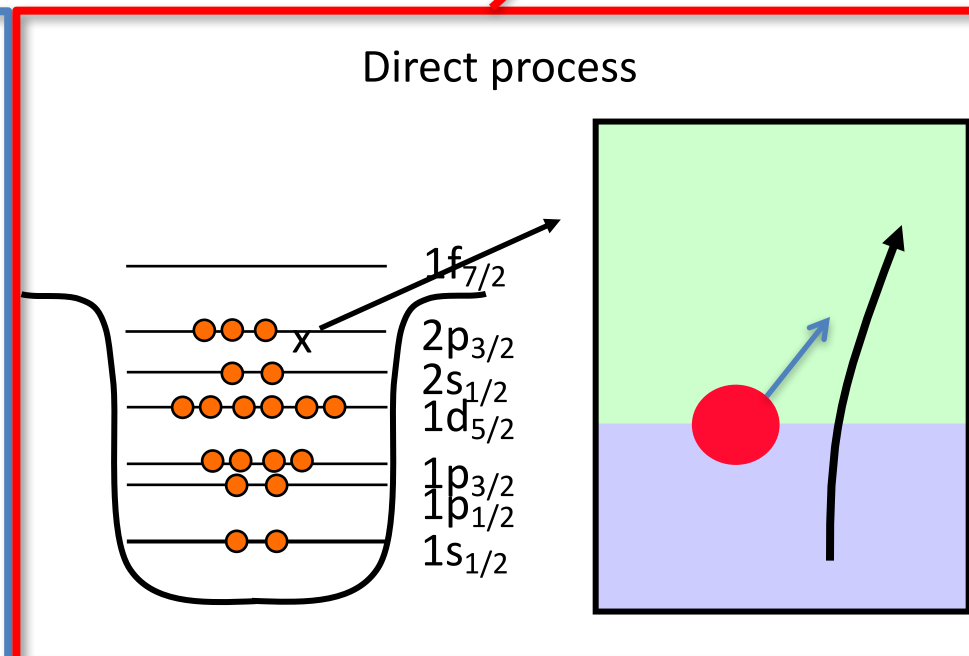
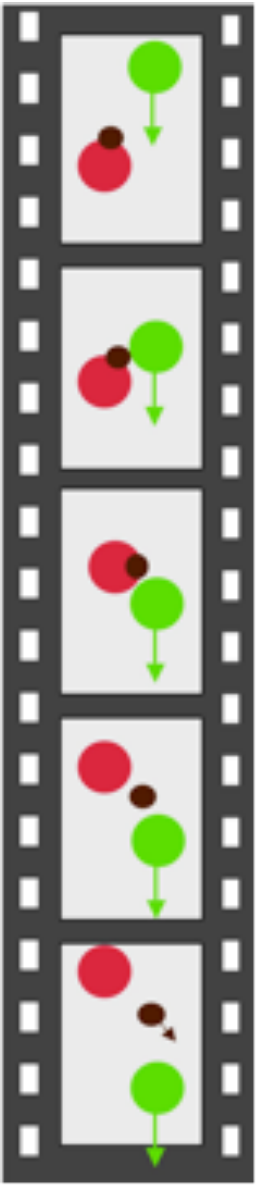
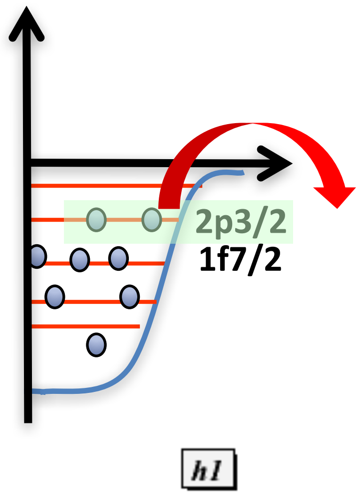


Illustration: time-dependent Schrödinger Eq. for nuclear break-up



^{58}Ni break-up @44 MeV/A

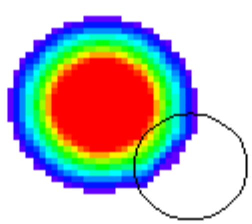


$$i\hbar\partial_t|\Phi_\alpha(t)\rangle = \left\{\frac{\mathbf{p}^2}{2m} + V_P(\vec{\mathbf{r}},t) + V_T(\vec{\mathbf{r}},t)\right\}|\Phi_\alpha(t)\rangle$$

Wood-Saxon potentials

$$V_{P/T}(\vec{r},t) = \frac{V_0}{1+\exp\{|\vec{\mathbf{r}}-\vec{\mathbf{r}}_{T/P}(t)|/a\}}$$

+ 3D Split-operator



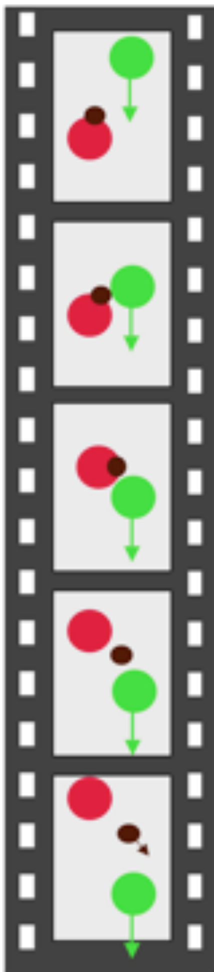
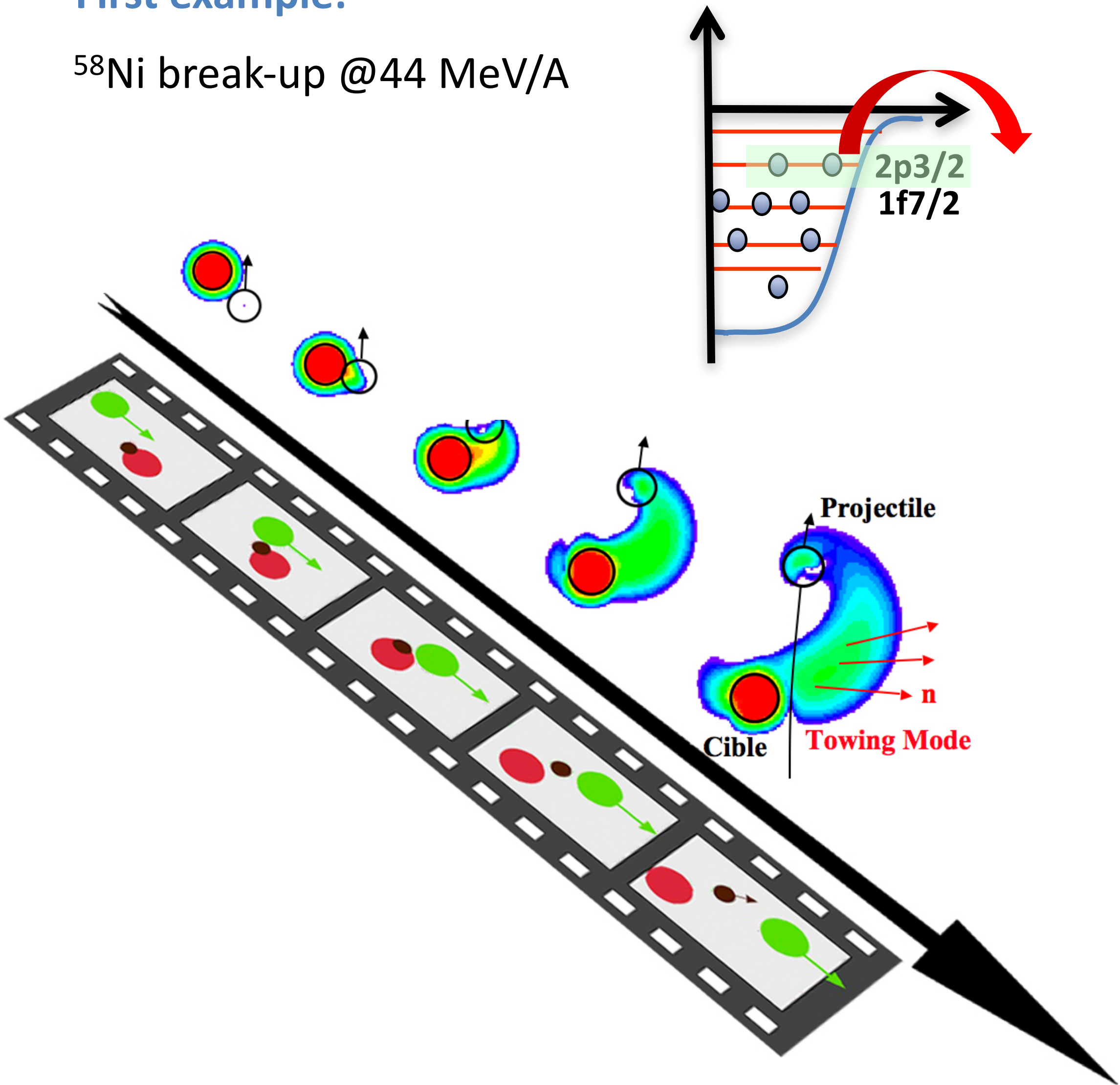


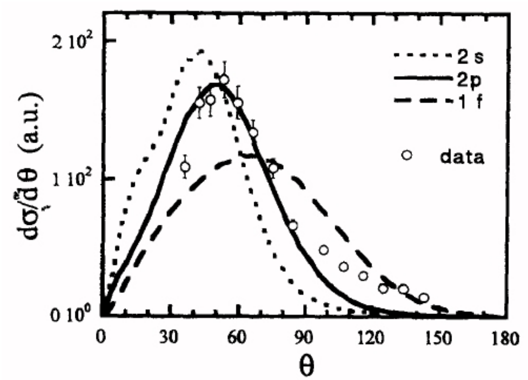
Illustration: time-dependent Schrödinger Eq. for nuclear break-up

First example:

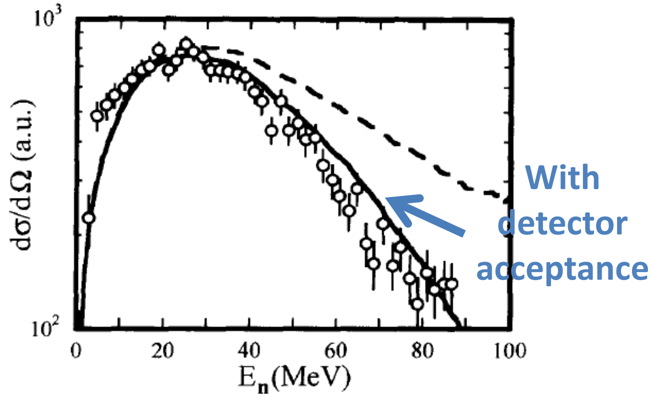
^{58}Ni break-up @44 MeV/A



Angular distribution:



Kinetic Energy distribution:

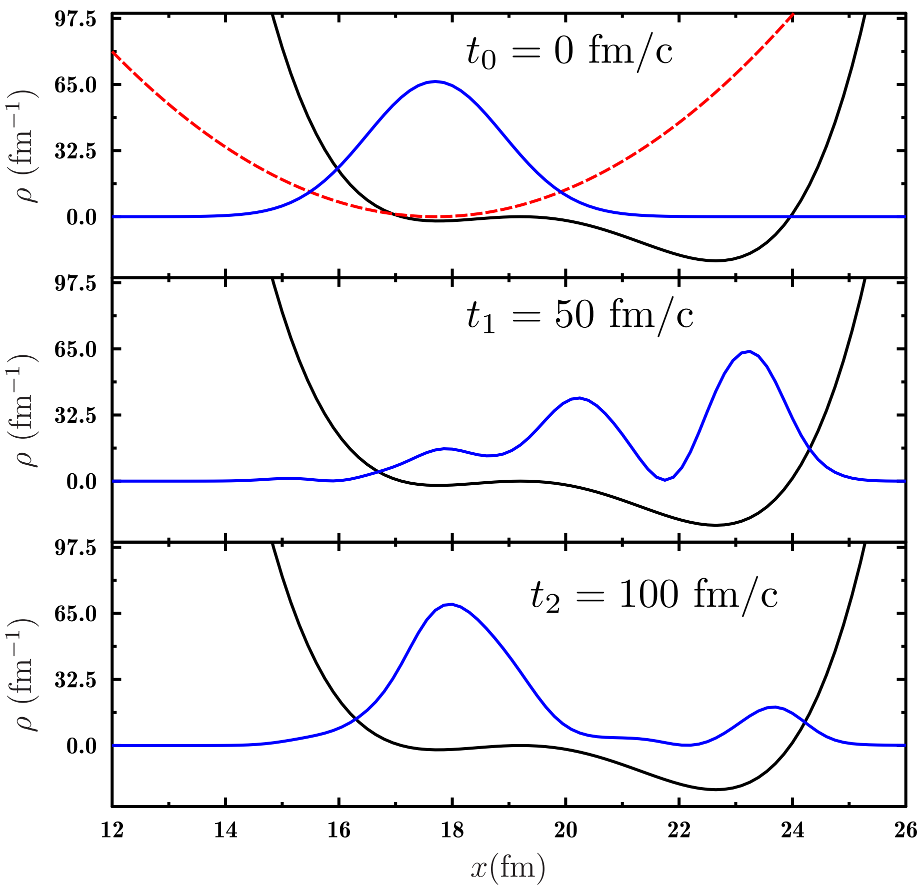


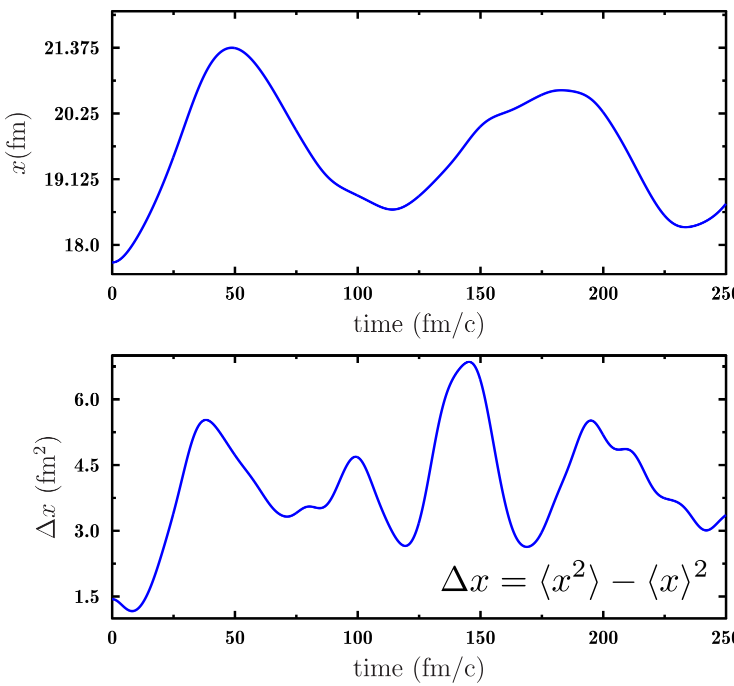
DL, Scarpaci, Chomaz, NPA658 (1999)

Observables, Densities
and
information/complexity reduction

Observable evolution

$$|\Psi(t)\rangle \Rightarrow \langle\hat{O}(t)\rangle = \langle\Psi(t)|\hat{O}|\Psi(t)\rangle$$





Density definition

$$D(t) = |\Psi(t)\rangle\langle\Psi(t)| \Rightarrow \langle O(t)\rangle = \mathrm{Tr}(OD(t))$$

Reminder: Ehrenfest, Liouville von-Neumann evolution

From the Schrödinger Equation

$$-i\hbar\frac{d}{dt}\langle\Psi| = \langle\Psi|H \qquad \text{and} \qquad i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle$$

Liouville von-Neumann Equation

$$i\hbar\frac{d}{dt}D = \left(i\hbar\frac{d}{dt}|\Psi\rangle\right)\langle\Psi| + |\Psi\rangle\left(i\hbar\frac{d}{dt}\langle\Psi|\right) = H|\Psi\rangle\langle\Psi| - |\Psi\rangle\langle\Psi|H$$

$$\Rightarrow \quad i\hbar\frac{d}{dt}D = [H, D]$$

Ehrenfest Theorem

$$i\hbar\frac{d}{dt}\langle O\rangle = \mathrm{Tr}\left(O\frac{dD}{dt}\right) = \mathrm{Tr}\left(O[H, D]\right)$$

$$\Rightarrow \quad i\hbar\frac{d}{dt}\langle O\rangle = \mathrm{Tr}\left([O, H]D\right) = \langle[O, H]\rangle$$

Dimension N N^2 N^2

Densities can describe systems that could not easily be described by a single wave-packet.

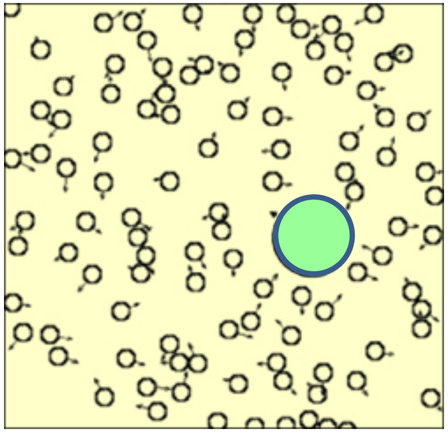
Example 1: Quantum statistical Mechanics

$$D = \sum |\Psi_i\rangle \mathcal{P}_i \langle \Psi_i|$$

$$D^2 - D = \sum |\Psi_i\rangle (\mathcal{P}_i^2 - \mathcal{P}_i) \langle \Psi_i|$$

N.B.: $D^2 = D$ → pure state case

Example 2: Non-equilibrium quantum dynamics with dissipation/irreversible process

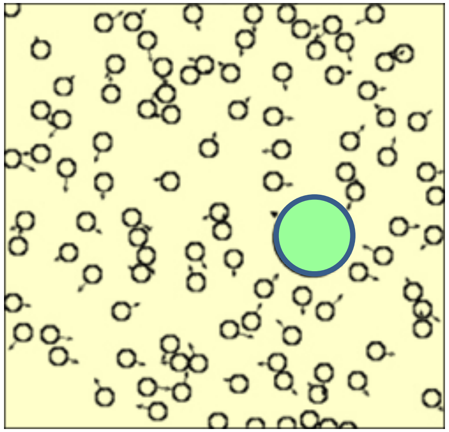


Lindblad equation

$$\frac{d}{dt} D = \frac{1}{i\hbar}[H, D(t)] - \frac{1}{2\hbar^2} \sum_k \gamma_k \left(2A_k D(t) A_k - A_k A_k D(t) - D(t) A_k A_k\right)$$

Non-Hamiltonian evolution

Why we need to select specific degrees of freedom?



-In most realistic situations, the number of DOF is very large

-All DOF cannot be followed in time simultaneously

-Some DOF are irrelevant for the considered process.

Information reduction

-The idea is to focus on the relevant DOF.

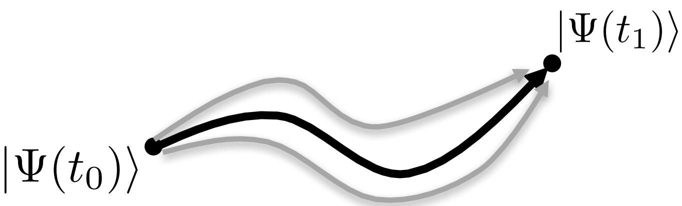
⇒ Use of variational principles.

-Dilemma: lots of interesting aspects come from the coupling between relevant and irrelevant DOF.

⇒ Necessity to account for this coupling

Minimize the action

$$S = \int_{t_0}^{t_1} ds \, \langle \Psi(t) | \, i\hbar\partial_t - H \, | \Psi(t) \rangle$$



under the constraint

$$|\delta\Psi(t_0)\rangle = 0 \quad \text{and} \quad \langle \delta\Psi(t_1)| = 0$$

How does it works?

Using the component $\Psi_i(t) = \langle i | \Psi(t) \rangle$

$$\Rightarrow \quad S = \int_{t_0}^{t_1} ds \sum_i \left\{ i\hbar \Psi_i^*(t) \partial_t \Psi_i(t) - \underbrace{\sum_j \Psi_i^*(t) H_{ij} \Psi_j(t)}_{\mathcal{H}[\Psi, \Psi^*]} \right\}$$

Variation with respect to:

$\delta\Psi_i^*$

$$i\hbar\partial_t \Psi_i = \partial\mathcal{H}/\partial\Psi_i^* = \sum_j H_{ij}\Psi_j$$

$$i\hbar\partial_t |\Psi\rangle = H|\Psi\rangle$$

$\delta\Psi_i$ (after integration by part)

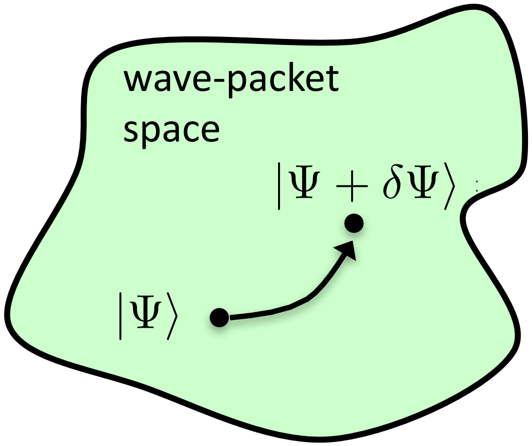
$$i\hbar\partial_t \Psi_i^* = -\partial\mathcal{H}/\partial\Psi_i = -\sum_j H_{ij}\Psi_j^*$$

$$-i\hbar\partial_t \langle\Psi| = \langle\Psi|H$$

Variational principle in quantum mechanics

Selection of degrees of freedom

Selection of trial states with specific rules of variation:



$$|\Psi + \delta\Psi\rangle = (1 + \sum_\alpha \delta q_\alpha A_\alpha + \cdots)|\Psi\rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha}|\Psi\rangle$$

$\{A_\alpha\}$: generator of the transformation

often $|\Psi(\mathbf{Q})\rangle \equiv |\mathbf{Q}\rangle = R(\mathbf{Q})|\Psi(0)\rangle = e^{\mathbf{Q}.\mathbf{A}}|\Psi(0)\rangle$

Wave-function variation → Variation of $(q_1, \cdots, q_N)$ parameters

Interest

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

$$\langle \delta\mathbf{Q}| = \langle \mathbf{Q}| \sum_\alpha \delta q^*_\alpha(t) A_\alpha$$

$$|\delta\mathbf{Q}\rangle = \sum_\alpha \delta q_\alpha A_\alpha |\mathbf{Q}\rangle$$

→

$$i\hbar\langle \mathbf{Q}|A_\alpha|\dot{\mathbf{Q}}\rangle = \langle \mathbf{Q}|A_\alpha H|\mathbf{Q}\rangle$$

$$i\hbar\langle \dot{\mathbf{Q}}|A_\alpha|\mathbf{Q}\rangle = -\langle \mathbf{Q}|H A_\alpha|\mathbf{Q}\rangle$$

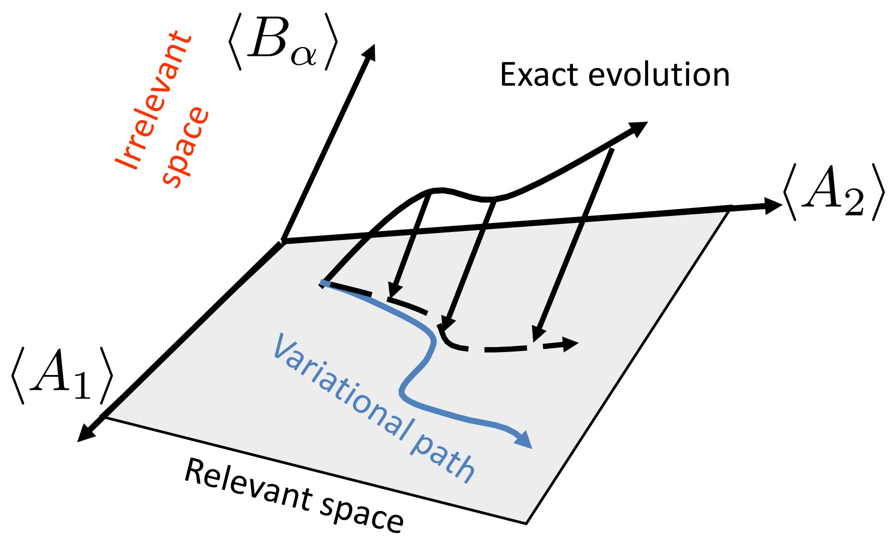
→

$$i\hbar\frac{d\langle A_\alpha\rangle}{dt} = \langle [A_\alpha, H]\rangle$$

Ehrenfest theorem

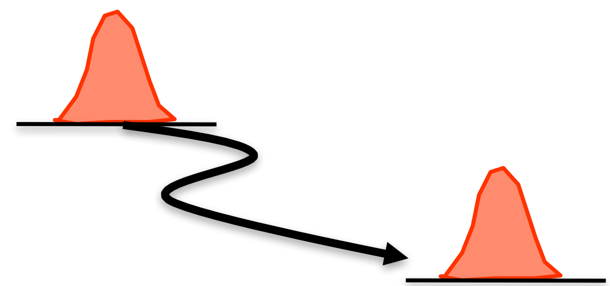
Variational principle in quantum mechanics

Selection of degrees of freedom



The use of variational principle with specific class of trial states insure optimal dynamics of the variables $\langle A_\alpha \rangle$ for short time

Examples



Coherent states

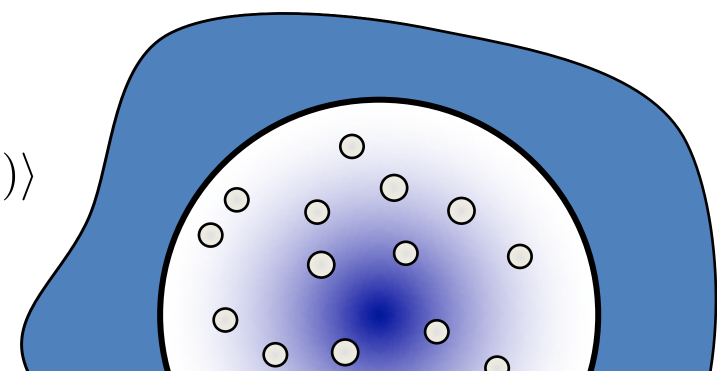
$$|\alpha + \delta\alpha\rangle \propto e^{\delta\alpha a^\dagger - \delta\alpha^* a}|\alpha\rangle$$

optimal for $\langle x \rangle, \langle p \rangle$

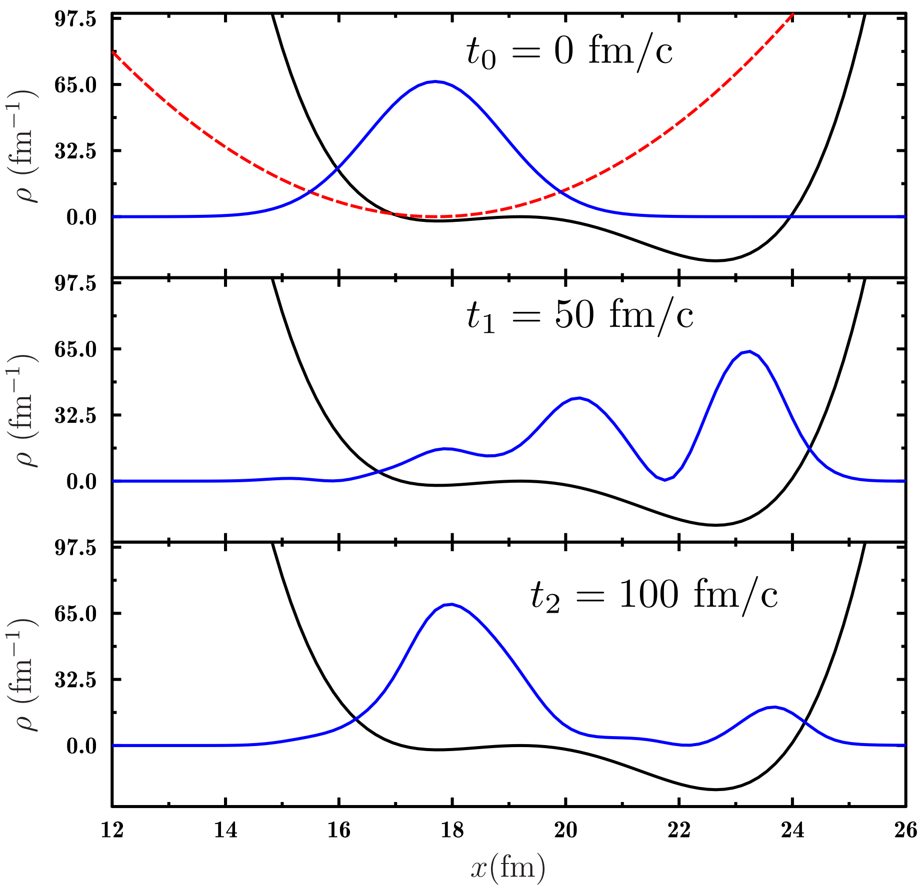
Independent part. states

$$|\Psi(Z + \delta Z)\rangle \propto e^{\sum_{ij} \delta Z_{ij} a_i^\dagger a_j}|\Psi(Z)\rangle$$

optimal for $\langle a_i^\dagger a_j \rangle$



Goal: Find an approximation of the dynamics imposing that the state remains Gaussian



$$(x, p) \Rightarrow (a, a^\dagger)$$

$$x = \frac{1}{\sqrt{2\eta}}\left(a + a^\dagger\right) \qquad p = i\hbar\sqrt{\frac{\eta}{2}}\left(a^\dagger - a\right)$$

$$\Rightarrow \quad a = \sqrt{\frac{\eta}{2}}x + \frac{i}{\hbar\sqrt{2\eta}}p$$

Coherent states might be defined as eigenstates of a with complex eigenvalues

$$\langle x|a|\alpha\rangle = \left\{\frac{1}{\sqrt{2\eta}}\frac{\partial}{\partial x} + \sqrt{\frac{\eta}{2}}x\right\}\Phi_\alpha(x) = \alpha\Phi_\alpha(x)$$

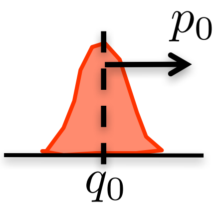
$$\Phi_\alpha(x) = \left(\frac{\eta}{\pi}\right)^{1/4}\exp\left(-\frac{\eta}{2}\left(x - q_0\right)^2 + i\frac{p_0 x}{\hbar} - i\frac{p_0 q_0}{2\hbar}\right)$$

Example of Information reduction

Gaussian coherent state

Information reduction with coherent state

$$\Phi_\alpha(x) = \left(\frac{\eta}{\pi}\right)^{1/4} \exp\left(-\frac{\eta}{2}(x-q_0)^2 + i\frac{p_0 x}{\hbar} - i\frac{p_0 q_0}{2\hbar}\right) = \Phi_{(p_0,q_0)}(x)$$



with $\langle x \rangle = q_0 \qquad \langle p \rangle = p_0$

⇨ All the information on the system is contained in (p_0, q_0)

⇨ For any observable $\langle O \rangle = \mathcal{O}(p_0, q_0)$

Example: $\Delta x = \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{2\eta}(\alpha^2 + (\alpha^*)^2 + 2\alpha\alpha^* + 1 - \{\alpha + \alpha^*\}^2) = \frac{1}{2\eta}$

⇨ $\langle x^2 \rangle = q_0^2 + \frac{1}{2\eta}$

Similarly $\langle p^2 \rangle = p_0^2 + \hbar^2 \eta / 2$,

$$\langle x^3 \rangle = q_0^3 + \frac{3}{2\eta} q_0, \qquad \langle x^4 \rangle = q_0^4 + \frac{3}{\eta} q_0^2 + \frac{3}{4\eta^2}, \qquad \ldots$$

Gaussian coherent state

Variational principle

$$\langle\alpha|i\hbar\partial_t|\alpha\rangle = \frac{1}{2}(p_0\dot{q}_0 - q_0\dot{p}_0)$$

$$\langle\alpha|H|\alpha\rangle = \frac{\langle p^2\rangle}{2m} + \frac{a}{2}\langle x^2\rangle + \frac{b}{3}\langle x^3\rangle + \frac{c}{4}\langle x^4\rangle = \mathcal{H}(p_0, q_0)$$

$$\frac{dq_0}{dt} = \frac{\partial\mathcal{H}}{\partial p_0}$$

$$\frac{dp_0}{dt} = -\frac{\partial\mathcal{H}}{\partial q_0}$$

Like classical Hamilton Eq.

Explicit Equation of motion

$$\frac{dq_0}{dt} = \frac{p_0}{m}$$

$$\frac{dp_0}{dt} = -aq_0 - b\left(q_0^2 + \frac{1}{2\eta}\right) - c\left(q_0^3 + \frac{3}{2\eta}q_0\right)$$

Comparison with direct Ehrenfest Theorem application

$$\frac{d}{dt}\langle x\rangle = -\frac{i}{\hbar}\langle[x, H]\rangle = \frac{\langle p\rangle}{m} = \frac{p_0}{m}$$

$$\frac{d}{dt}\langle p\rangle = -\frac{i}{\hbar}\langle[p, H]\rangle = -a\langle x\rangle - b\langle x^2\rangle - c\langle x^3\rangle$$

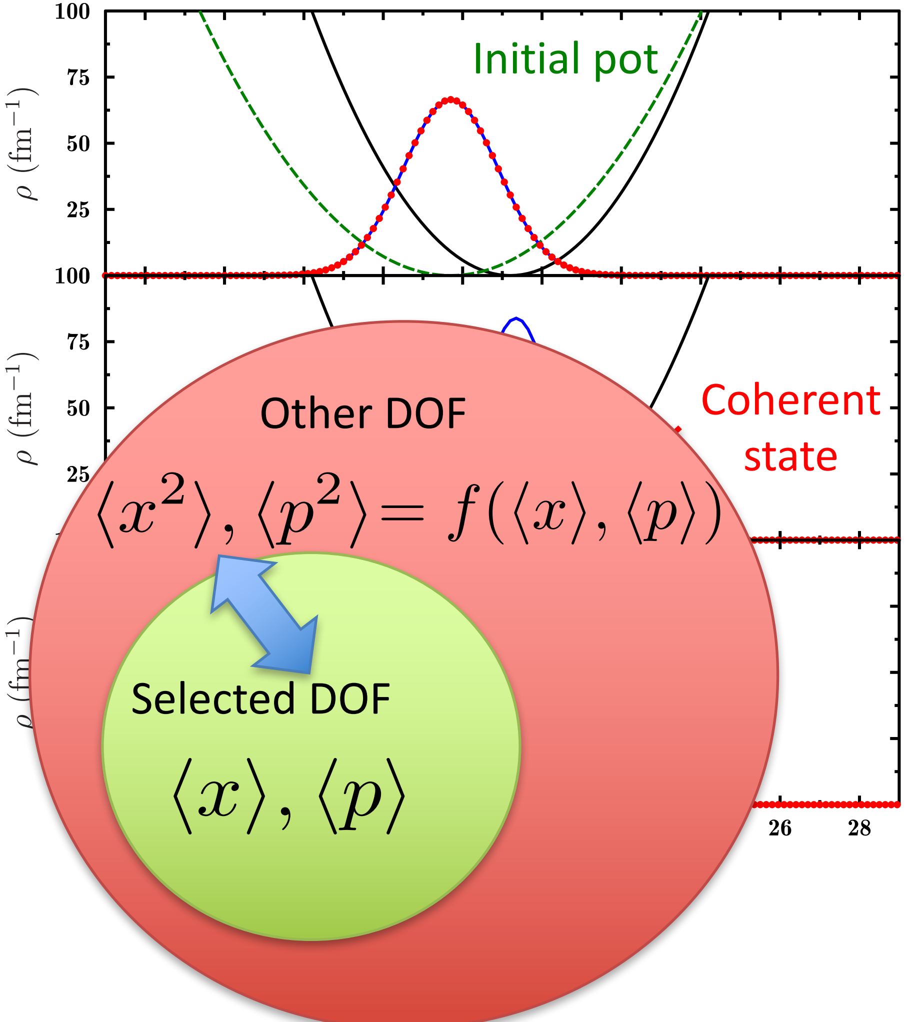
with

$$\langle x\rangle = q_0 \qquad \langle x^2\rangle = q_0^2 + \frac{1}{2\eta} \qquad \langle x^3\rangle = q_0^3 + \frac{3}{2\eta}q_0$$

The equivalence only holds for relevant degrees of freedom!

Gaussian state in harmonic potential

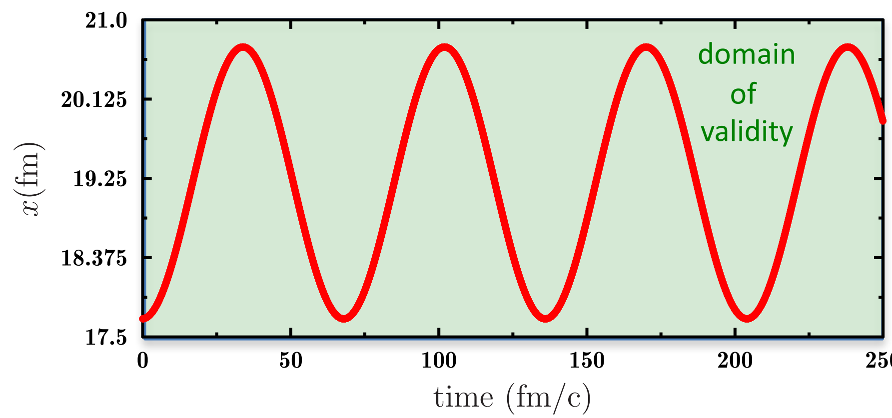
$$H = \frac{p^2}{2m} + \frac{1}{2}ax^2 + \frac{1}{3}bx^3 + \frac{1}{4}cx^4$$



Case 1 $b = c = 0$

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m} \qquad \frac{d}{dt}\langle p\rangle = -a\langle x\rangle$$

Evolution of x and p is exact



Gaussian state in slightly anharmonic potential

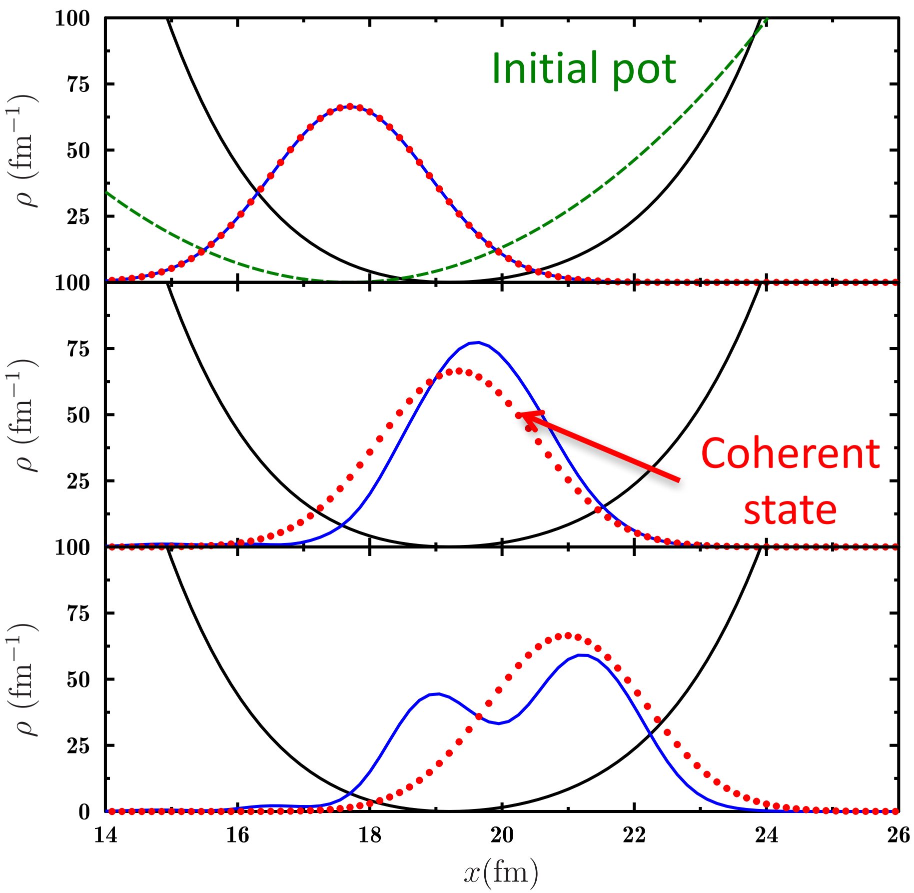
$$H = \frac{p^2}{2m} + \frac{1}{2}ax^2 + \frac{1}{3}bx^3 + \frac{1}{4}cx^4$$

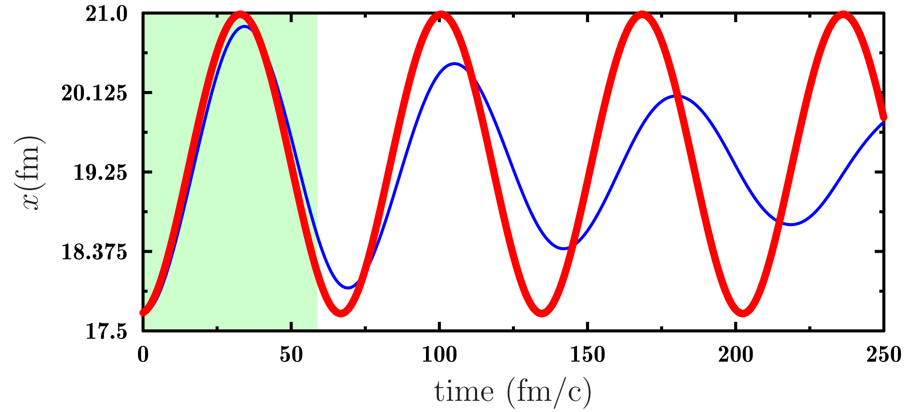
Case 2

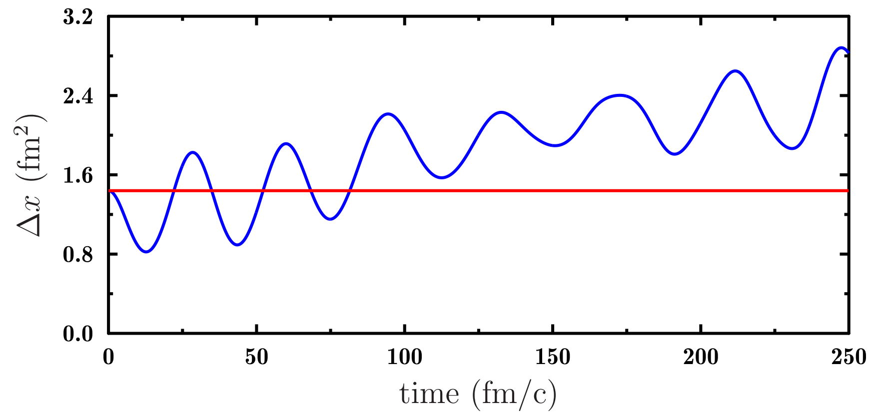
$b \neq 0$

$c \neq 0$

$b, c \ll a$







Due to the coupling to irrelevant DOF

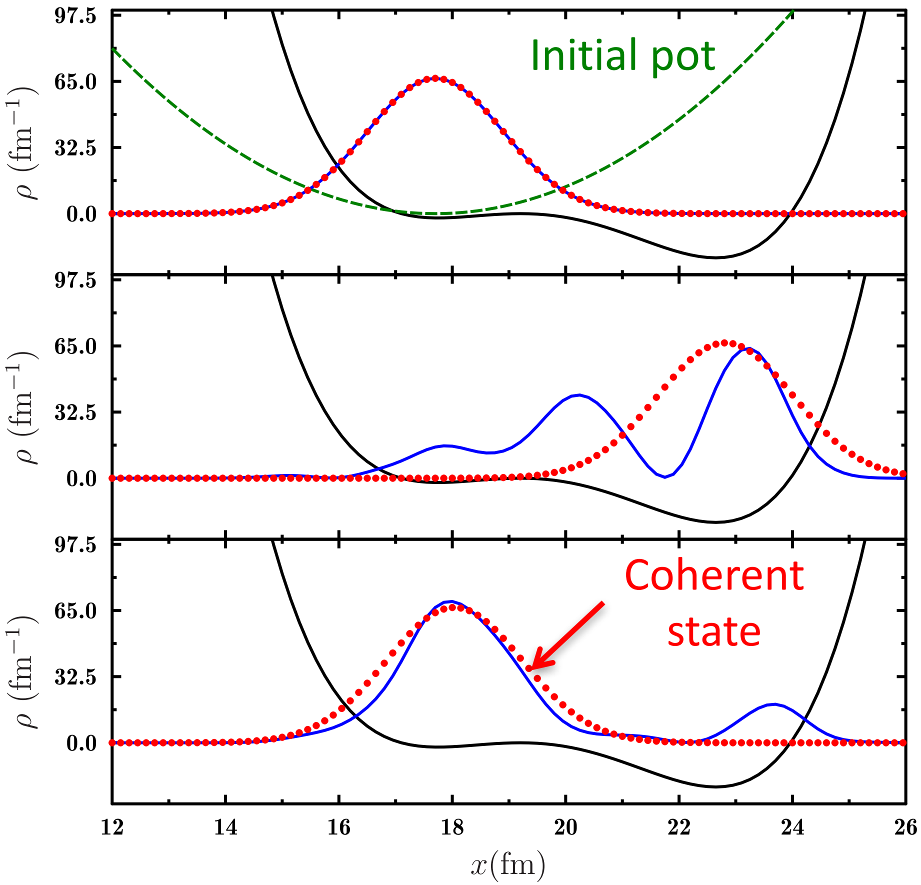
Damping might occur

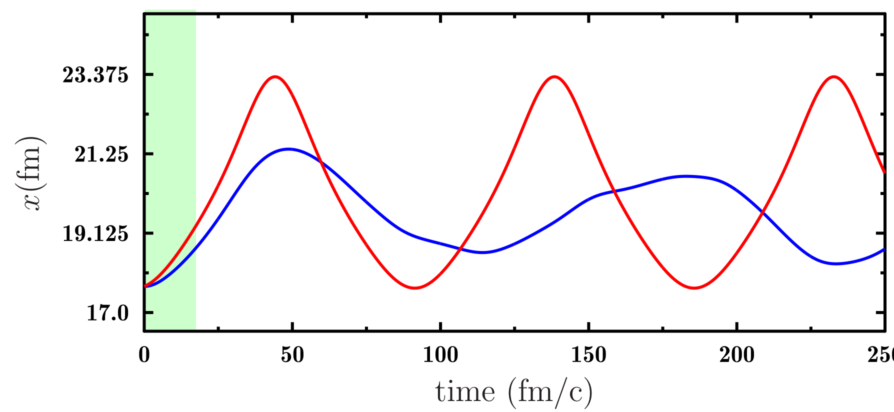
Example of Information reduction

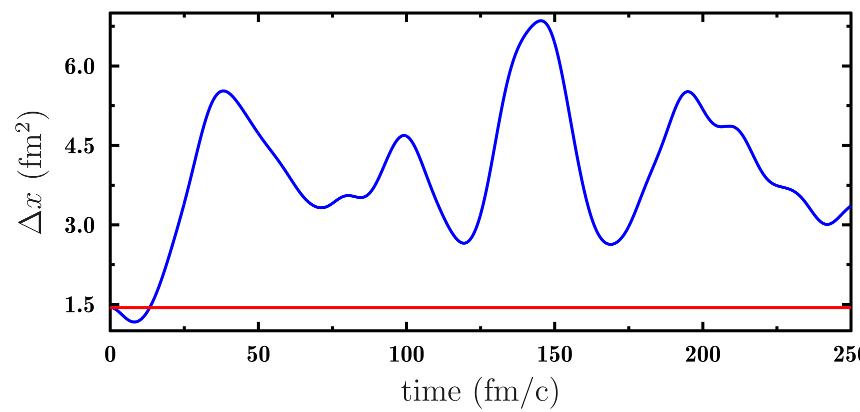
Gaussian state in strongly potential

$$H = \frac{p^2}{2m} + \frac{1}{2}ax^2 + \frac{1}{3}bx^3 + \frac{1}{4}cx^4$$

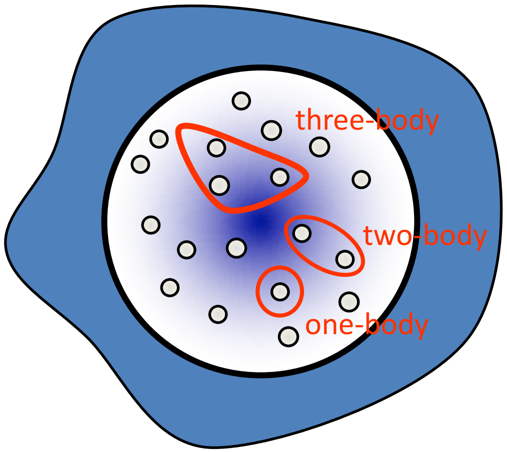
Case 3: $b \neq 0$, $c \neq 0$ $\qquad b, c \sim a$







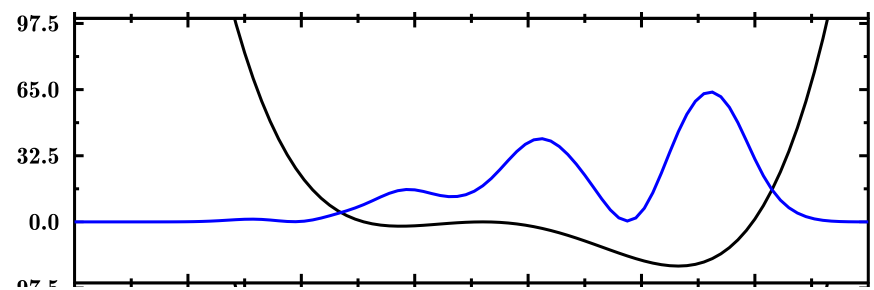
Strongly anharmonic potential induces a strong coupling between relevant and irrelevant space (and the approximation fails)



Nuclei are complex
quantum
many-body systems

quantum

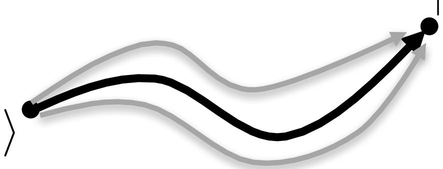
$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}+V(x)\right\}\Psi(x,t)$$



Wave	Density Matrix	Observable space
$\lvert\Psi(t)\rangle$	$D(t)=\lvert\Psi(t)\rangle\langle\Psi(t)\rvert$	$\langle O(t)\rangle=\mathrm{Tr}(OD(t))$

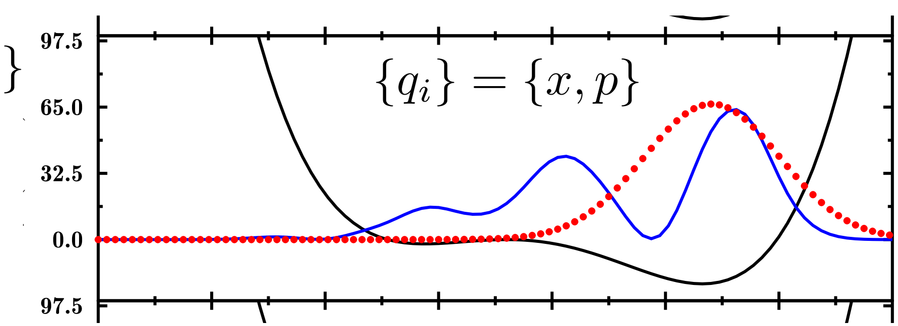
Complexity reduction

$$\lvert\Psi+\delta\Psi\rangle=e^{\sum_\alpha \delta q_\alpha A_\alpha}\lvert\Psi\rangle$$



$\Psi_i \longrightarrow \{q_i\}$

Optimal dyn. for the $\langle A_\alpha\rangle$

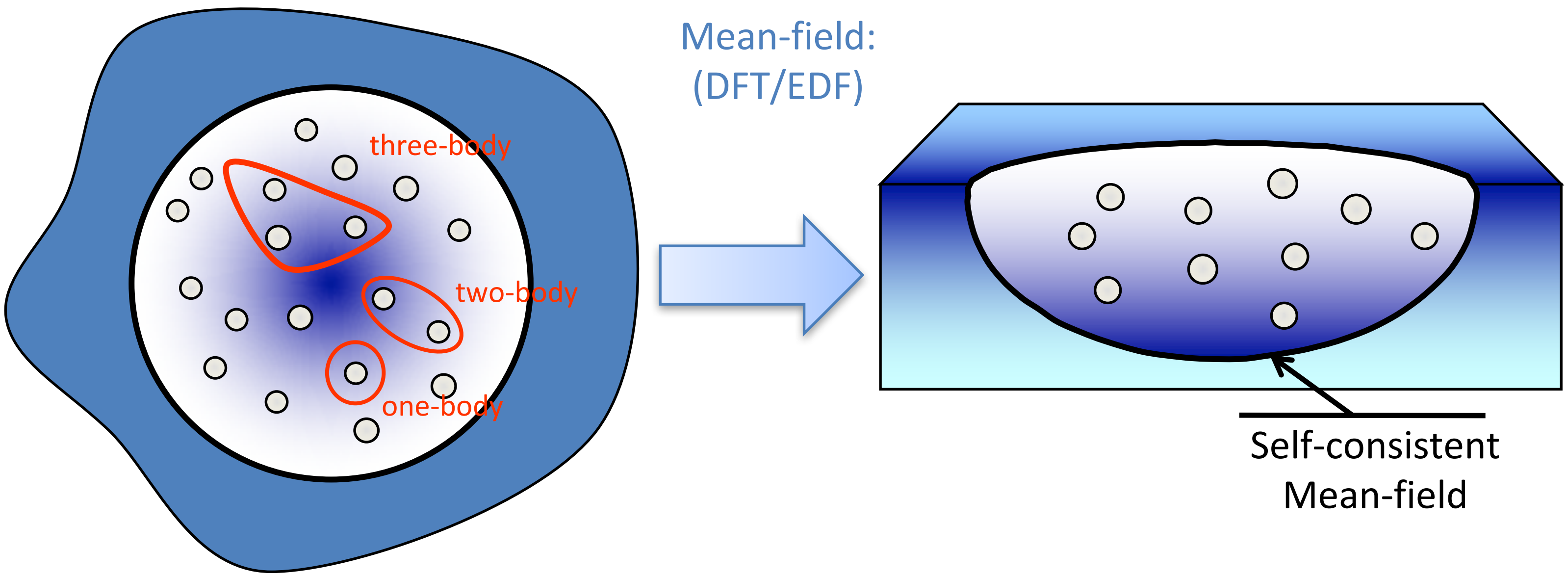


Application to the nuclear Many-Body problem

The Nuclear Energy Density Functional: Goal

Starting point: $$H = \sum_i T(i) + \sum_{i<j} V^{(2)}(i,j) + \sum_{i<j<k} V^{(3)}(i,j,k)$$

Goal: Map the nuclear many-body problem into an "independent" particle problem



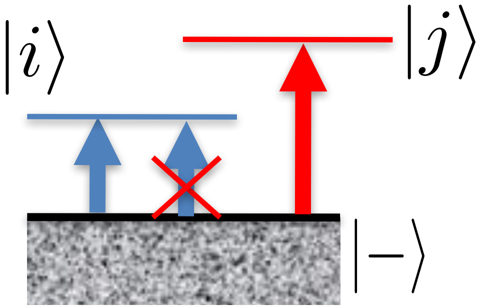
"Simple" Trial state:

$$\Psi(r_1, \cdots, r_{12}, \cdots, r_{123}, \cdots)$$

In the EDF, particles behaves as Independent particles interacting through an effective average potential

Strategy

- Identify relevant degrees of freedom (one-body DOF)
- Use appropriate trial states in the variational principle (Slater Det. wave-function)



$|-\rangle$ Vacuum

By definition: $a_i|-\rangle = 0$

Single-particle creation: $a_i^\dagger|-\rangle = |i\rangle$

Single-particle annihilation: $a_i|j\rangle = |-\rangle\langle i|j\rangle$

Two-body states: $a_i^\dagger a_j^\dagger|-\rangle = |ij\rangle$

$(a_i^\dagger)^2|-\rangle = 0$ (fermions)

Fermionic anti-commutation rules:

$$[\, a_i^\dagger, a_j^\dagger \,]_+ = a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$$

$$[\, a_i, a_j \,]_+ = a_i a_j + a_j a_i = 0$$

$$[\, a_i, a_j^\dagger \,]_+ = a_i a_j^\dagger + a_j^\dagger a_i = \langle i|j\rangle$$

Observable expressions

one-body $$O^{(1)} = \sum_{ij} \langle i|O_1|j\rangle a_j^\dagger a_i$$

two-body $$O^{(2)} = \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{O}_{12}|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

three-body $$O^{(3)} = \frac{1}{6}\sum_{ijk,lmn} \langle ijk|\tilde{O}_{123}|lmn\rangle a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n$$

Density matrices

Definition	Information content	Size
one-body: $\langle i\|\rho^{(1)}\|j\rangle = \langle a_j^\dagger a_i\rangle$	$\langle O^{(1)}\rangle = \mathrm{Tr}(O^{(1)}\rho^{(1)})$	$[\Omega]^2$
two-body: $\langle kl\|\rho^{(2)}\|ij\rangle = \langle a_i^\dagger a_j^\dagger a_l a_k\rangle$	$\langle O^{(2)}\rangle = \frac{1}{4}\mathrm{Tr}(\tilde{O}^{(2)}\rho^{(2)})$	$[\Omega(\Omega-1)/2]^2$
three-body: $\langle klm\|\rho^{(3)}\|ijn\rangle = \langle a_i^\dagger a_j^\dagger a_n^\dagger a_m a_l a_k\rangle$	$\langle O^{(3)}\rangle = \frac{1}{6}\mathrm{Tr}(\tilde{O}^{(3)}\rho^{(3)})$	$[\Omega(\Omega-1)(\Omega-2)/3!]^2$

$[\Omega]$: size of the single-particle space

Reduction of information to one-body DOF

The two-particles case $|i,j\rangle = a_i^\dagger a_j^\dagger |-\rangle$

$$\Phi_{ij}(r_1,r_2) = \langle r_2 r_1 | i,j\rangle = \langle -| a_{r_2} a_{r_1} a_i^\dagger a_j^\dagger |-\rangle$$
$$= \langle r_1|i\rangle\langle r_2|j\rangle - \langle r_2|i\rangle\langle r_1|j\rangle = \phi_i(r_1)\phi_j(r_2) - \phi_i(r_2)\phi_j(r_1)$$

$$\Rightarrow \quad \Phi_{ij}(r_1,r_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_i(r_1) & \phi_i(r_2) \\ \phi_j(r_1) & \phi_j(r_2) \end{vmatrix} = \frac{1}{\sqrt{2!}} \mathcal{A}(\phi_i(r_1), \phi_i(r_2))$$

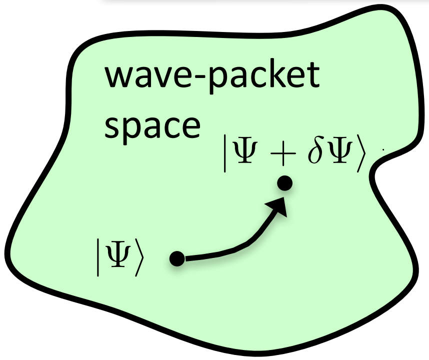
The N-particles case $|i_1, \cdots, i_N\rangle = \frac{1}{\sqrt{N!}} a_{i_1}^\dagger \cdots a_{i_N}^\dagger |-\rangle$

Associated density matrices

one-body $\langle r|\rho^{(1)}|r'\rangle = \langle r| \left(\sum_i |i\rangle\langle i| \right) |r'\rangle \quad \Rightarrow \quad \rho_1 = \sum |i\rangle\langle i|$

two-body $\rho_{12} = \rho_1 \rho_2 (1 - P_{12})$ (with $P_{12}|ij\rangle = |ji\rangle$)

three-body $\rho_{123} = \rho_1\rho_2\rho_3(1-P_{12})(1-P_{13}-P_{23})$



$$|\Psi + \delta\Psi\rangle = \left(1 + \sum_\alpha \delta q_\alpha A_\alpha + \cdots\right)|\Psi\rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha}|\Psi\rangle$$

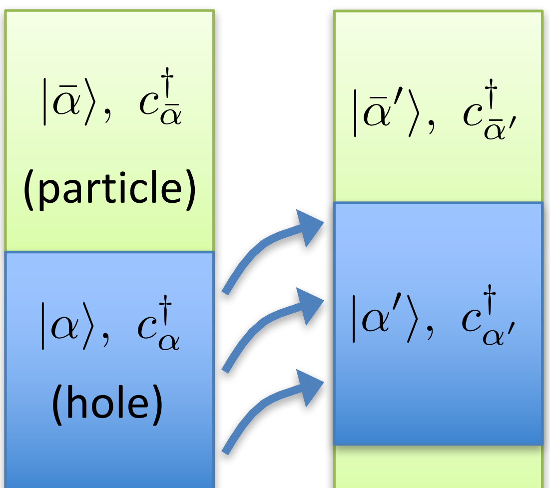
Here $|\Psi\rangle \propto \prod_{\alpha=1}^{N} c^\dagger_\alpha |-\rangle$

We complete occupied states $\sum_\alpha |\alpha\rangle\langle\alpha| + \sum_{\bar\alpha} |\bar\alpha\rangle\langle\bar\alpha| = 1$

The new state $|\Psi + \delta\Psi\rangle = e^{\sum_{\beta\bar\beta} \delta Z_{\beta\bar\beta} a^\dagger_{\bar\beta} a_\beta}|\Psi\rangle = e^{\hat{Z}}|\Psi\rangle$

Is a Slater determinant $|\Psi + \delta\Psi\rangle = \prod_{\alpha'=1}^{N} c^\dagger_{\alpha'}|-\rangle$

Single-particle space



Proof: $e^{\hat{Z}}|\Psi\rangle = e^{\hat{Z}} c^\dagger_{\alpha_1} e^{-\hat{Z}} e^{\hat{Z}} c^\dagger_{\alpha_2} e^{-\hat{Z}} \cdots e^{\hat{Z}} c^\dagger_{\alpha_N} e^{-\hat{Z}} |-\rangle$

$$e^{\hat{Z}} c^\dagger_{\alpha_i} e^{-\hat{Z}} = c^\dagger_{\alpha_i} + [\hat{Z}, c^\dagger_{\alpha_i}] + \frac{1}{2!}[\hat{Z}, [\hat{Z}, c^\dagger_{\alpha_i}]] + \cdots$$

$$[\hat{Z}, c^\dagger_{\alpha_i}] = \sum_\beta Z_{\alpha_i\bar\beta} c^\dagger_{\bar\beta}$$

$$e^{\hat{Z}} c^\dagger_{\alpha_i} e^{-\hat{Z}} = c^\dagger_{\alpha'_i} = c^\dagger_{\alpha_i} + \sum_\beta Z_{\alpha_i\bar\beta} c^\dagger_{\bar\beta}$$

From variational principle

$$S = \int_{t_0}^{t_1} ds \, \langle \Psi(t) | \, i\hbar\partial_t - H \, | \Psi(t) \rangle \Rightarrow S = \int_{t_0}^{t_1} dt \sum_{\alpha} \int_{\mathbf{r}} d^3\mathbf{r} \Big\{ i\hbar\phi_\alpha^*(i)\partial_t\phi_\alpha^*(i) - \mathcal{H}(\phi_\alpha, \phi_\alpha^*) \Big\}$$

For two-body hamiltonian

$$\mathcal{H} = \sum_{ij\alpha} t_{ij}\phi_\alpha^*(i)\phi_\alpha(j) + \frac{1}{2}\sum_{ijkl\alpha\beta} \tilde{v}_{ij,kl}\phi_\alpha^*(i)\phi_\beta^*(j)\phi_\alpha(k)\phi_\beta(l)$$

Mean-field equation of motion (in r-space)

$$\Rightarrow \boxed{i\hbar\partial_t\phi_\alpha(\mathbf{r}) = -\frac{\hbar^2}{2m}\Delta\phi_\alpha(\mathbf{r}) + U_{\mathrm{H}}(\mathbf{r})\phi_\alpha(\mathbf{r}) + \int d\mathbf{r}' U_{\mathrm{ex}}(\mathbf{r},\mathbf{r}')\phi_\alpha(\mathbf{r}')}$$

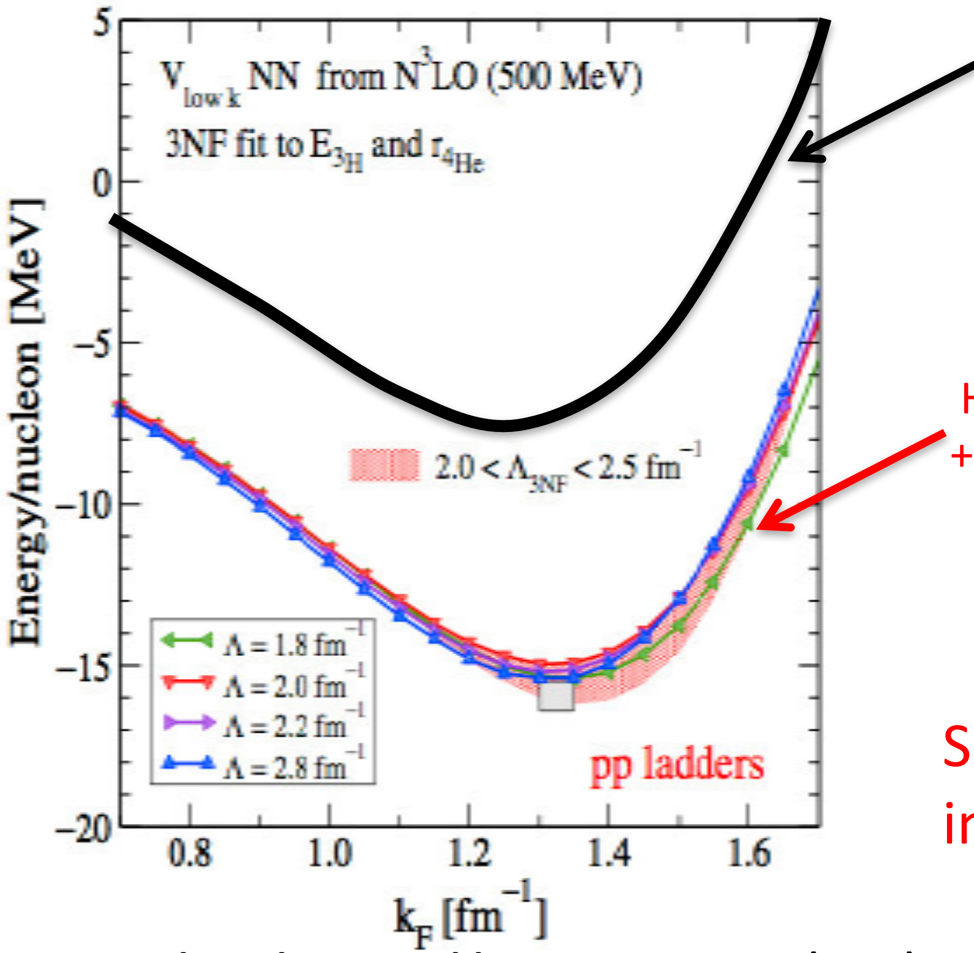
Direct term $U_{\mathrm{H}}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\mathbf{r}')$

Exchange term $U_{\mathrm{ex}}(\mathbf{r},\mathbf{r}') = -v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r},\mathbf{r}')$

From Ehrenfest.

$$i\hbar\frac{d\langle A_\alpha\rangle}{dt} = \langle [A_\alpha, H] \rangle \Rightarrow i\hbar\frac{d}{dt}\langle a_i^\dagger a_j \rangle = \langle [a_i^\dagger a_j, H] \rangle \Rightarrow i\hbar\partial_t\rho = [h_{\mathrm{MF}}[\rho], \rho]$$

Calculation from bare soft NN interaction



Hartree-Fock only

Hartree-Fock + perturbation theory

Bogner, Schwenk, Furnstahl, Nogga, NPA 763 (2005) .

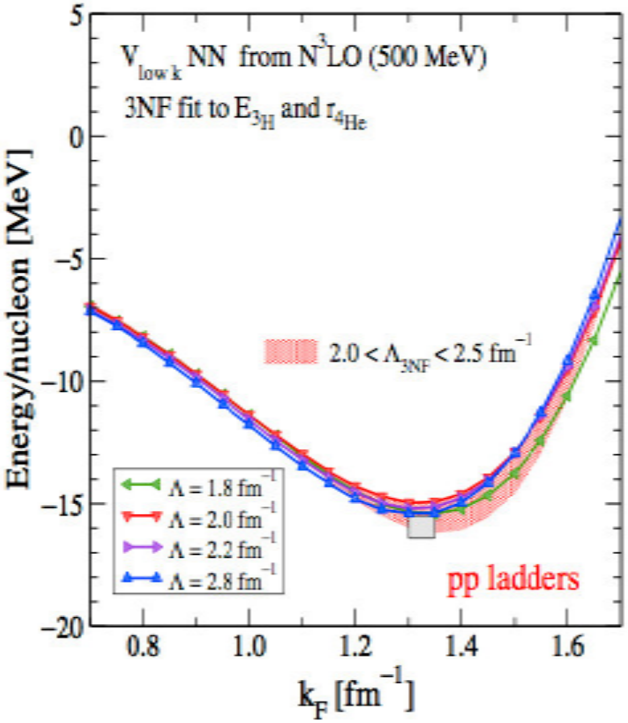
So, why is mean-field theory so important in nuclear physics?

Nuclear Equation of state

Ab-initio

Bare soft NN interaction

Hartree Fock+3body
+pert. theory

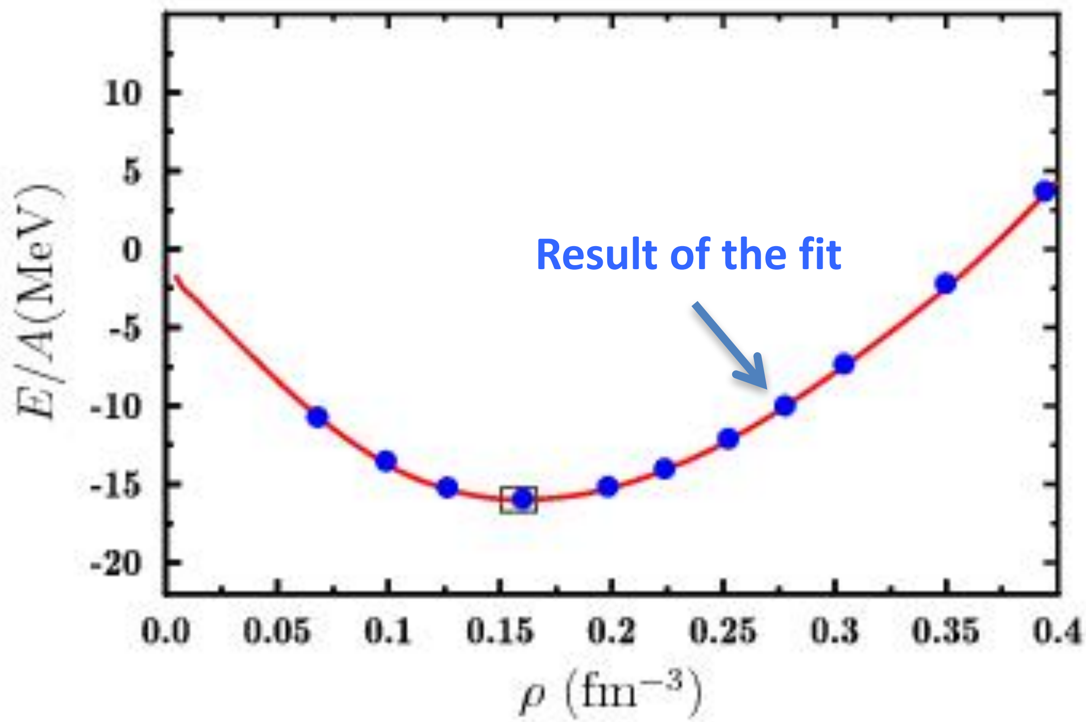


Energy Density Functional

$$|\Psi\rangle \propto \prod_{\alpha=1}^{N} c_\alpha^\dagger |-\rangle \Rightarrow \rho = \sum |\alpha\rangle\langle\alpha|$$

$$E = \left\langle \frac{p^2}{2m} \right\rangle + U[\rho]$$

with $U[\rho] = \sum_n c_n \rho^n$



Nuclear Energy Density Functional based on effective interaction

Illustration with the Skyrme Functional

Vautherin, Brink, PRC (1972)

$$
\begin{aligned}
v(\mathbf{r}_1-\mathbf{r}_2) &= t_0\,(1+x_0\hat{P}_\sigma)\,\delta(\mathbf{r}) \\
&+\tfrac{1}{2}t_1\,(1+x_1\hat{P}_\sigma)\big[\mathbf{P}'^2\,\delta(\mathbf{r})+\delta(\mathbf{r})\,\mathbf{P}^2\big] \\
&+t_2\,(1+x_2\hat{P}_\sigma)\,\mathbf{P}'\cdot\delta(\mathbf{r})\,\mathbf{P} \\
&+iW_0\sigma.\big[\mathbf{P}'\times\delta(\mathbf{r})\,\mathbf{P}\big] \\
&+\tfrac{1}{6}t_3\,(1+x_3\hat{P}_\sigma)\,\rho^\alpha(\mathbf{R})\,\delta(\mathbf{r})
\end{aligned}
$$

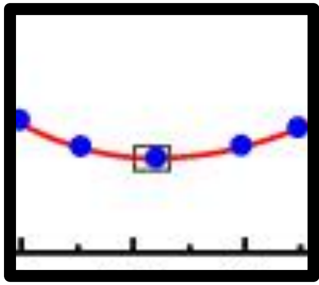
$$
\mathcal{E} = \langle\Psi|H(\rho)|\Psi\rangle = \int \mathcal{H}(r)d^3\mathbf{r}
$$

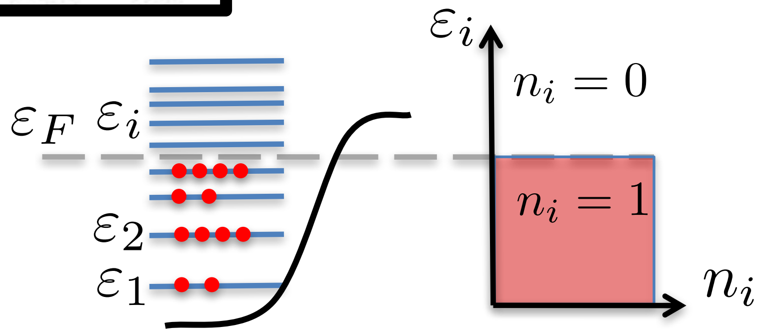
$$
\begin{aligned}
\mathcal{H} = \mathcal{K}+\mathcal{H}_0+\mathcal{H}_3+\mathcal{H}_{\rm eff} \\
+\mathcal{H}_{\rm fin}+\mathcal{H}_{\rm so}+\mathcal{H}_{\rm sg}+\mathcal{H}_{\rm Coul}
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{H}_0 &= \tfrac{1}{4}t_0\big[(2+x_0)\rho^2-(2x_0+1)(\rho_p^2+\rho_n^2)\big] \\
\mathcal{H}_3 &= \tfrac{1}{24}t_3\rho^\alpha\big[(2+x_3)\rho^2-(2x_3+1)(\rho_p^2+\rho_n^2)\big] \\
\mathcal{H}_{\rm eff} &= \tfrac{1}{8}\big[t_1(2+x_1)+t_2(2+x_2)\big]\tau\rho \\
&+ \tfrac{1}{8}\big[t_2(2x_2+1)-t_1(2x_2+1)\big](\tau_p\rho_p+\tau_n\rho_n) \\
\mathcal{H}_{\rm fin} &= \tfrac{1}{32}\big[3t_1(2+x_1)-t_2(2+x_2)\big](\nabla\rho)^2 \\
&- \tfrac{1}{32}\big[3t_1(2x_1+1)+t_2(2x_2+1)\big]\big[(\nabla\rho_p)^2+(\nabla\rho_n)^2\big] \\
\mathcal{H}_{\rm so} &= \tfrac{1}{2}W_0\big[\mathbf{J}.\nabla\rho+\mathbf{J}_p.\nabla\rho_p+\mathbf{J}_n.\nabla\rho_n\big] \\
\mathcal{H}_{\rm sg} &= -\tfrac{1}{16}(t_1x_1+t_2x_2)\mathbf{J}^2+\tfrac{1}{16}(t_1-t_2)\big[\mathbf{J}_p^2+\mathbf{J}_n^2\big]
\end{aligned}
$$

Functional of $\rho, \rho_n, \rho_p, \tau, \tau_n, \tau_p, \mathbf{J}, \ldots$

Around 10-14 parameters to be adjusted

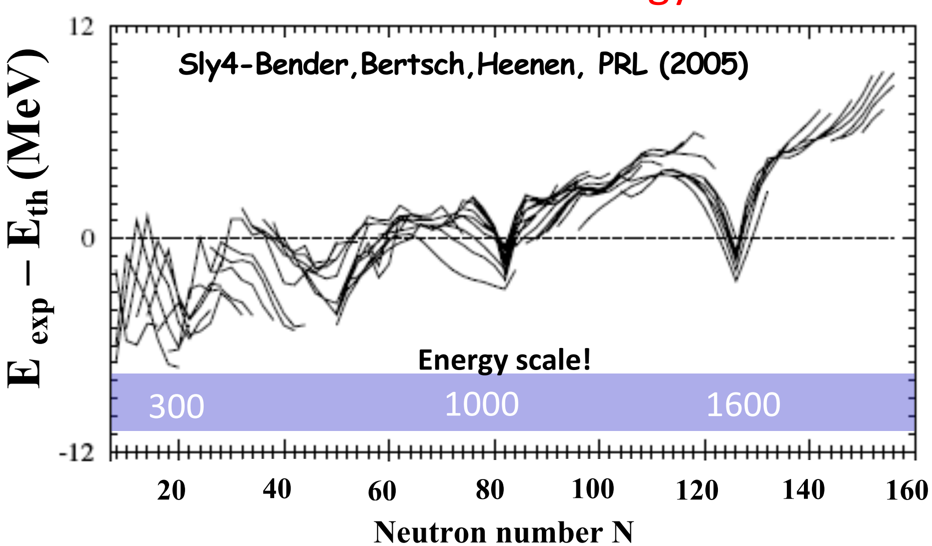




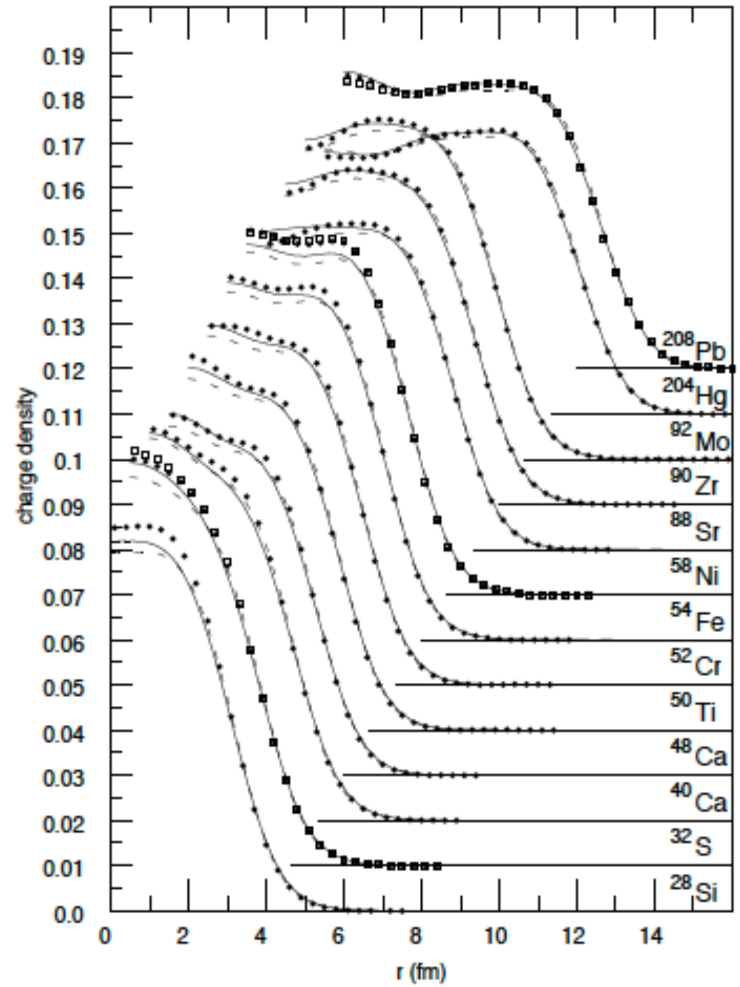
In practice

$$\{\varphi_\alpha\} \Longrightarrow \rho \Longrightarrow h_{\mathrm{MF}}[\rho] \Longrightarrow \{\varphi_\alpha\} \Longrightarrow \cdots$$

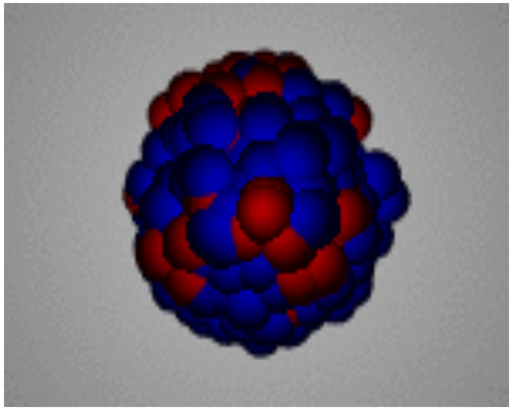
Ground state Energy



Ground state density

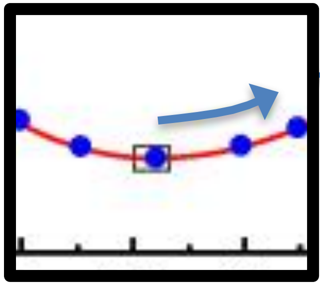


Time-Dependent Mean-Field
For collective motion



First step towards non equilibrium

Constrained calculations



Nuclei at various shapes $\delta\langle\Psi|H-\lambda Q-E|\Psi\rangle=0$

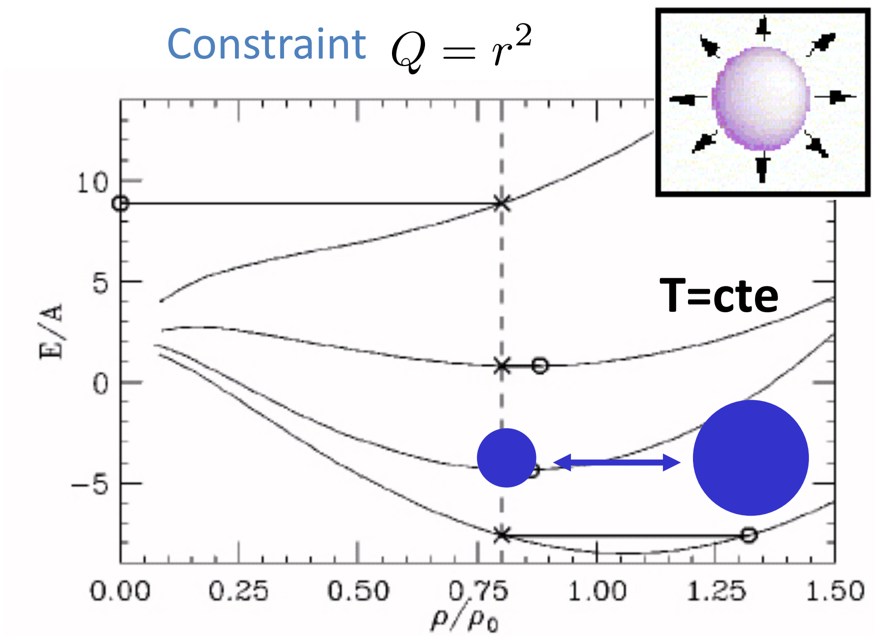
Thermodynamics of nuclei $\delta\langle\Psi|H-TS-\mu N|\Psi\rangle=0$ with $S=-\mathrm{Tr}(D\ln D)$

Here $\rho=\sum|i\rangle n_i\langle i|$ $\quad S[n_i]=-\sum_i[n_i\log(n_i)+(1-n_i)\log(1-n_i)]$

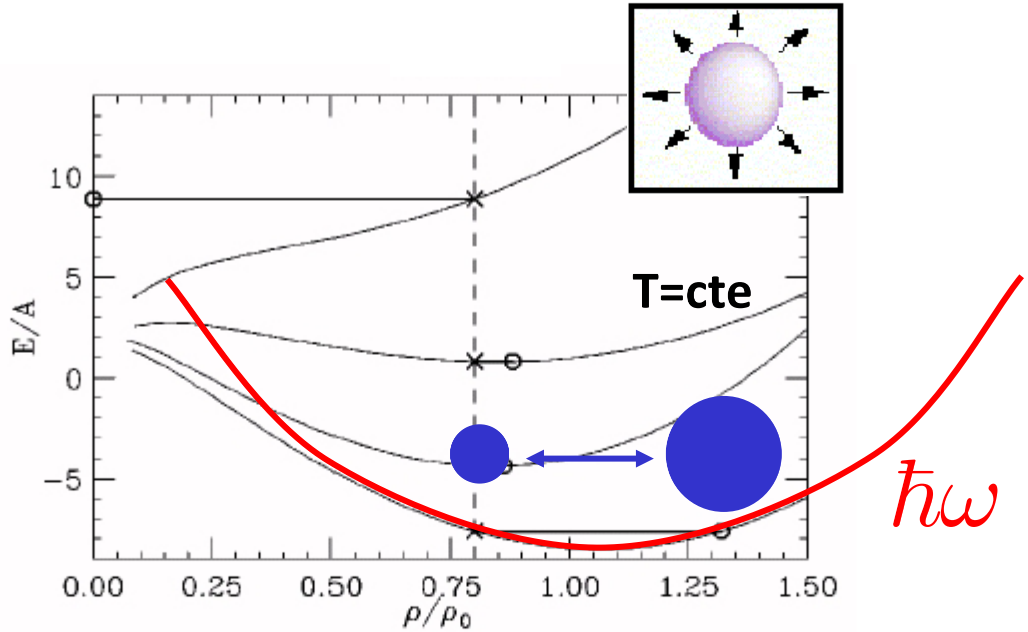
$\Rightarrow\quad n_i=1/(1+exp\{(\varepsilon_i-\mu)/T\})$

Monopole vibration

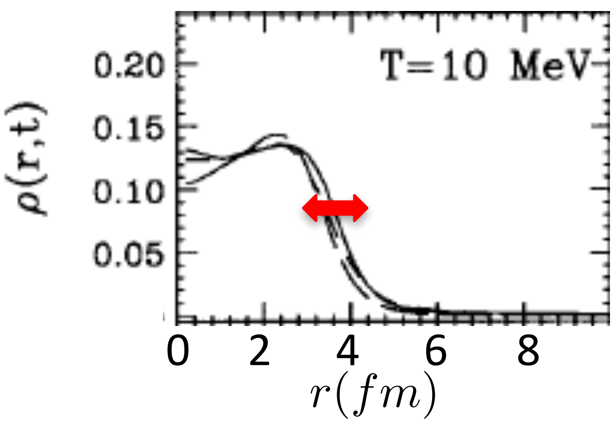
Constraint $Q=r^2$

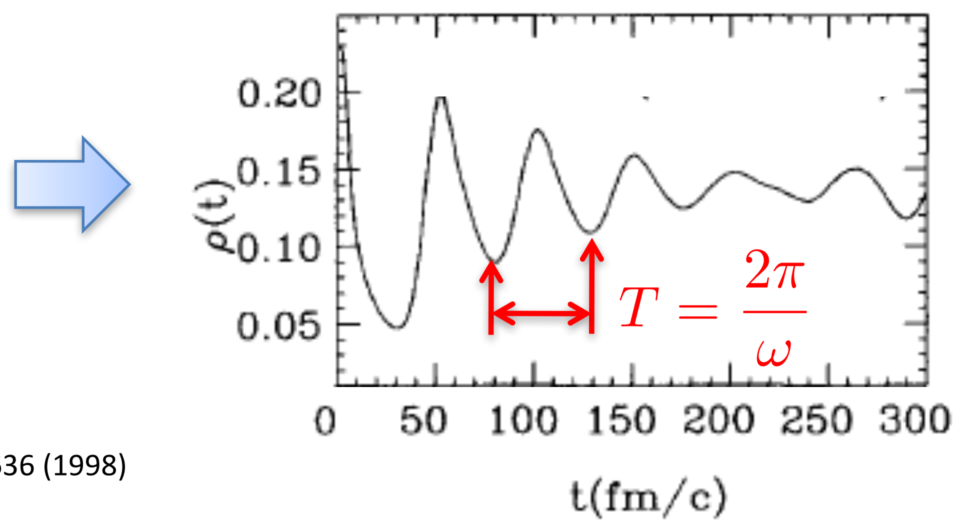


Constrained mean-field versus dynamics



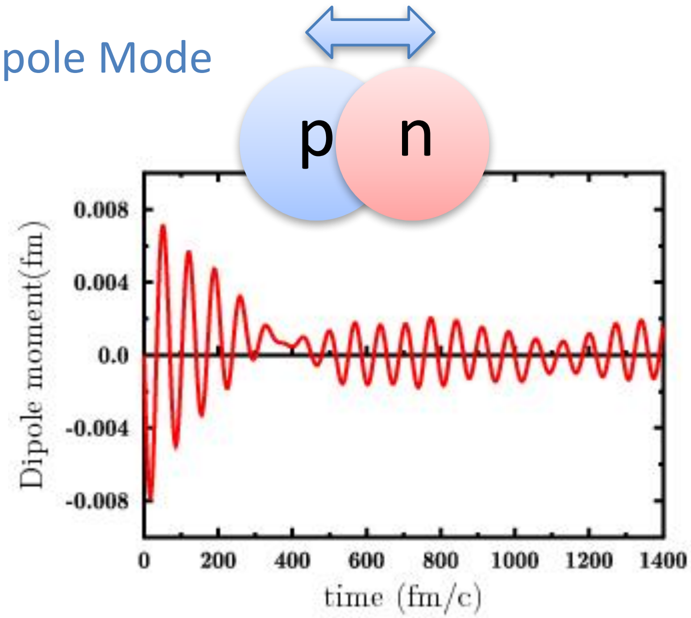
Time evolution

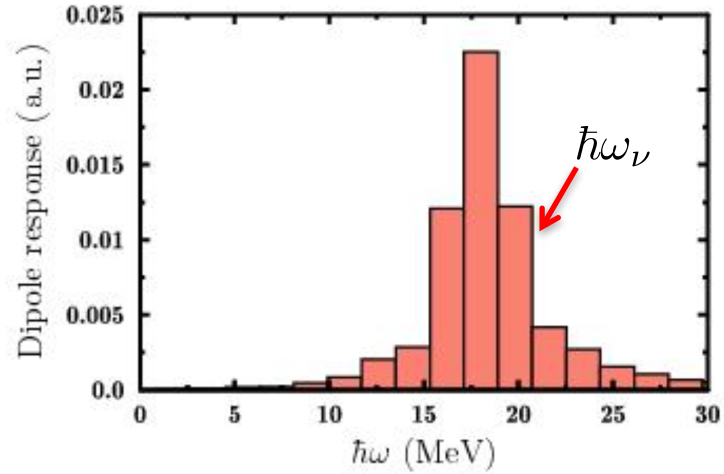




From DL, Ph. Chomaz, Nucl. Phys. A636 (1998)

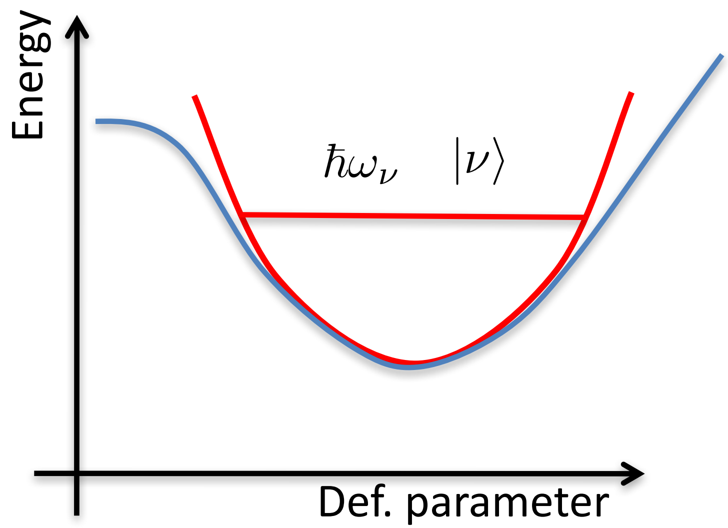
Dipole Mode





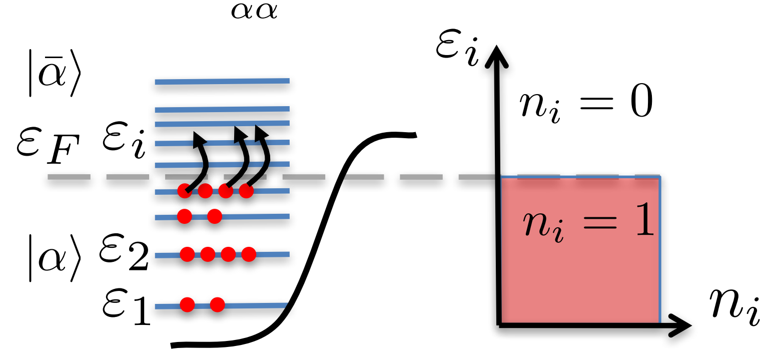
Note: small amplitude limit of TDHF is RPA

Nature of the collective states

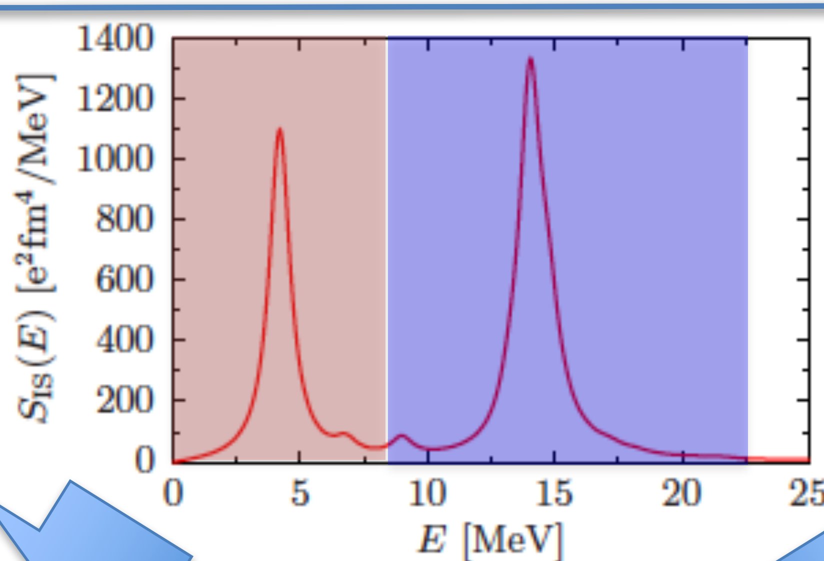


Particle-hole decomposition

$$|\nu\rangle \propto \sum_{\alpha\bar{\alpha}} X^{\nu}_{\bar{\alpha}\alpha} a^{\dagger}_{\bar{\alpha}} a_{\alpha} |\Psi_0\rangle$$

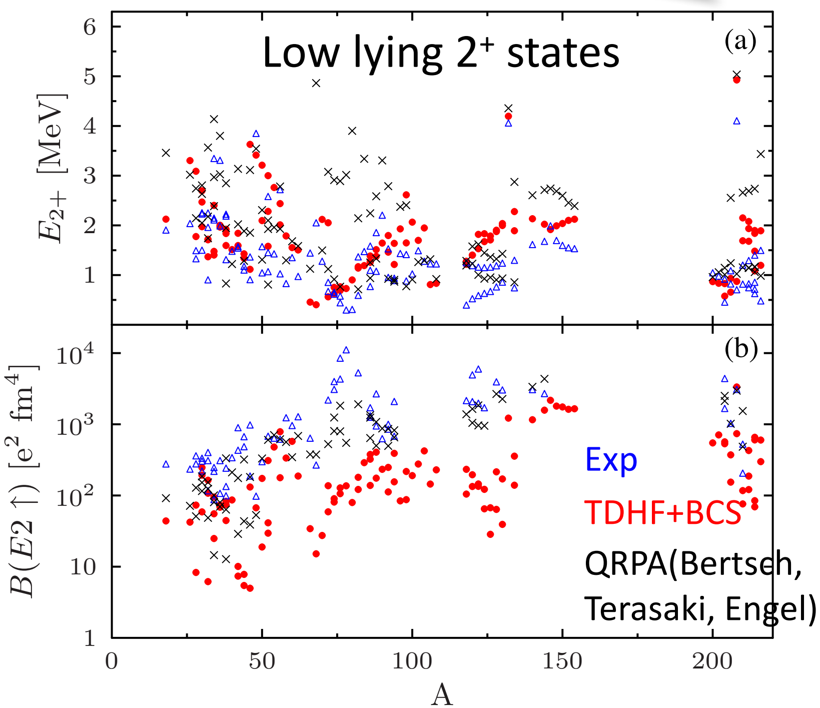


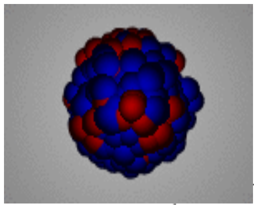
The RPA is also a way to re-quantize TDHF

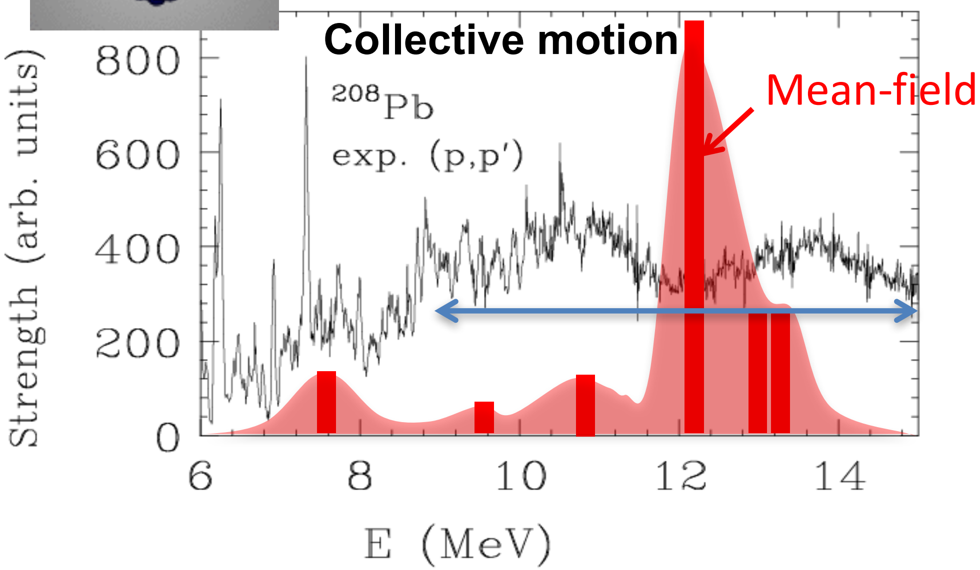


Low-lying sector

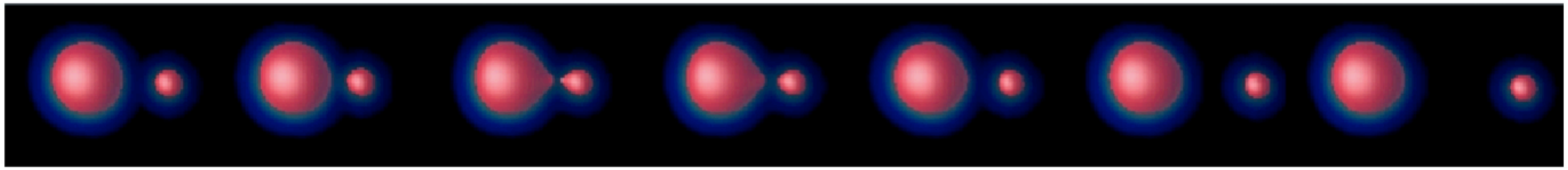
Collective sector

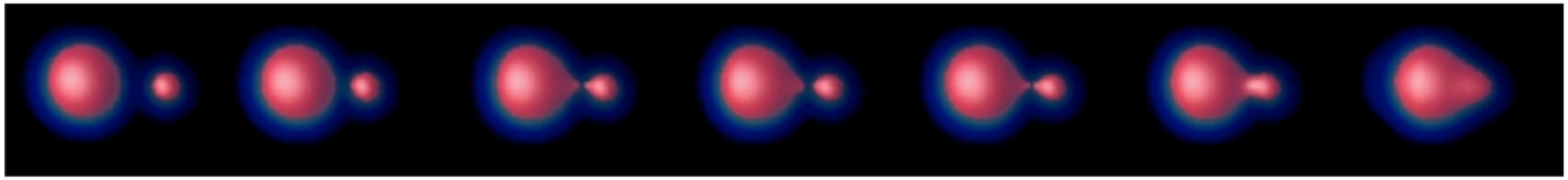


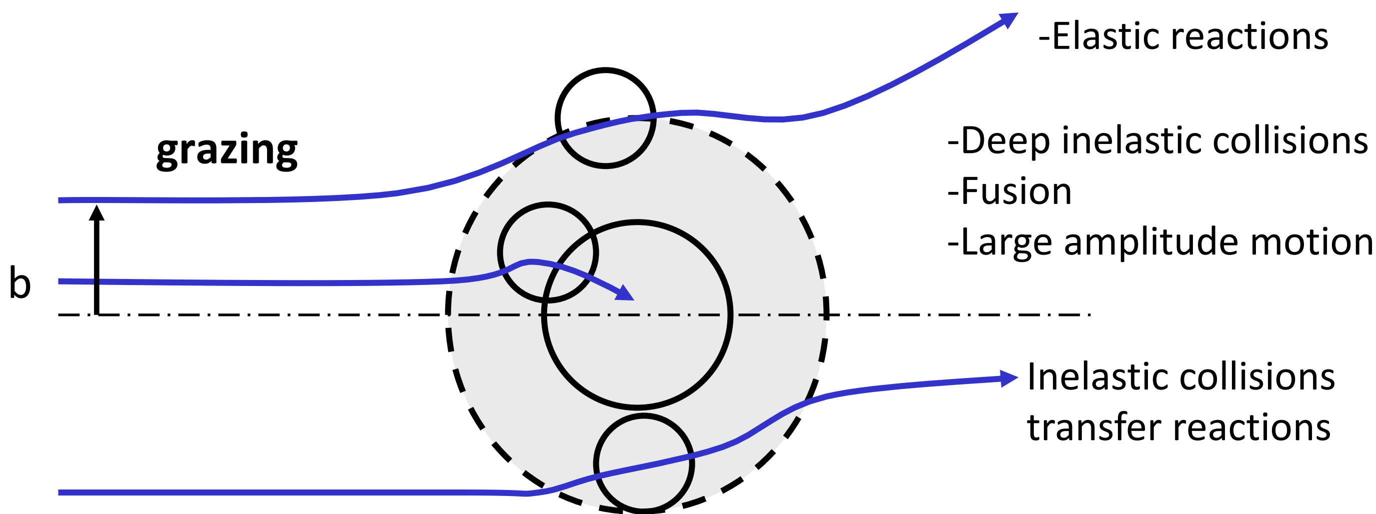




Time-Dependent Mean-Field
for low energy collisions

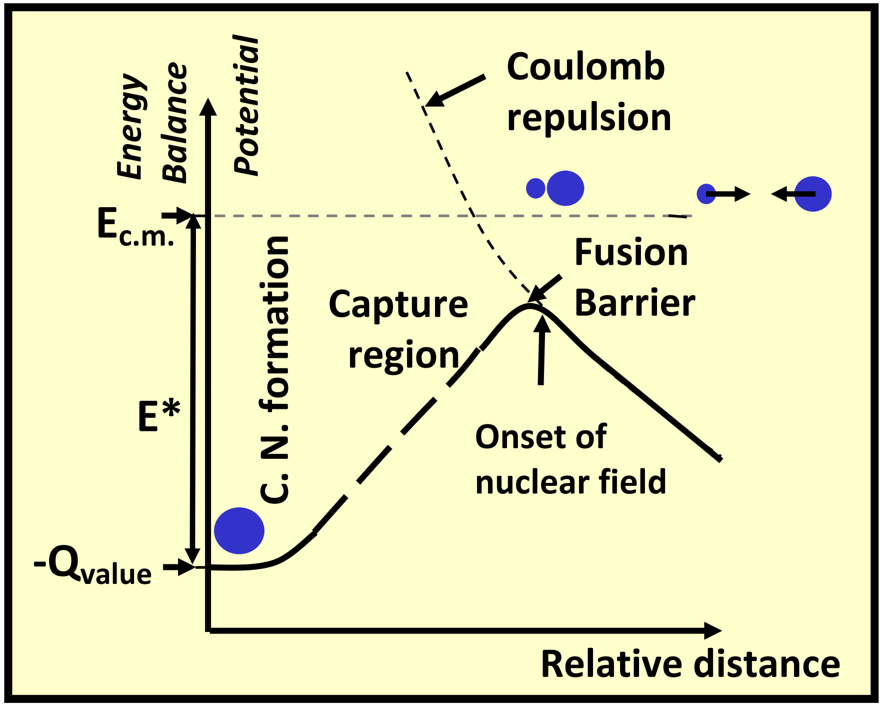






Adapted from: W. Nörenberg and H.A. Weidenmüller, *Introduction to Heavy-Ion theory*, Springer-Verlag 1981.

Macroscopic aspects:



Important parameters

Mass/Charge:

Projectile (N_P, Z_P)

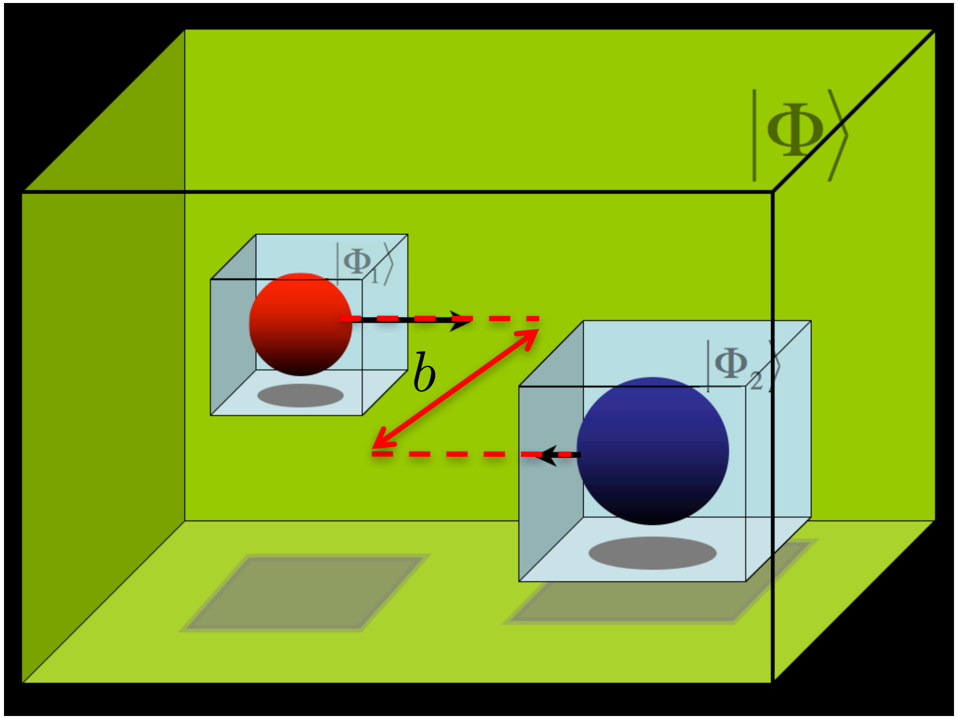
Target (N_T, Z_T)

Impact parameter: b

$$L = r \wedge p = b p_{ini}$$

Beam Energy: E_B/A

$$E_B^{Fus} \simeq 5\ MeV.A$$



Step 1

Initialize both nuclei separately

Step 2

Put both in a 3D Mesh (in the c.m.)

Step 3

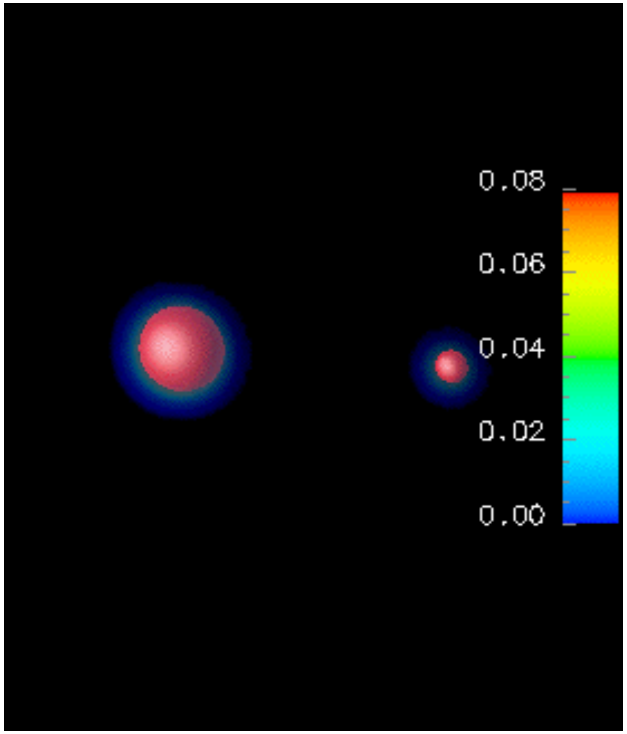
Boost wave-packets $|\phi_\alpha^{T/P}\rangle \rightarrow e^{-ip_{T/P}r/\hbar}|\phi_\alpha^{T/P}\rangle$

Step 4

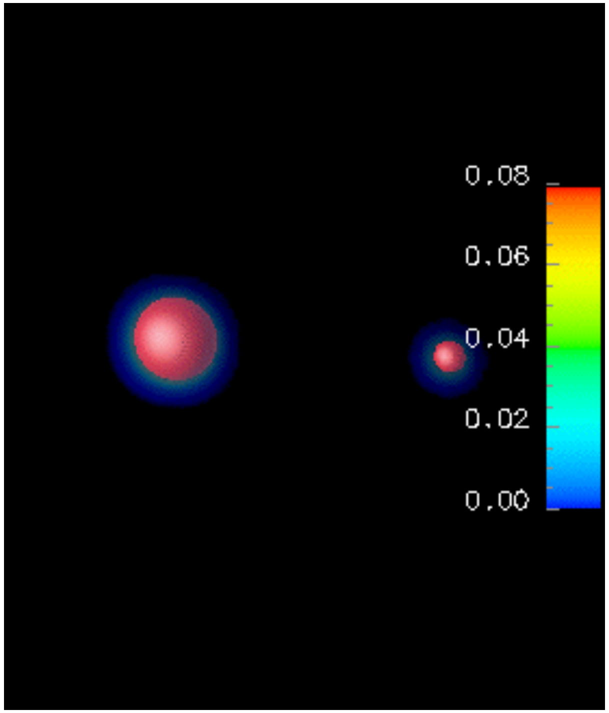
Perform evolution

Some illustration of mean-field evolution

$^{16}O+^{208}Pb$ @ 74.44 MeV

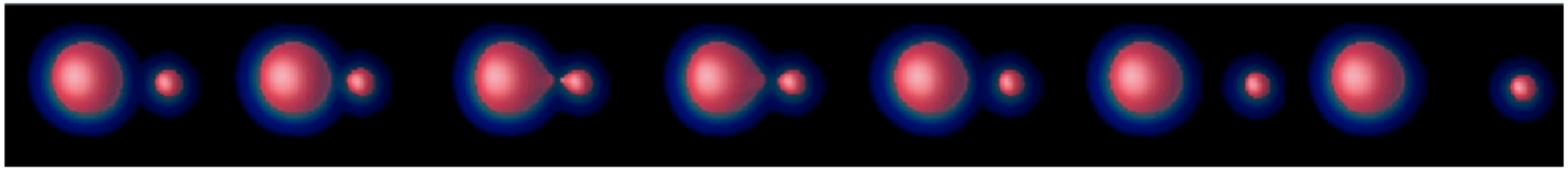


$^{16}O+^{208}Pb$ @ 74.45 MeV

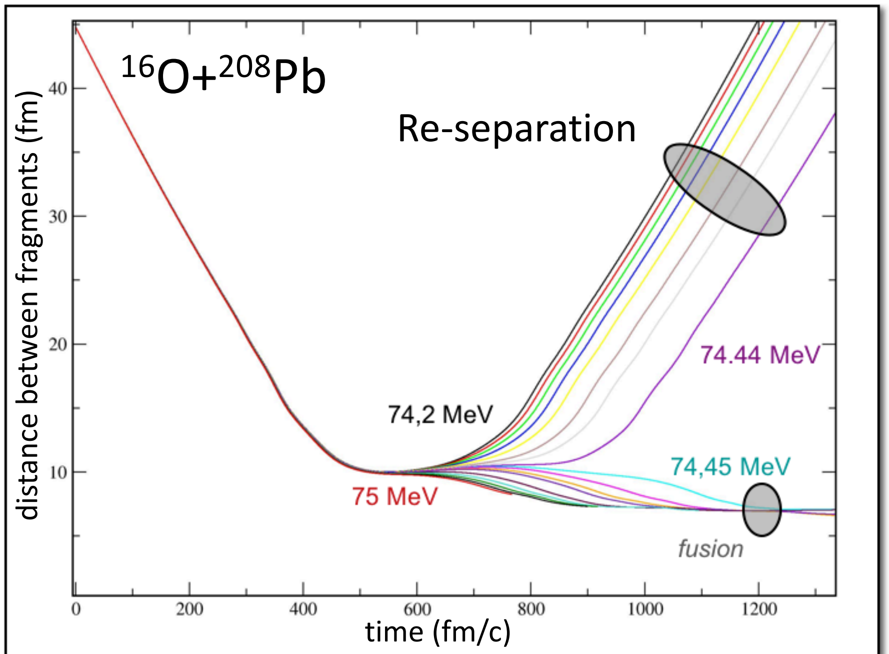


Example of application: reaction time

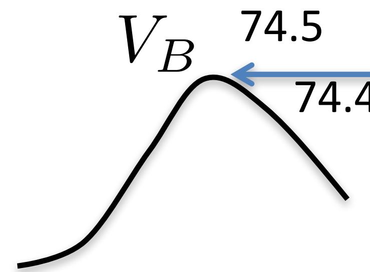
Re-separation



time

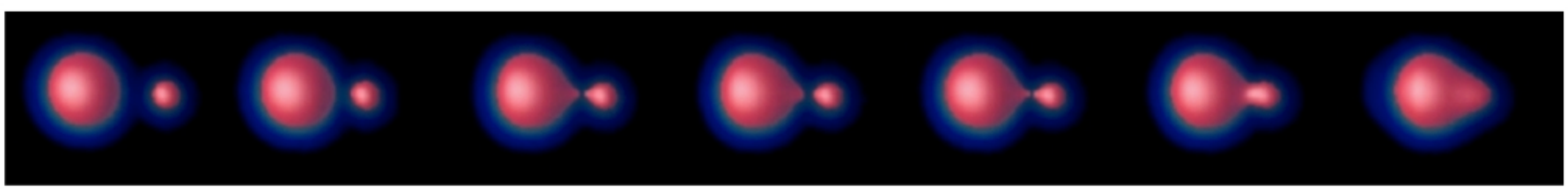


di-nuclear



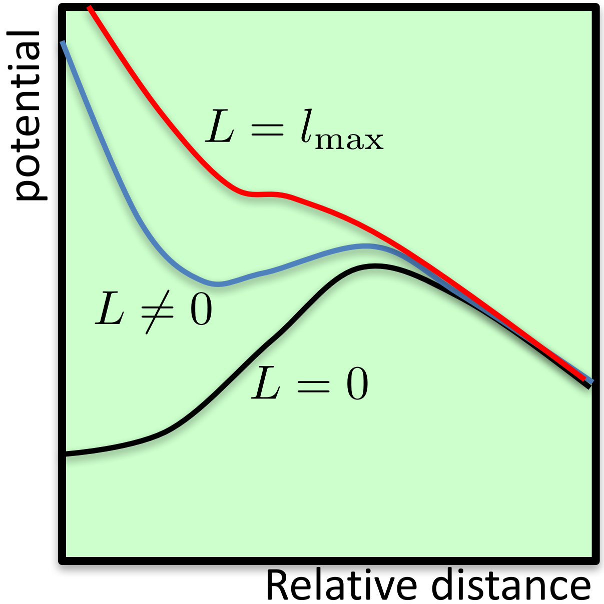
mono-nuclear

Fusion



Simenel, Avez, DL, (2008) arXiv:0806.2614.

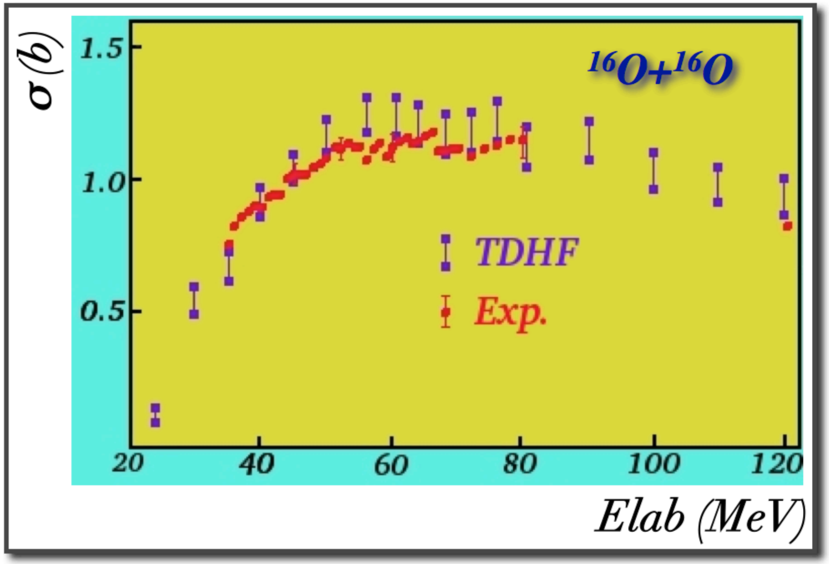
Example of application: fusion cross-sections



$$L = r \wedge p = b p_{ini} \qquad H = \frac{p^2}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)$$

For a given energy $\sigma_F = \pi b_{\rm crit}^2 = \left(\frac{\pi \hbar^2 l_{\rm crit}^2}{2\mu}\right) \frac{1}{E}$

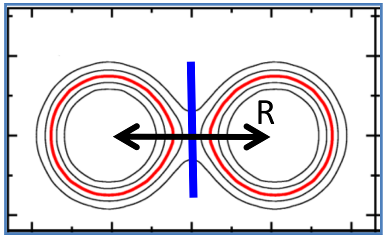
$$\sigma_{\rm Fus}(E) \simeq \frac{\pi \hbar^2}{2\mu E} (l_{max}(E) + 1)^2.$$



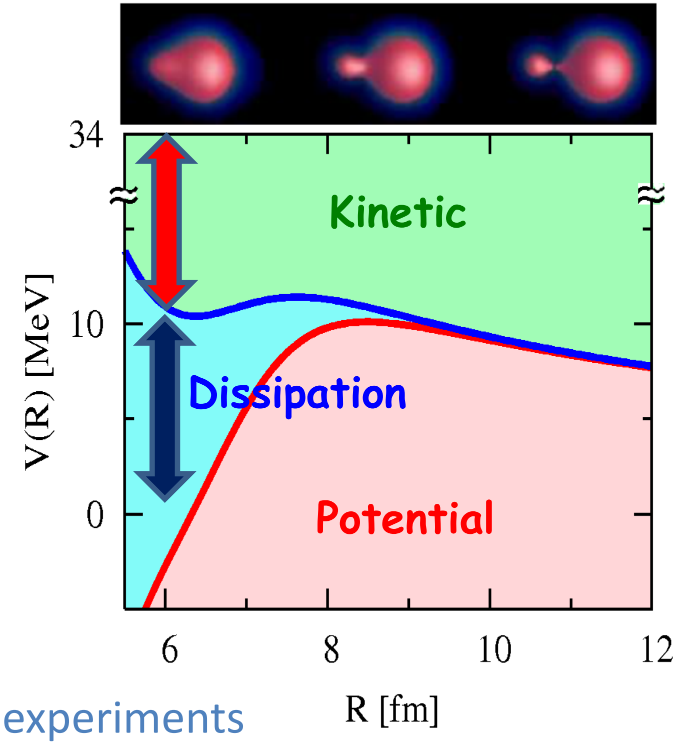
S.E. Koonin, Prog. Nucl. Part. Phys. 4 (79) 283.
K.T.R. Davies et al, Treat. Heavy Ion Sciences, 4 (85) 1.

Example of application: nucleus-nucleus potential/effect of dynamics

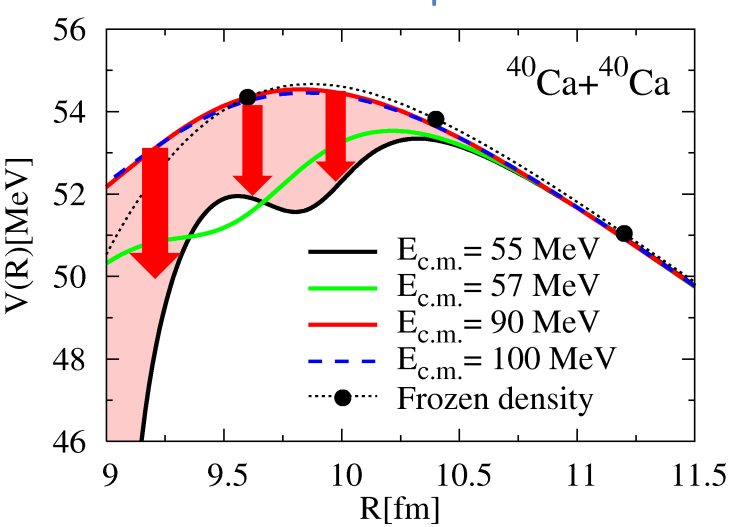
From microscopic to macroscopic world



$$\frac{dP}{dt} = -\frac{dV}{dR} - \gamma(R)\frac{dR}{dt}$$

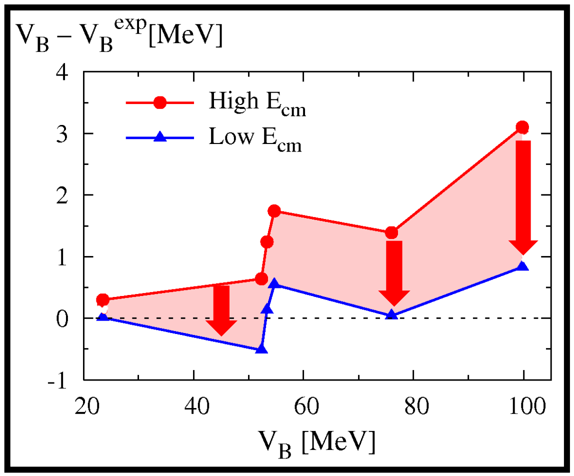


Nucleus-nucleus potential



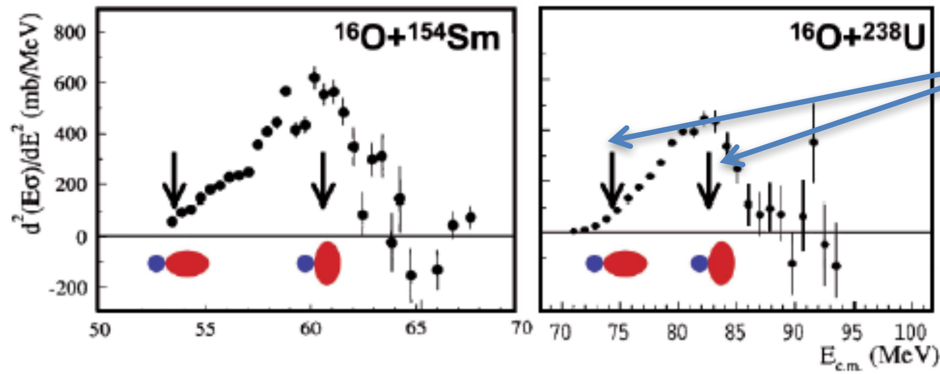
Washiyama, DL, PRC78 (2008).
Washiyama, DL, Ayik, PRC79 (2009).

Comparison with experiments



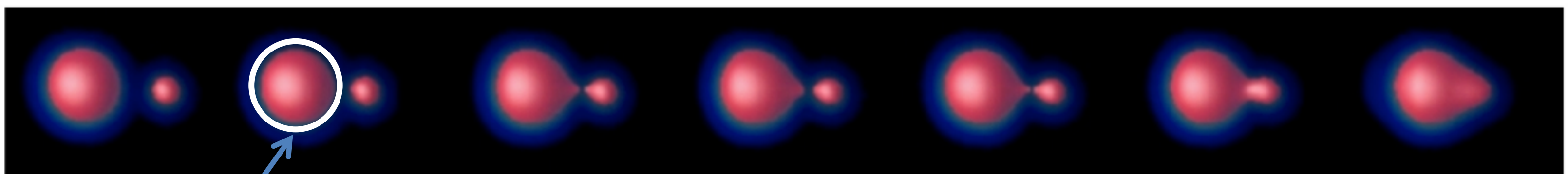
Very good agreement with experiment

Interplay between fusion and deformation is included in a semi-classical way:
Different orientation lead to different barriers



Barrier deduced
From TDHF

From Simenel, EPJA 48 (2012)

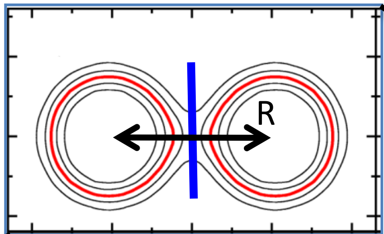


Vibrations can be excited during the approaching phase leading
to barrier fluctuations

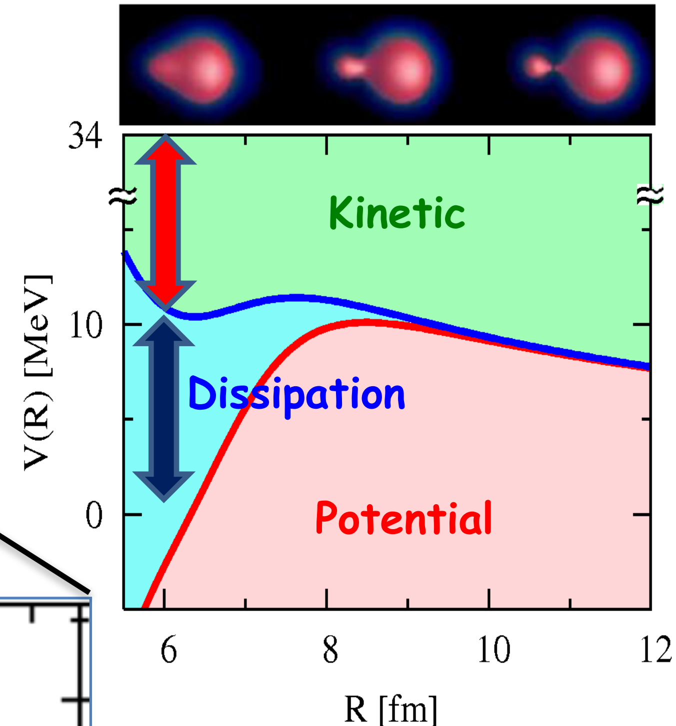
Important : the excited collective
degrees of freedom are not pre-selected

However, collective space is not quantized
Missing quantum fluctuations

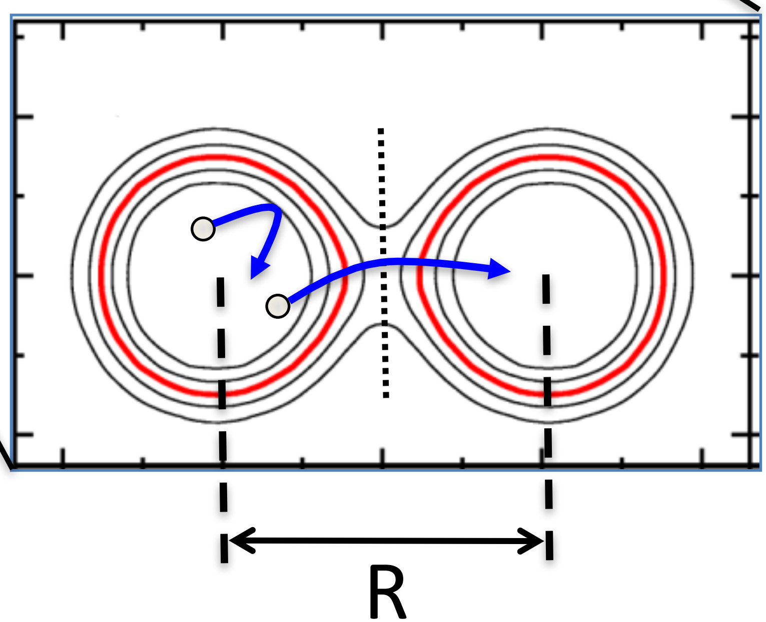
From microscopic to macroscopic world



$$\frac{dP}{dt} = -\frac{dV}{dR} - \gamma(R)\frac{dR}{dt}$$

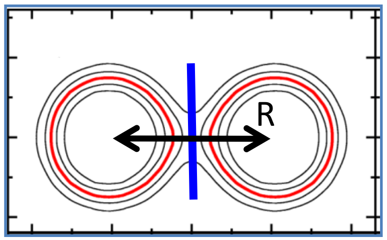


one-body origin of dissipation

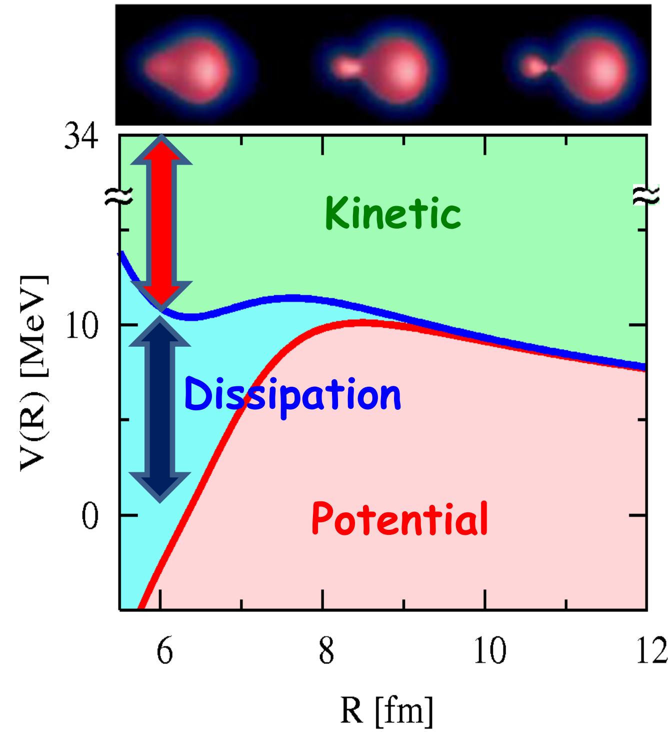


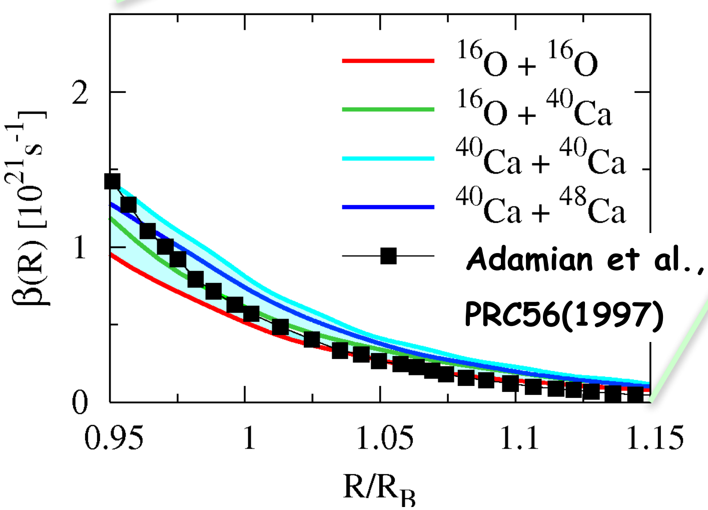
- -transfer of particle
- -reflection of particles

From microscopic to macroscopic world



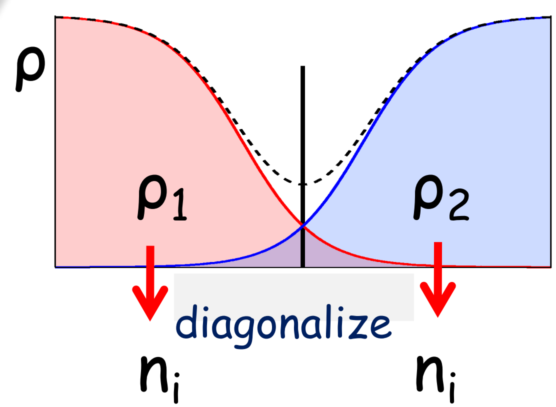
$$\frac{dP}{dt} = -\frac{dV}{dR} - \gamma(R)\frac{dR}{dt}$$





Washiyama, DL, PRC78 (2008).
Washiyama, DL, Ayik, PRC79 (2009).

Link with internal excitation



$$E^* \simeq \sum \varepsilon_i (n_i - n_i^0)$$

$$E^* \simeq E_{\rm diss}$$

Large Amplitude Collective Motion and dissipative aspects (multi-nucleon transfer, quasi-fission)

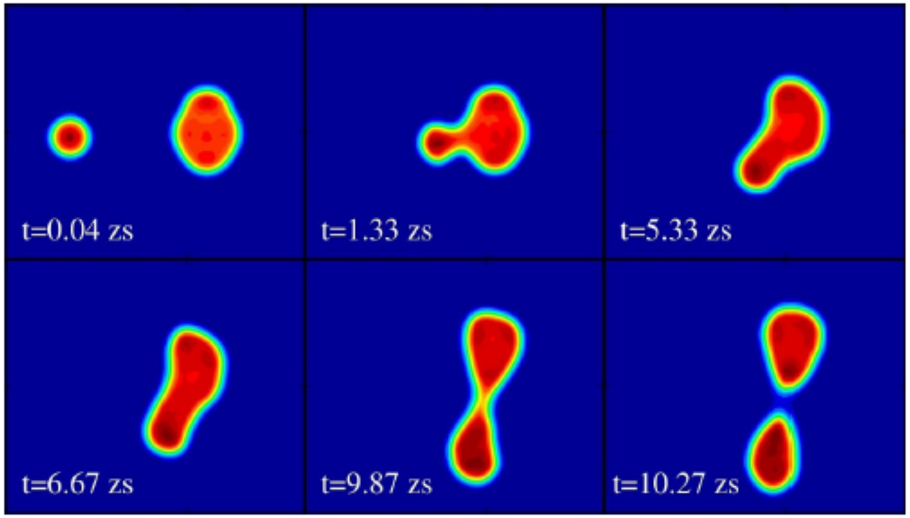
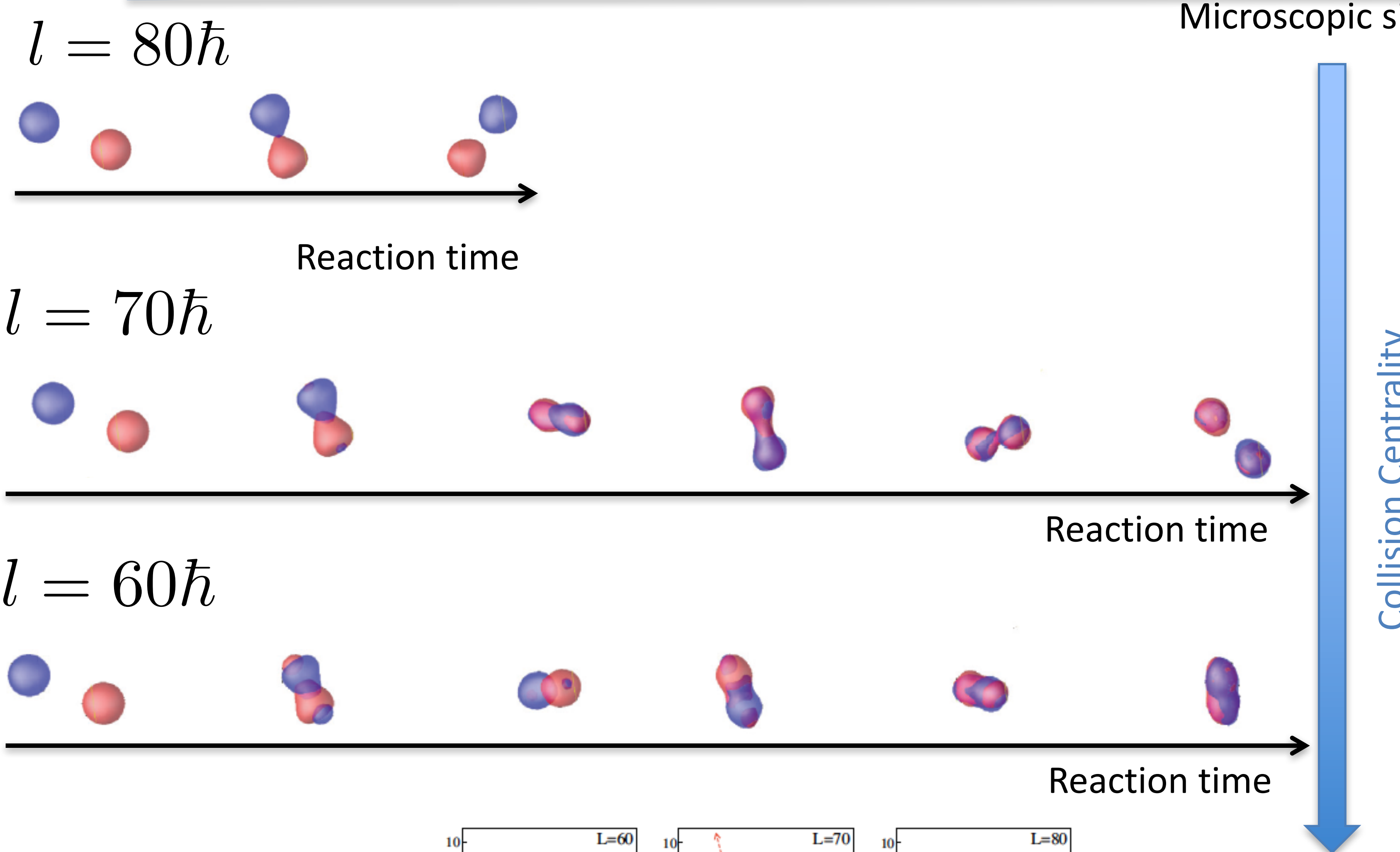


FIG. 1. (Color online) Quasifission in the reaction $^{40}Ca+^{238}U$ at $E_{c.m.} = 209$ MeV with impact parameter $b = 1.103$ fm ($L = 20$). Shown is a contour plot of the time evolution of the mass density.

Oberacker et al, Phys. Rev. C90 (2014)

Quasi-fission reactions

Microscopic simulation



Nuclei trajectory

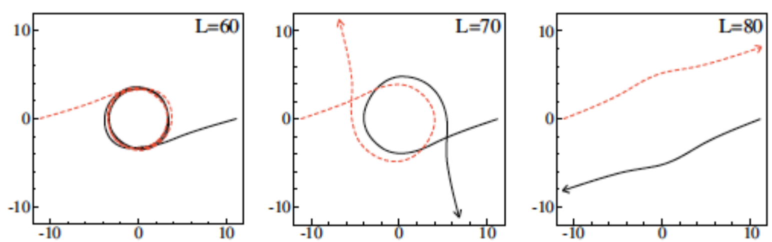


Fig. 32. Trajectories of the centers of mass of the fragments in $^{40}Ca + ^{40}Ca$ collisions at $E_{c.m.} = 128$ MeV.

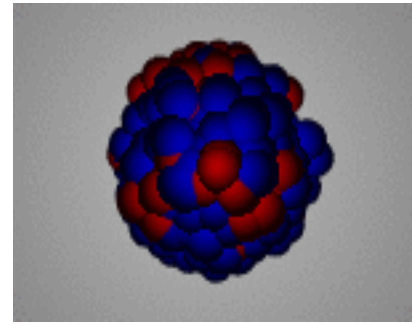
Gives access to time-scales

From Simenel, EPJA 48 (2012)

Effect of superfluidity
On nuclear reactions

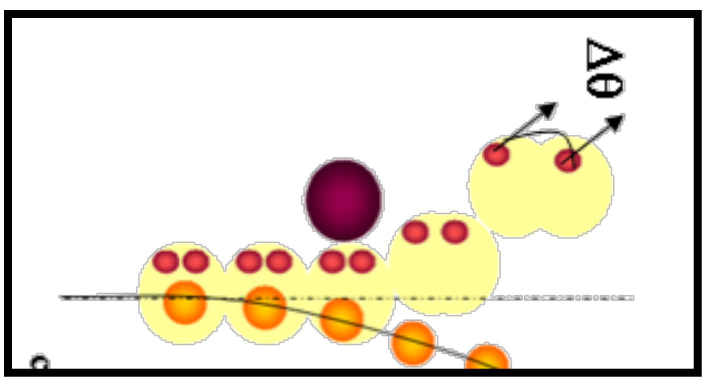
Goal

Systematic study of the pairing
Influence on nuclear dynamics



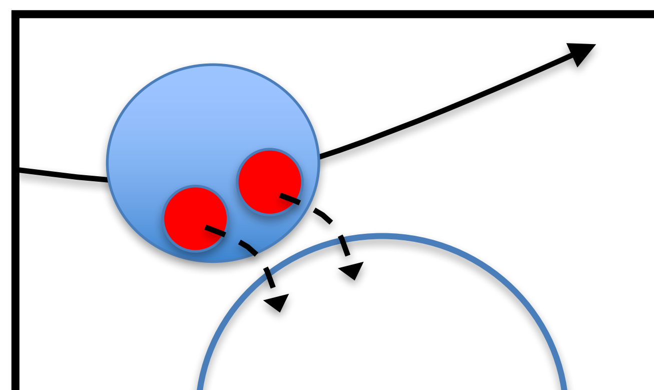
Scamps, Lacroix, PRC (2014)

2n-break-up reactions



Assié and Lacroix, PRL102 (2009)

2n-transfer reactions



Scamps, Lacroix, PRC 87 (2013)

EDF: Pairing correlations in nuclei

$$|\Phi_0\rangle = \Pi_i a_i^\dagger |-\rangle \;\Rightarrow\; |\Phi_0\rangle = \Pi \beta_\alpha^\dagger |-\rangle \quad \text{or} \quad |\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$$

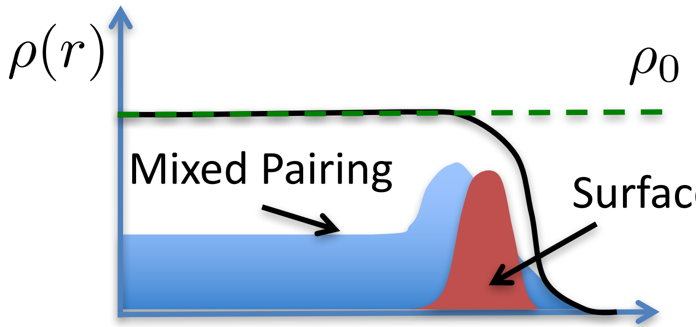
EDF: $$\mathcal{E}_{SR}[\rho, \kappa, \kappa^*] = \sum t_{ii}\rho_{ii} + \frac{1}{2}\sum \bar{v}^{\rho\rho}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum \bar{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\kappa^*_{i\bar{i}}\kappa_{j\bar{j}}$$

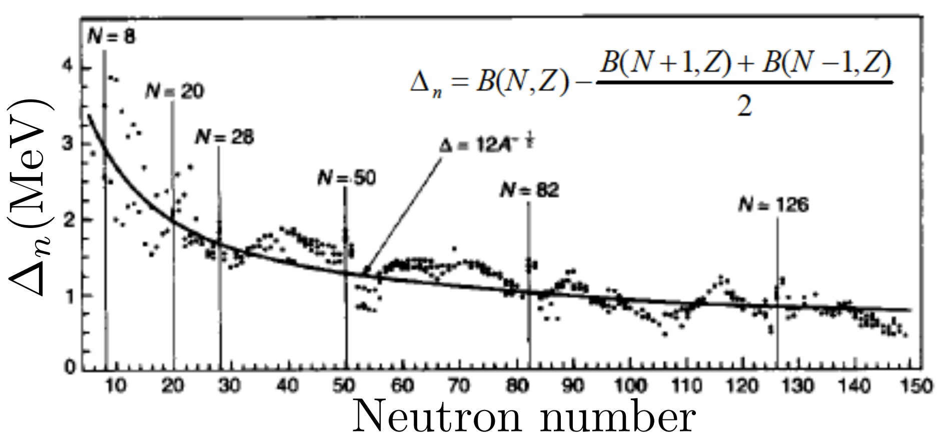
Pairing channel

$$\Phi_0 \rightarrow \{\rho, \kappa\} \rightarrow \mathcal{E}_{SR}$$

Pairing interaction

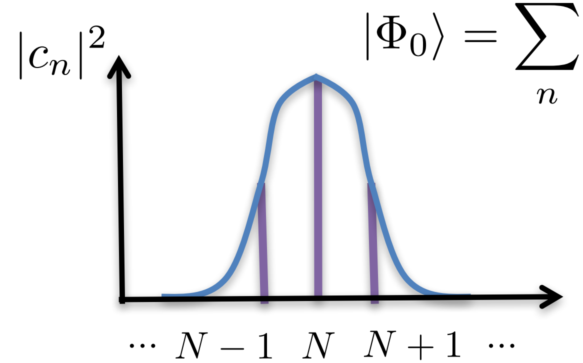
$$v^{\kappa\kappa} = v_0 \left(1 - \alpha \left[\frac{\rho}{\rho_0}\right]^\beta\right) \delta(r_1 - r_2)$$

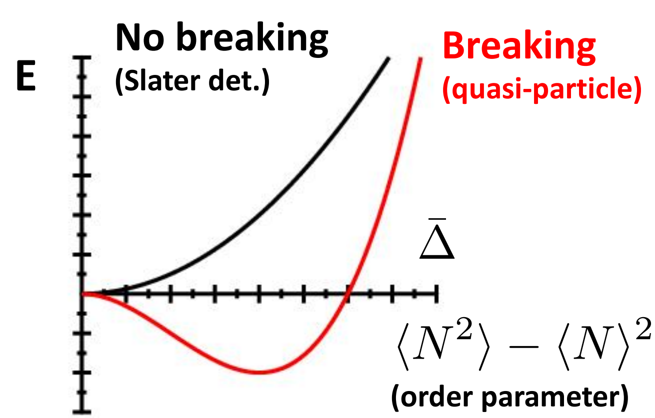




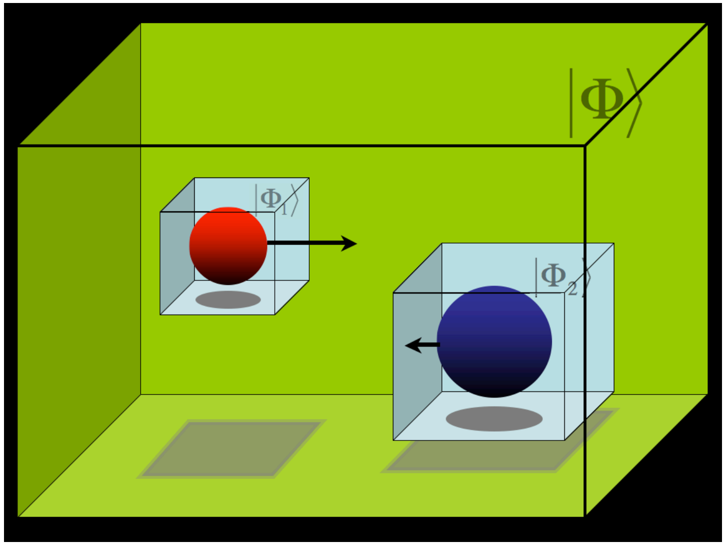
Particle number non-conservation

$$|\Phi_0\rangle = \sum_n c_n |\Psi_n\rangle$$





Nuclear reaction 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…)

BCS limit of TDHFB (also called Canonical basis TDHFB)

TDHFB = 1000 * (TDHF)

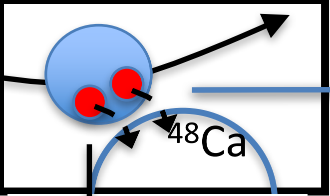
Neglect Δ_{ij}

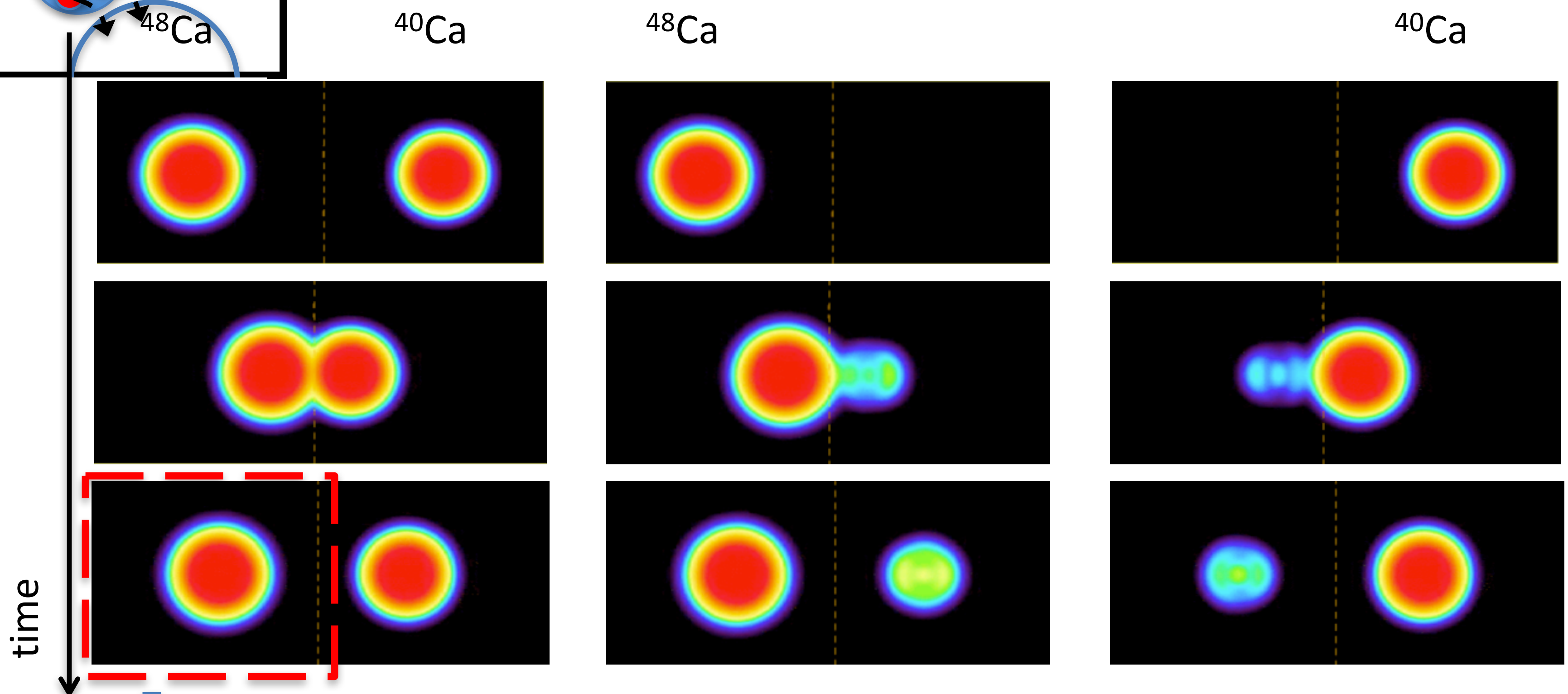
Avez, Simenel, and Chomaz, PRC78, (2008)

$$|\Phi(t)\rangle = \prod_{k>0}\left(u_k(t) + v_k(t)a^\dagger_k(t)a^\dagger_{\bar{k}}(t)\right)|-\rangle.$$

- Less demanding than TDHFB
- Reasonable results for collective motion — Ebata, Nakatsukasa et al, PRC82 (2010)
- Sometimes more predictive than TDHFB — Scamps, Lacroix, Bertsch, Washiyama, PRC85 (2012)

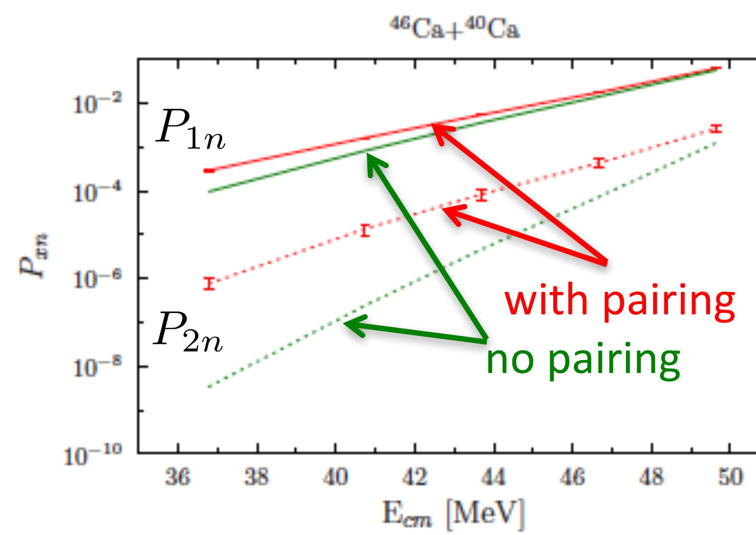
Transfer reaction below the Coulomb barrier





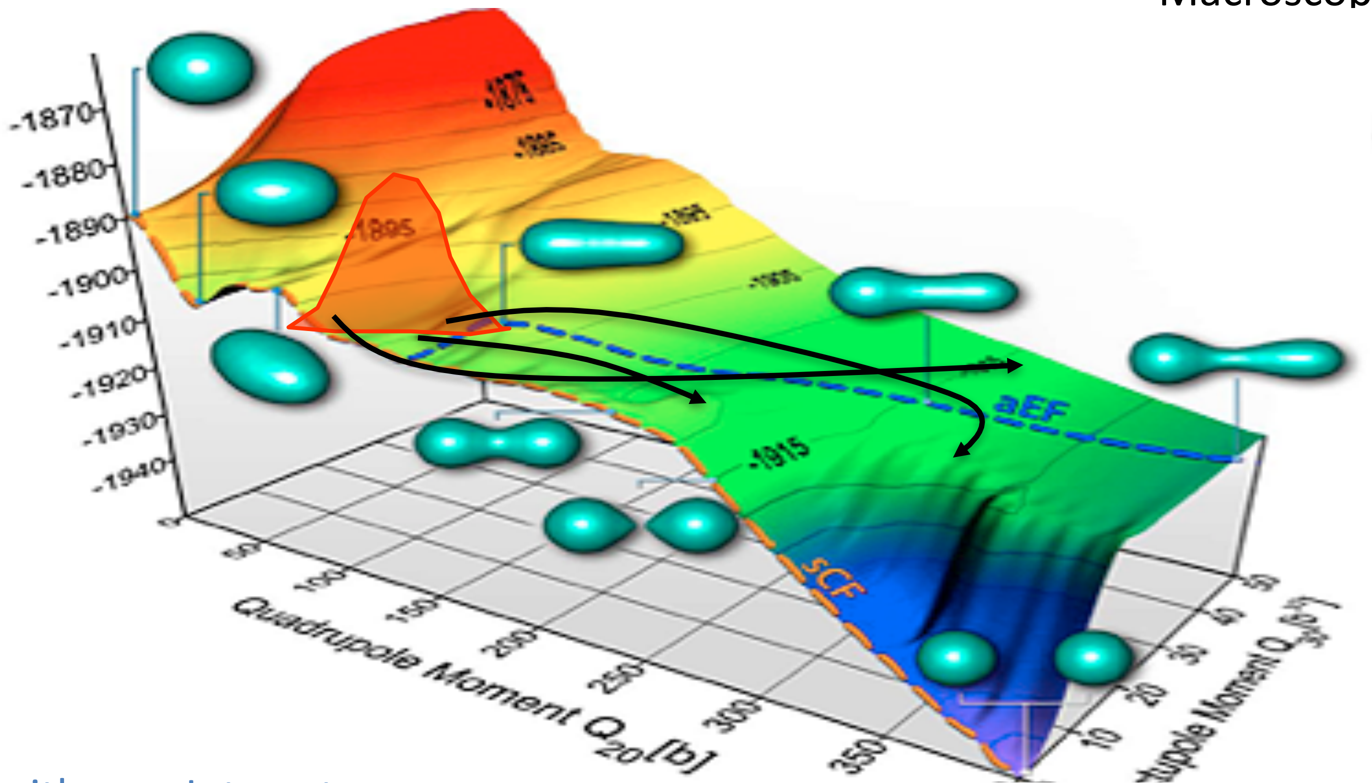
Extract one, two, …
nucleons transfer probabilities
$P_{1n}, \ P_{2n}, \ldots$

Scamps, Lacroix, PRC 87 (2013).



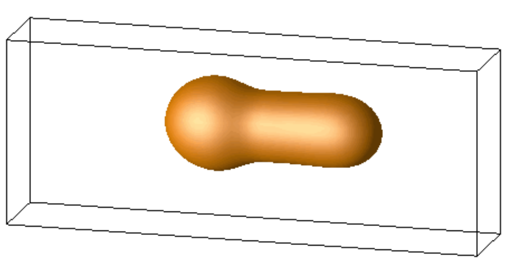
Fission process

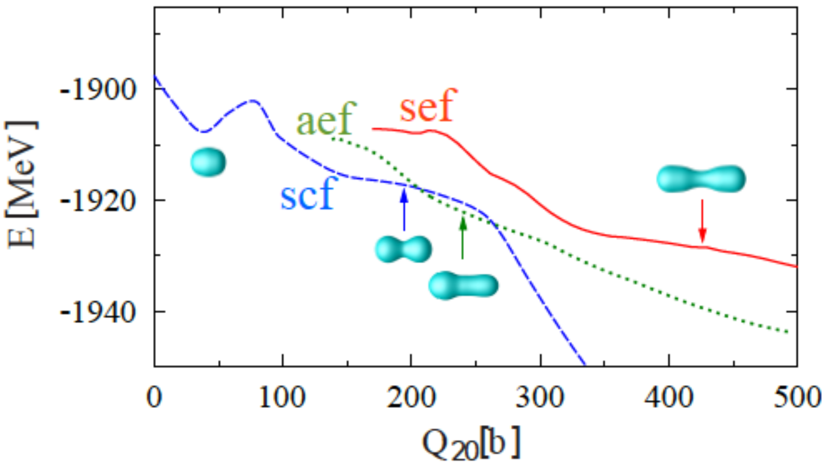
Macroscopic picture

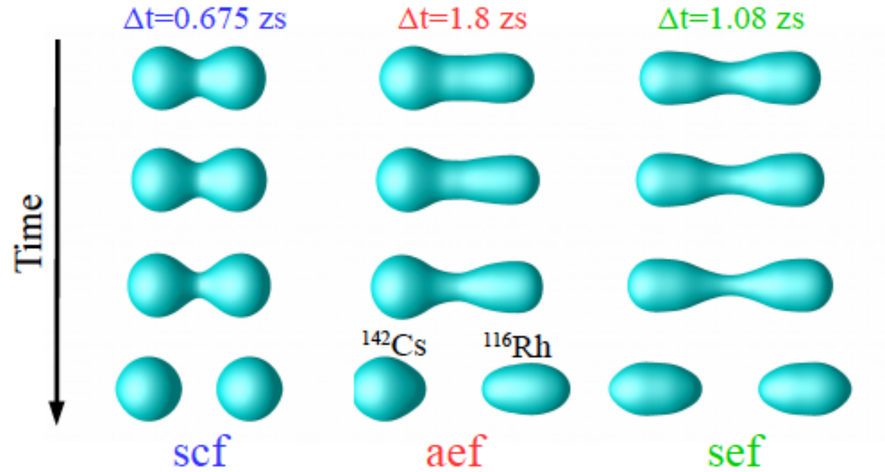


Direct contact with exp. Interest:

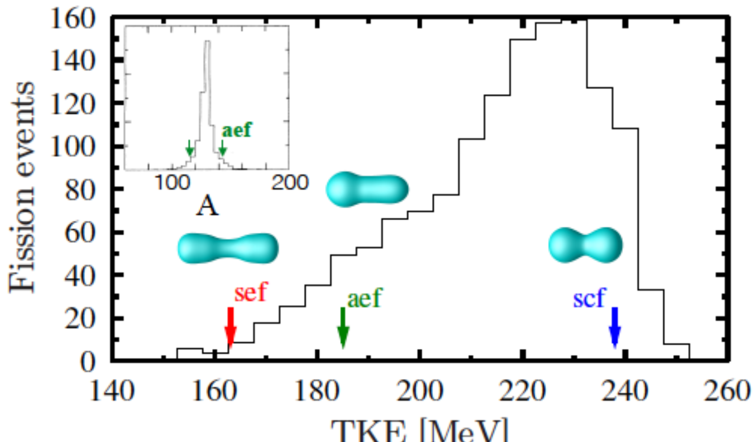
- The many-body facets of fission
- Fission life-time
- Exotic nuclei production
- Nuclear reactors





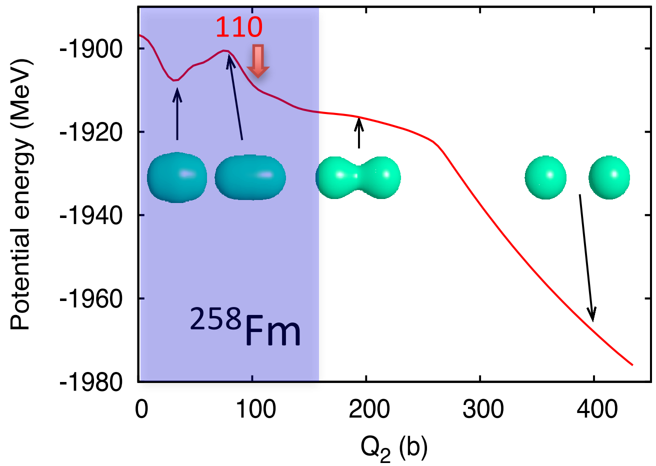


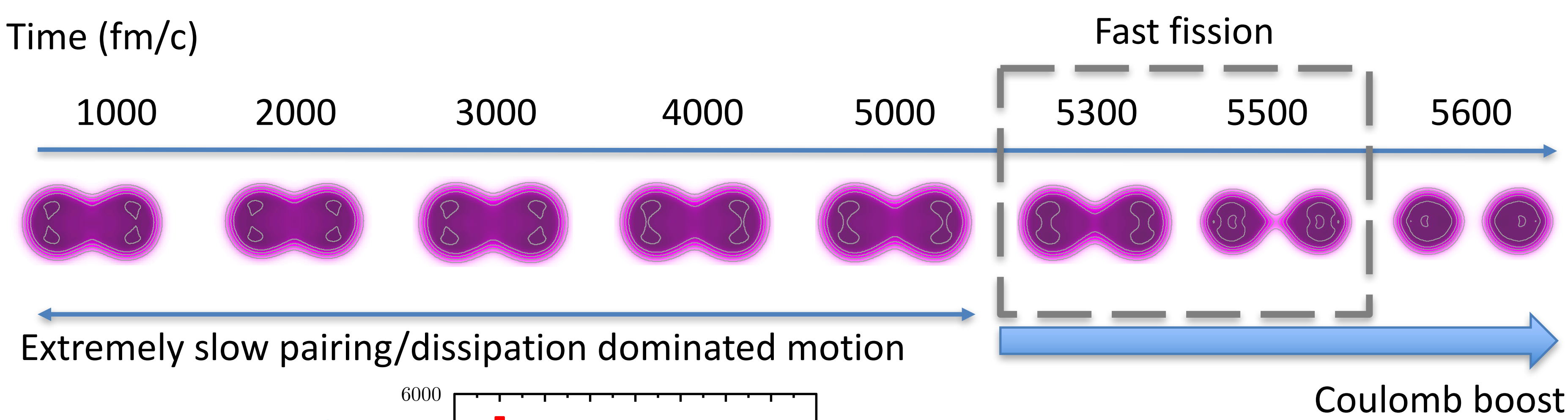
Experimental kinetic energy of the fissioning fragments



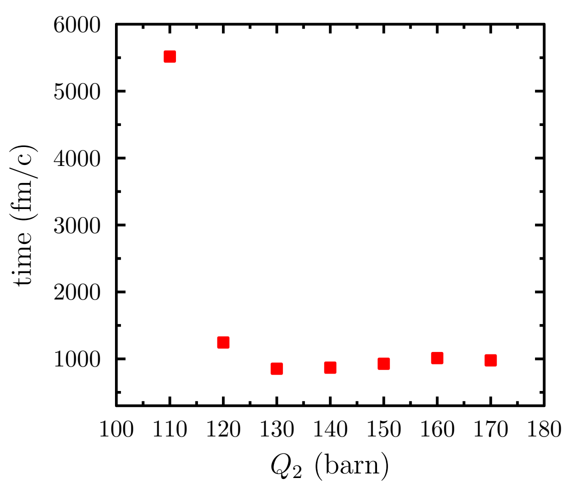
An additional remark on fission time scale:

Very sensitive to pairing type and much longer than anticipated





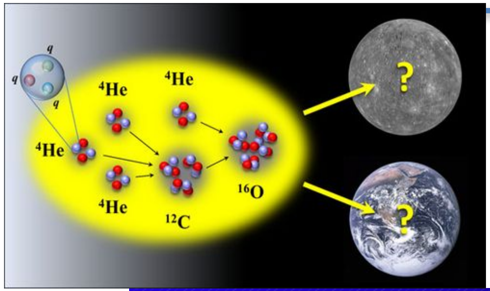
Fission time with TDHF+BCS



Confirms the finding of:

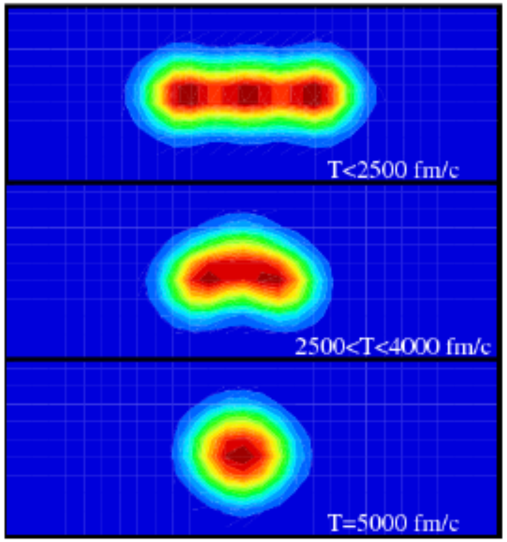
Bulgac, Magierski, Roche, and Stetcu
Phys. Rev. Lett. 116, 122504 (2016)

$$\alpha + \alpha + \alpha \rightarrow^{12} \mathrm{C}$$



Formation of ^{12}C In the Universe (also ^{16}O)

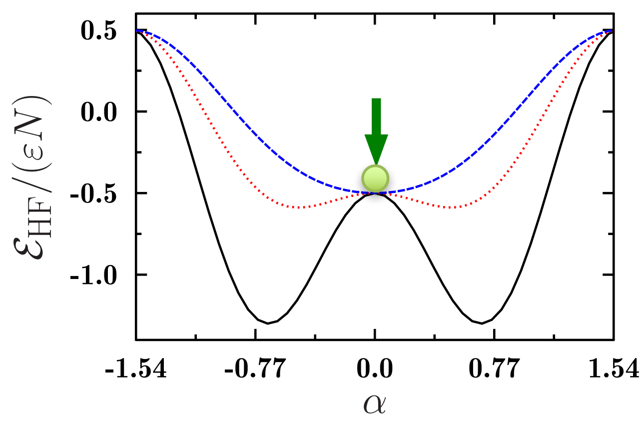
- ^{8}Be has 10^{-16}s lifetime and not found in nature
- In stars due to ^{4}He abundance small amount of ^{8}Be always present
- ^{4}He+^{8}Be combine to form resonant state of ^{12}C (Hoyle state)
- Excited state decays to ground state via an intermediate state
- Use TDHF to study the dynamics of this process



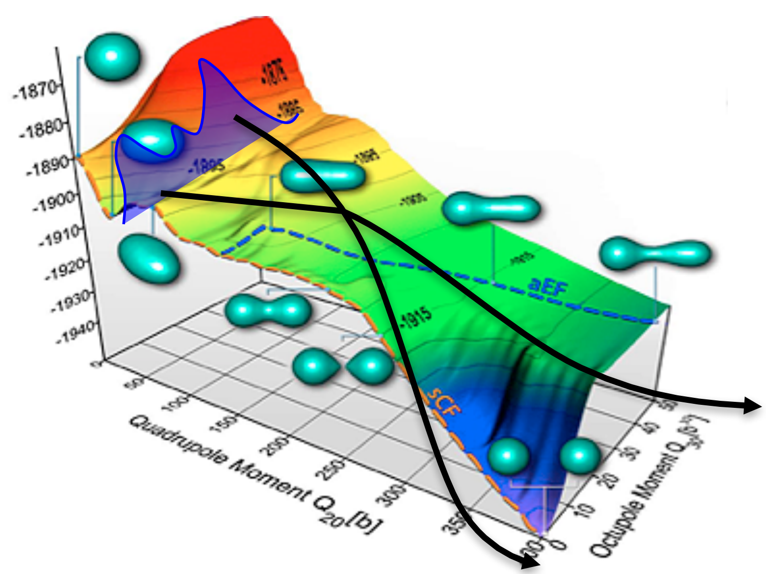
Umar, Maruhn, Itagaki, Oberaker
Phys. Rev. Lett. 104, 212503 (2010)

Beyond mean-field Approaches (deterministic and stochastic methods)

No spontaneous symmetry breaking

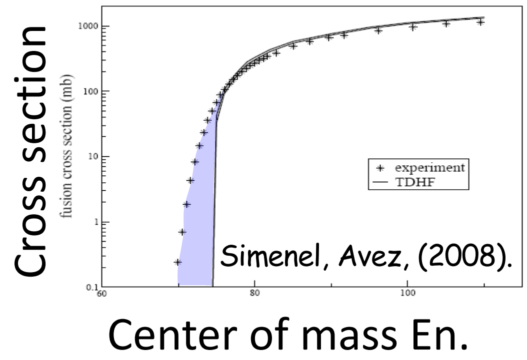


Mean-field is almost a classical theory in collective space



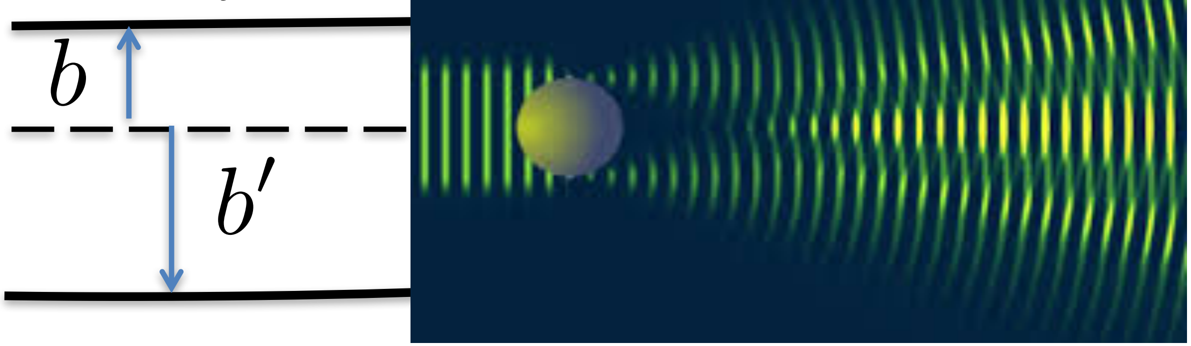
Absence of quantum effects

No tunneling in fusion cross-section

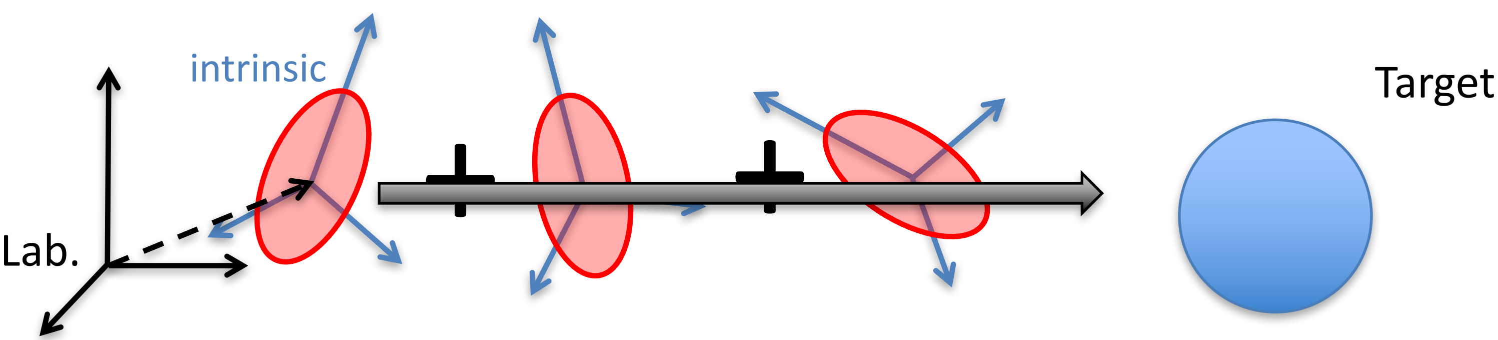


Absence of quantum interferences

Undistinguishable trajectories



Interfering trajectories can be constructive or destructive.



Beam Energy

5 MeV/A

10 MeV/A

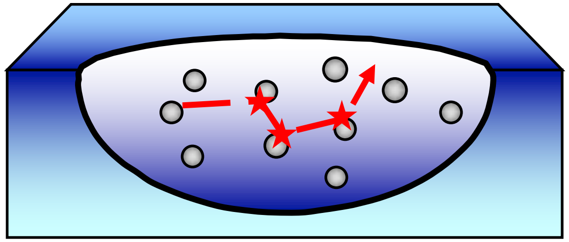
50 MeV/A

100 MeV/A

- Fusion
- Transfer★
- Break-up★ (Nuclear, Coulomb)
- Knock-out★

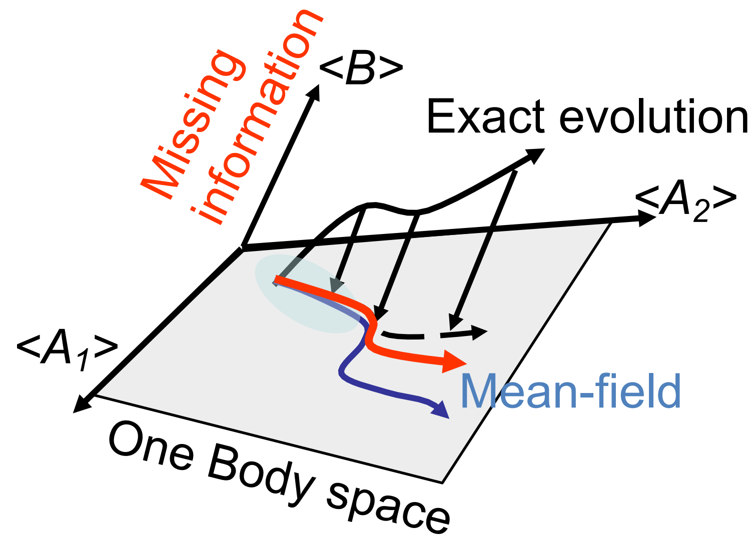
★Spectroscopic tools

Direct NN collisions



+Enhanced effect of the continuum In exotic nuclei

Y. Abe et al, Phys. Rep. 275 (1996)
DL, Ayik, Chomaz , Progress in Part. and Nucl. Phys. 52 (2004)



Short time evolution

$$i\hbar\frac{d}{dt}\rho_1 = [h_{MF},\rho_1] + Tr_2[v_{12}, C_{12}]$$

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

Correlation

$$C_{12} = \rho_{12} - (\rho_1\rho_2)_A$$

Approximate long time evolution+Projection (Nakajima-Zwanzig)

$$i\hbar\frac{d}{dt}\rho_1 = [h_{MF},\rho_1] + Tr_2[v_{12}, C_{12}]$$

with

$$C_{12}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} U_{12}(t,s) F_{12}(s) U_{12}^{\dagger}(t,s)\, ds + \delta C_{12}(t)$$

projected two-body effect

Propagated initial correlation

Dissipation (Extended TDHF)

$$i\hbar\frac{d}{dt}\rho = [h_{MF},\rho] + K(\rho)$$

Dissipation and fluctuation

$$i\hbar\frac{d}{dt}\rho = [h_{MF},\rho] + K(\rho) + \delta K(\rho)$$

Random initial condition

$$i\hbar\frac{\partial}{\partial t}\rho_1 = [h_1[\rho],\rho_1] + \frac{1}{2}\mathrm{Tr}_2[\bar{v}_{12}, C_{12}]$$

with

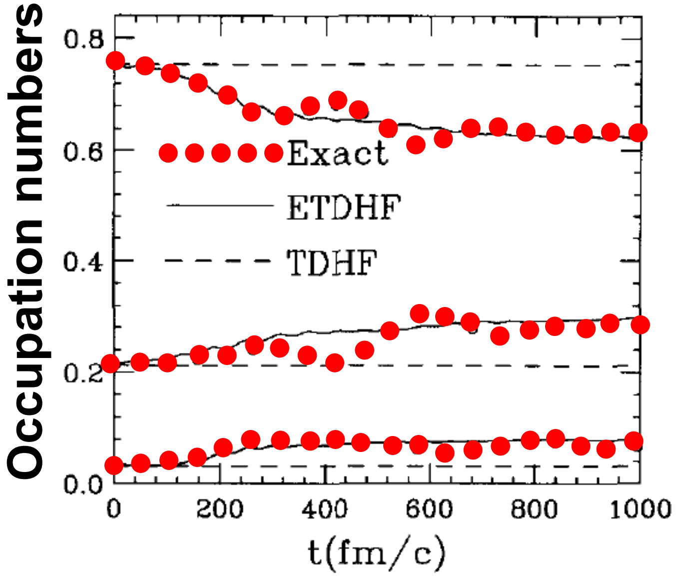
$$C_{12}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} U_{12}(t,s)\, F_{12}(s)\, U_{12}^{\dagger}(t,s)\, ds + \delta C_{12}(t)$$

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

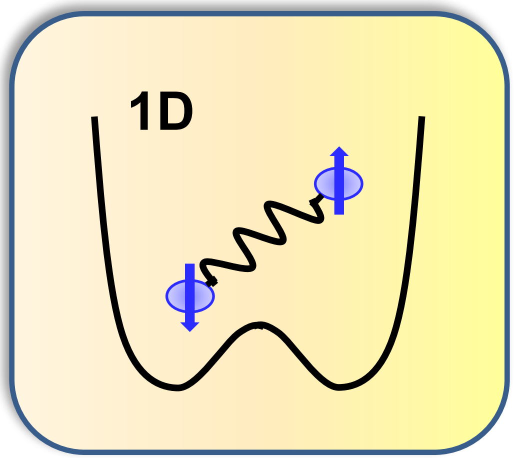
Non-Markovian master equation

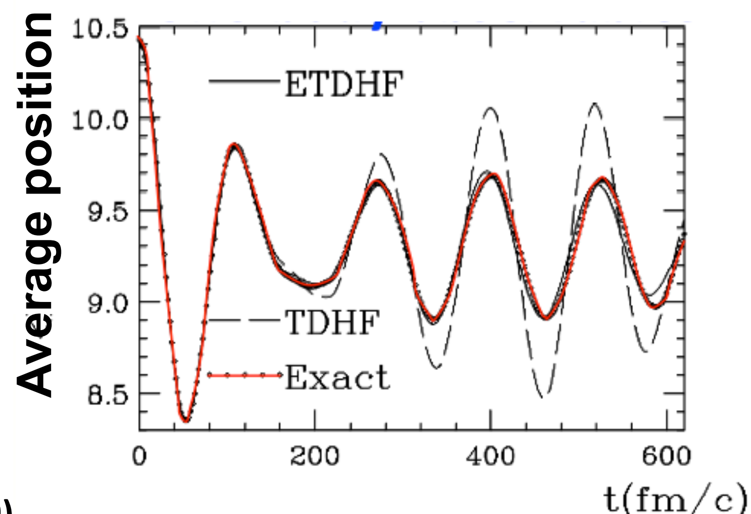
$$\frac{d}{dt}n_\lambda(t) = \int_{t_0}^{t} dt' \left\{\bar{n}_\lambda(t')\, \mathcal{W}_\lambda^{+}(t,t') - n_\lambda(t')\, \mathcal{W}_\lambda^{-}(t,t')\right\}$$

Occupation number evolution



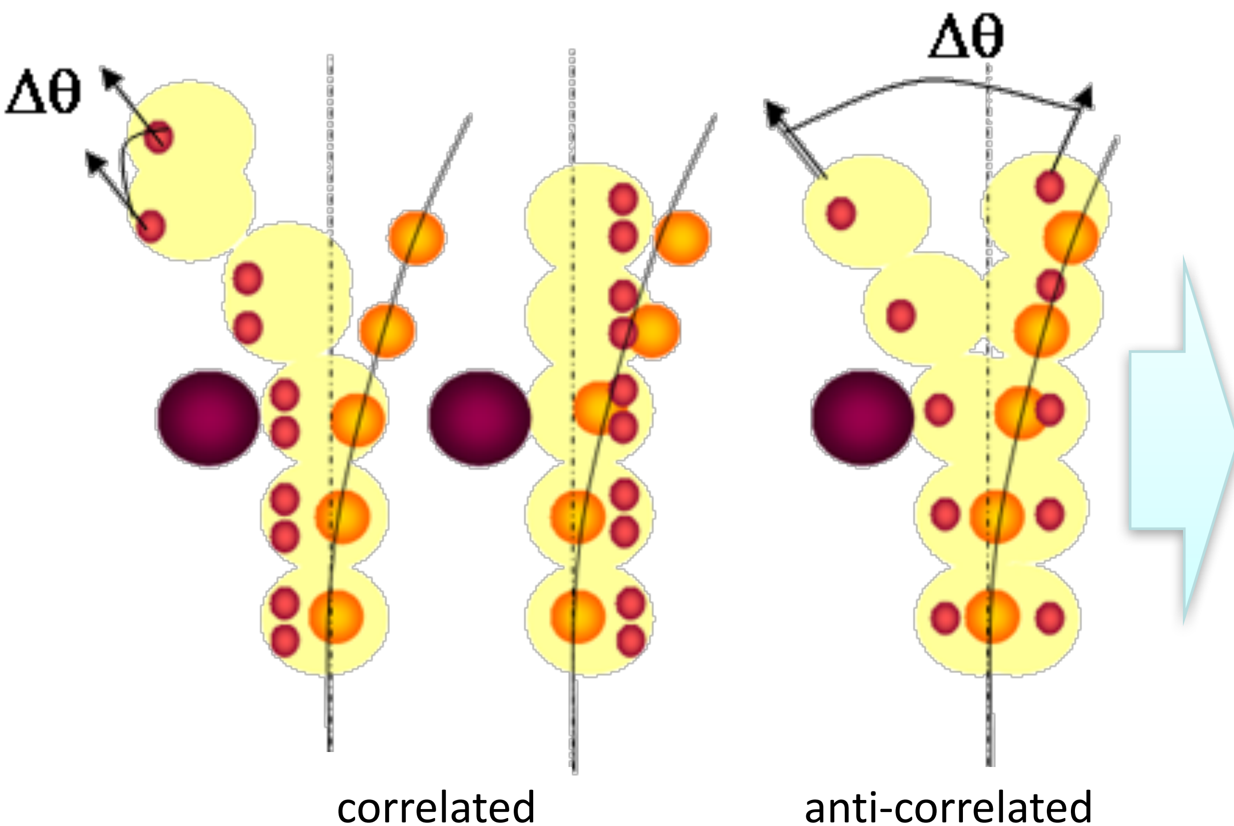
Example: two interacting fermions in 1dimension

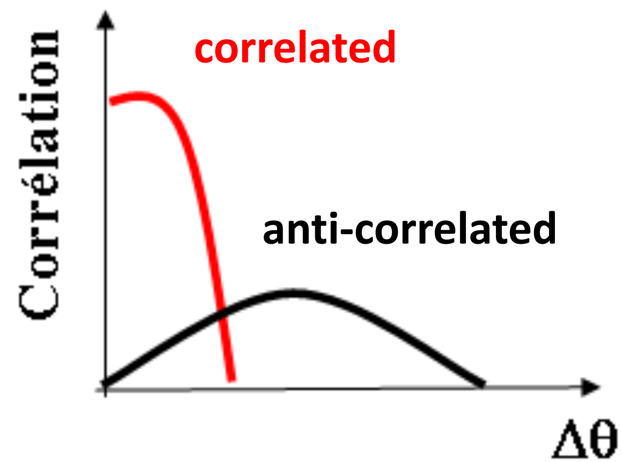




DL, Chomaz, Ayik, Nucl. Phys. A (1999).

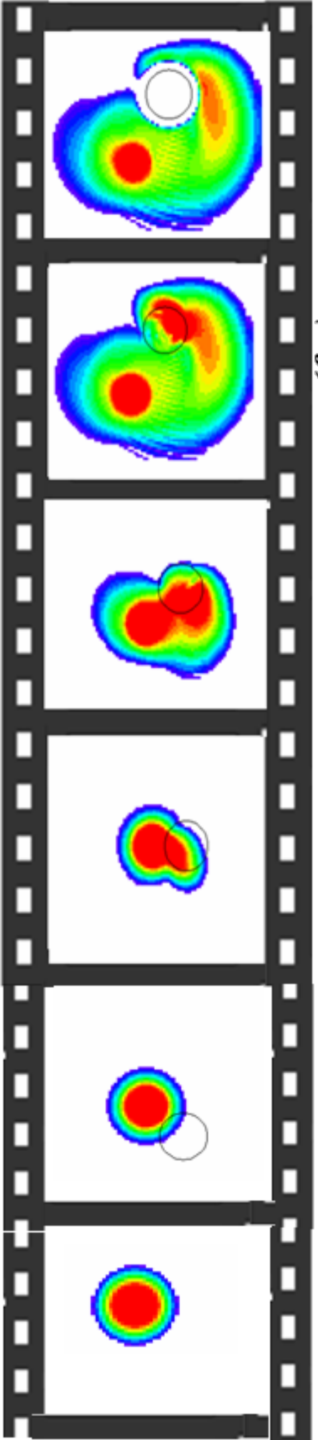
Physical Intuition

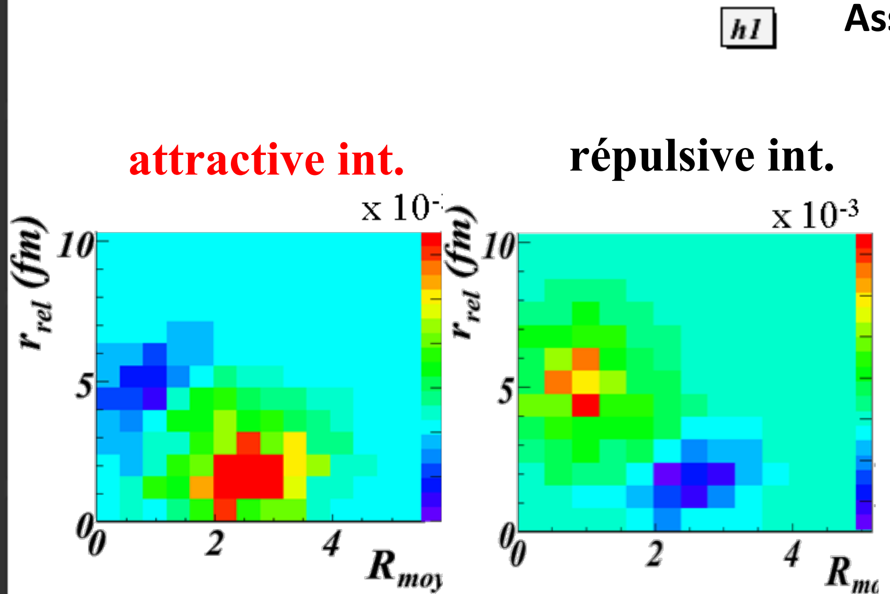


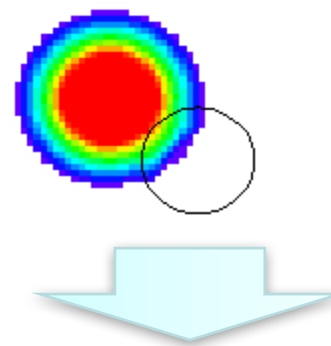


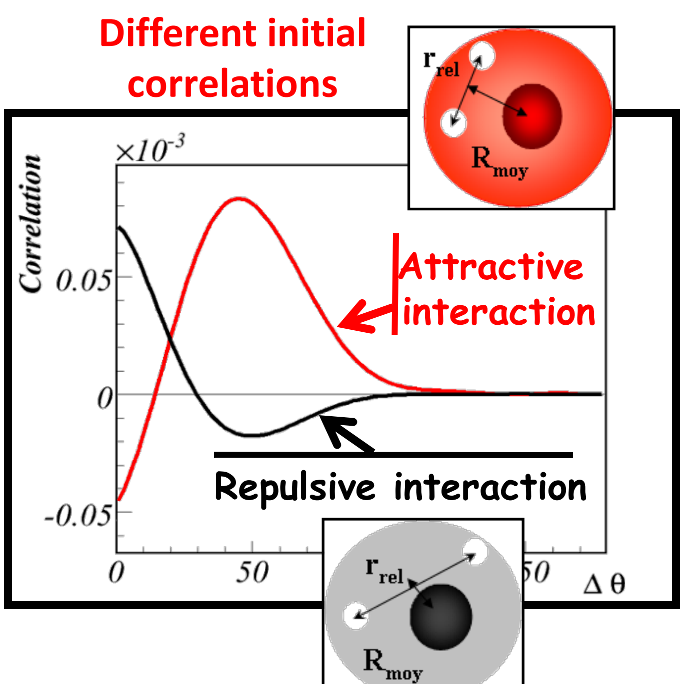
Nuclear break-up of correlated systems

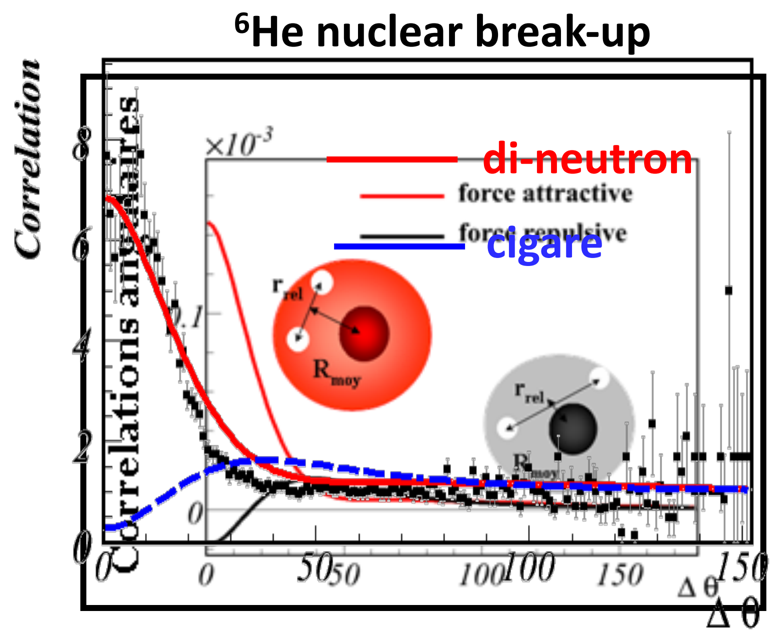
Assié, Lacroix, PRL (2009), arXiv:0901.0848





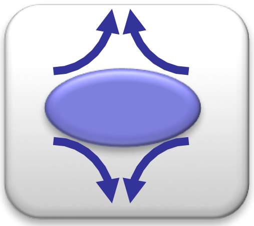


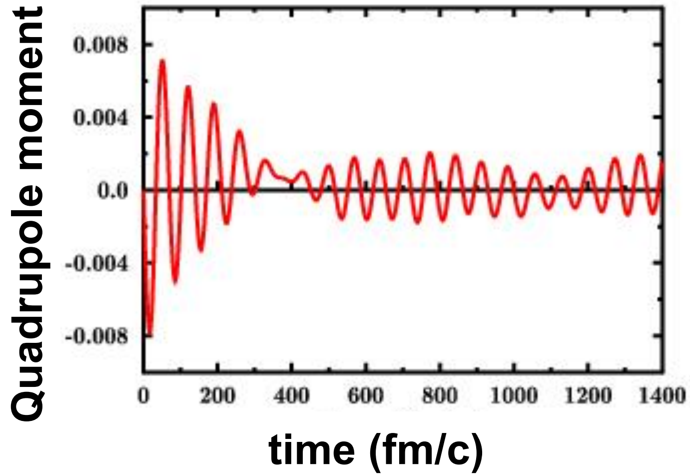




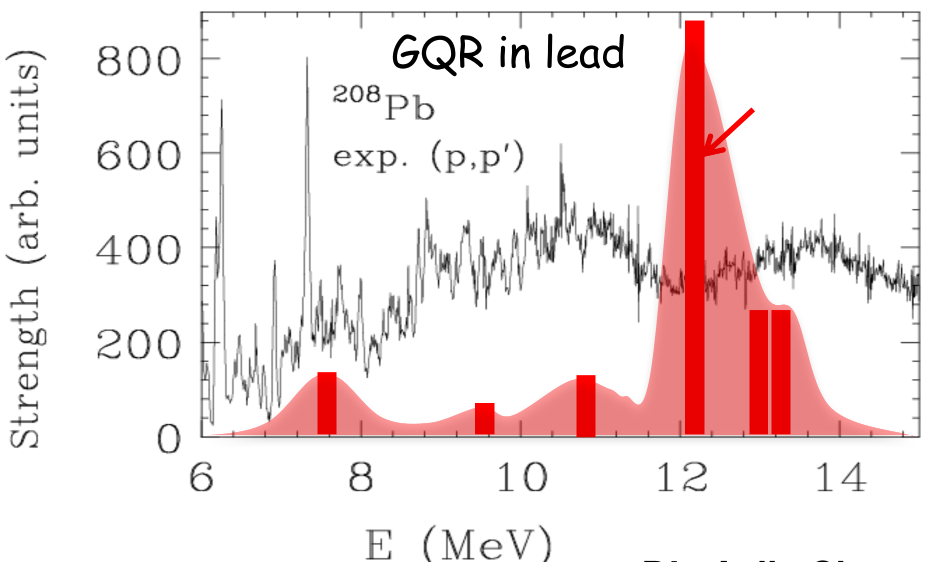
Assié, Scarpaci et al, EPJA (2009)

application to collective motion





Giant Quadrupole resonances

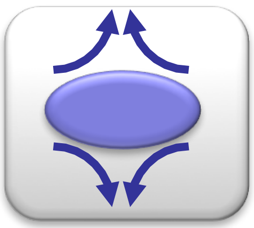


Mean energy is OK

Damping (dissipation) and fragmentation is missed

DL, Ayik, Chomaz, Prog. Part and Nucl. Phys. (2004)

application to collective motion

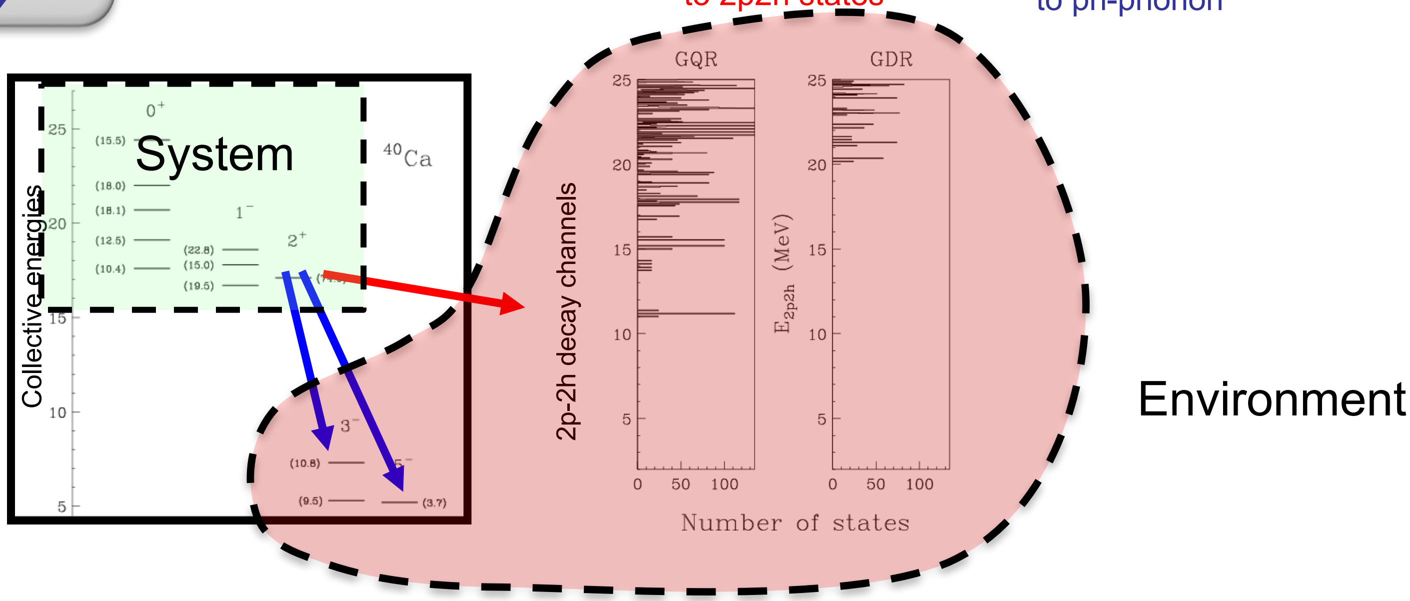


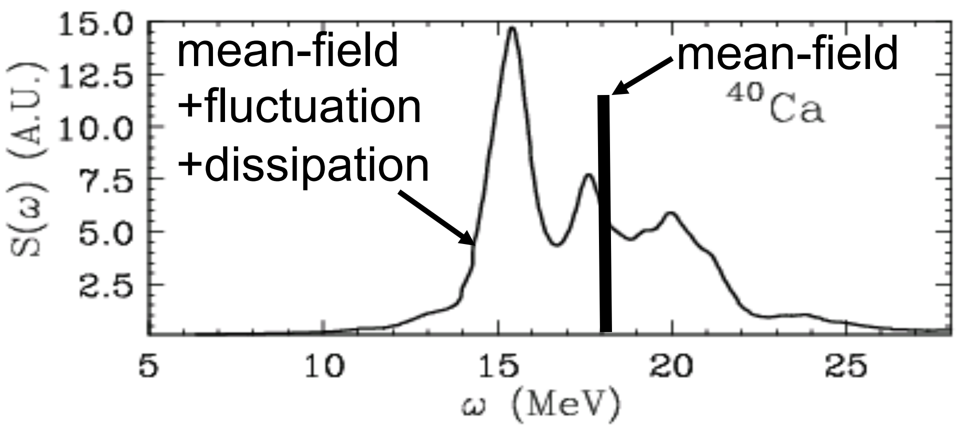
$$i\hbar\frac{\partial}{\partial t}\rho^{(n)} - [h(\rho^{(n)}), \rho^{(n)}] = K_I(\rho^{(n)}) + \delta K^{(n)}(t)$$

Mean-field

Coupling to 2p2h states

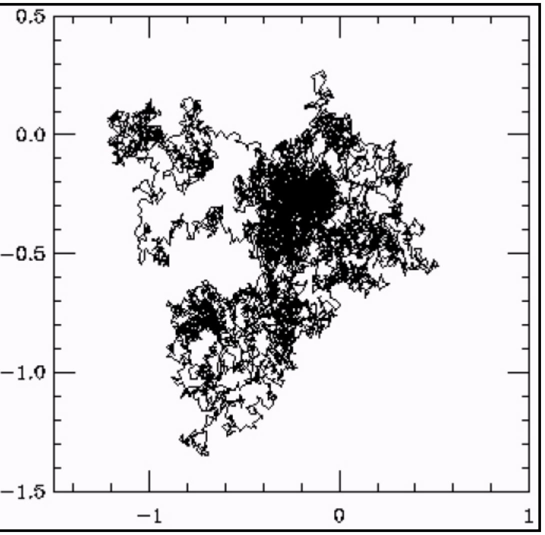
Coupling to ph-phonon





Incorporate dissipation in many-body system

Not so easy to use in Large amplitude Collective motion



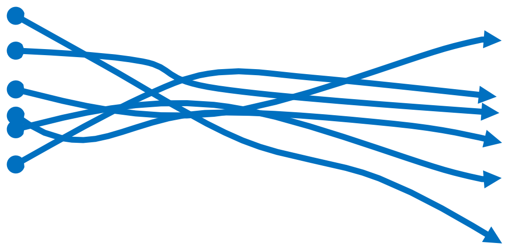
Stochastic methods

- To treat quantum fluctuations (stochastic mean-field)
- To treat direct two-body collisions (stochastic TDHF)
- To treat all correlations (Auxiliary field quantum Monte-Carlo)

Question: Is it possible to recover some of the quantum mechanics aspects by considering an ensemble of independent mean-field trajectories?

Stochastic Mean-Field

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



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

Stochastic TDHF

$|\Phi\rangle\langle\Phi|$

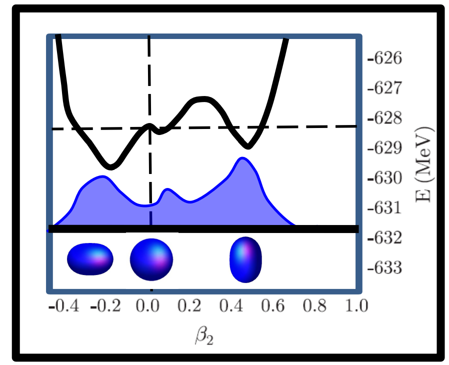
$\overline{|\Phi\rangle\langle\Phi|}$

Quantum Monte-Carlo

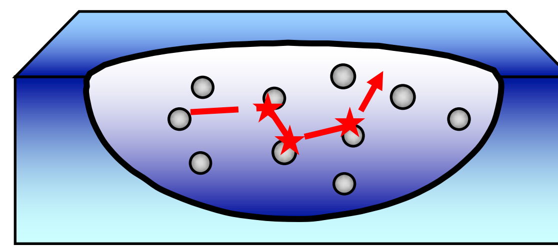
$|\Phi\rangle\langle\Phi|$

$\overline{|\Phi_a\rangle\langle\Phi_b|}$

Initial fluctuations



Correlations that built up in time
Direct NN collisions



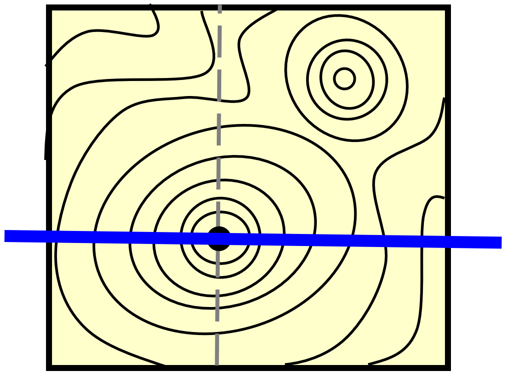
All Correlations

D. Lacroix and S. Ayik EPJA Review (2016)

Including quantum fluctuations
(Phase-space methods)

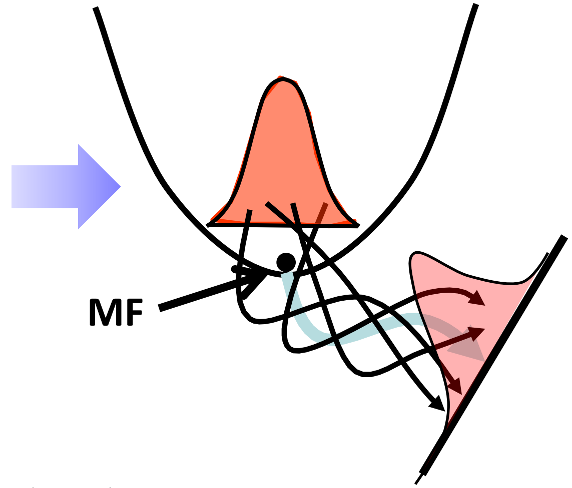
Strategy to construct a stochastic mean-field theory

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

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

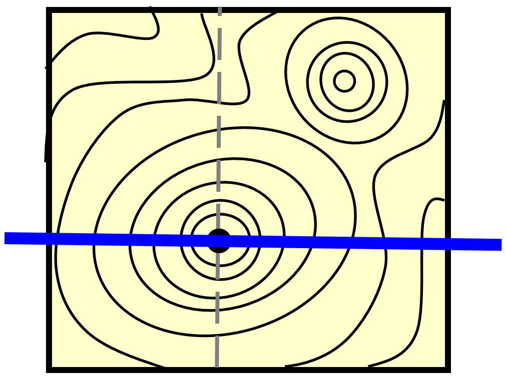
$$\{A_\alpha^{(n)}\}$$

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

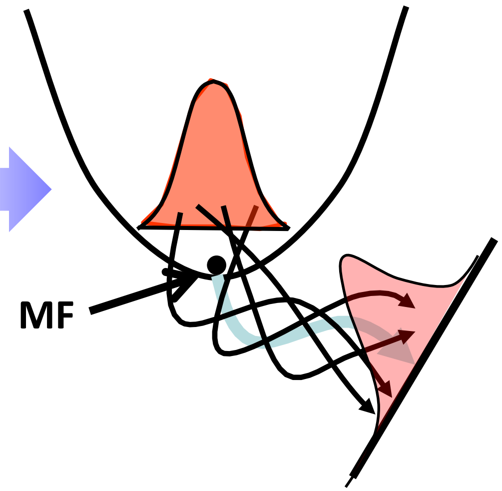
Constraint: $$\Sigma_C^2(t=0) = \sigma_Q^2(t=0)$$

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

Collective phase-space



Quantum fluctuations



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

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

The average properties of initial sampling should identify with properties of the mean-field.

SMF in density matrix space

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

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

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

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

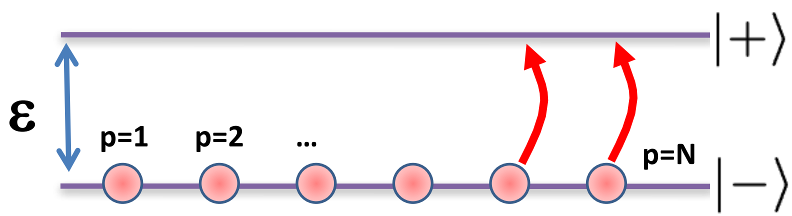
SMF in collective space

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

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

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

Lipkin Model



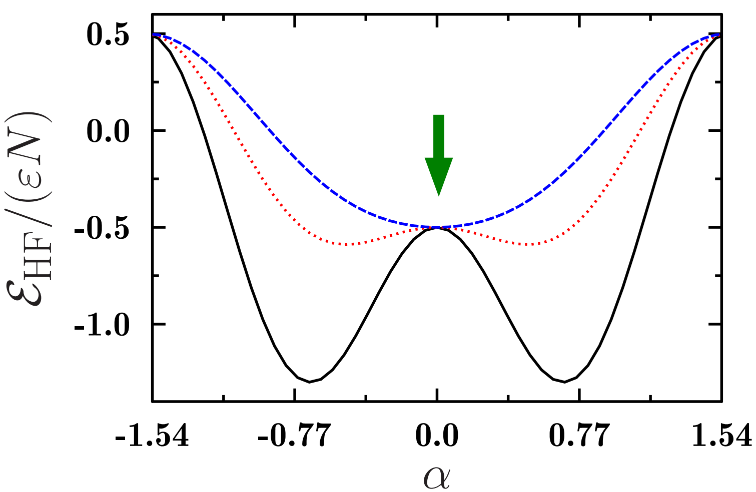
$$H = \varepsilon J_0 - \frac{V}{2}(J_+J_+ + J_-J_-)$$

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

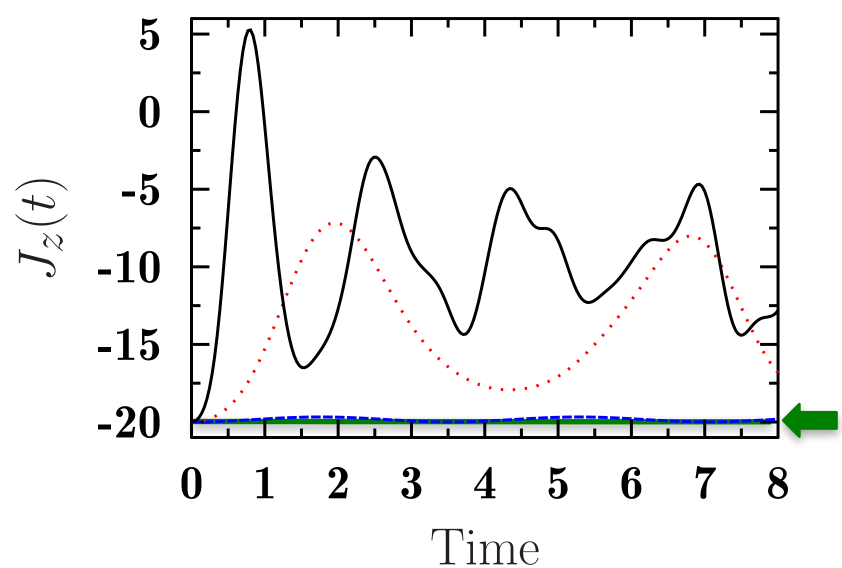
$$J_+ = \sum_{p=1}^{N} c^\dagger_{+,p}c_{-,p}, \quad J_- = J_+^\dagger, \qquad J_x = \frac{1}{2}(J_+ + J_-)$$

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

N=40 particles

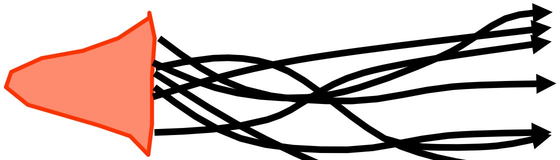


Exact dynamics

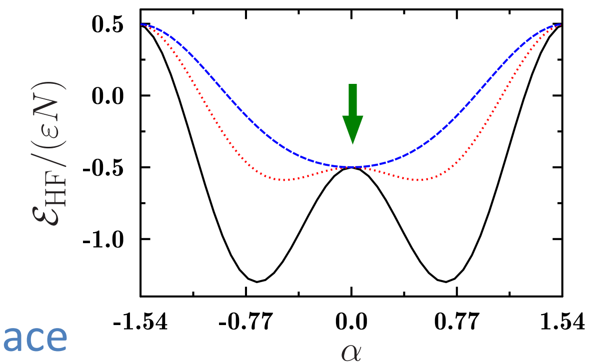


Mean-field is stationary

The stochastic mean-field solution



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



One-body observables

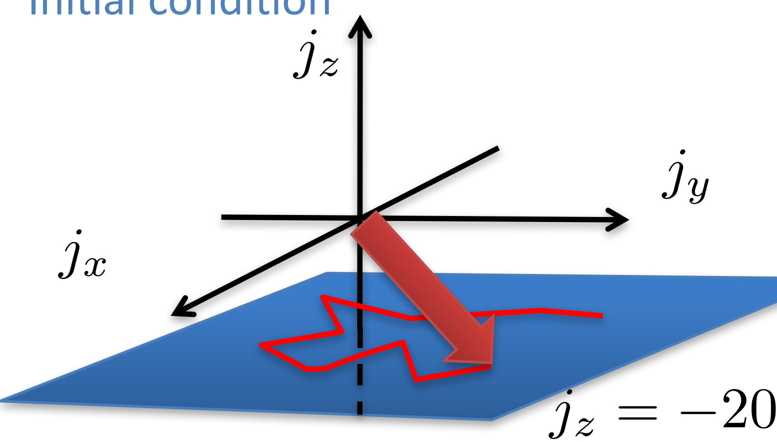
Formulation in quasi-spin space

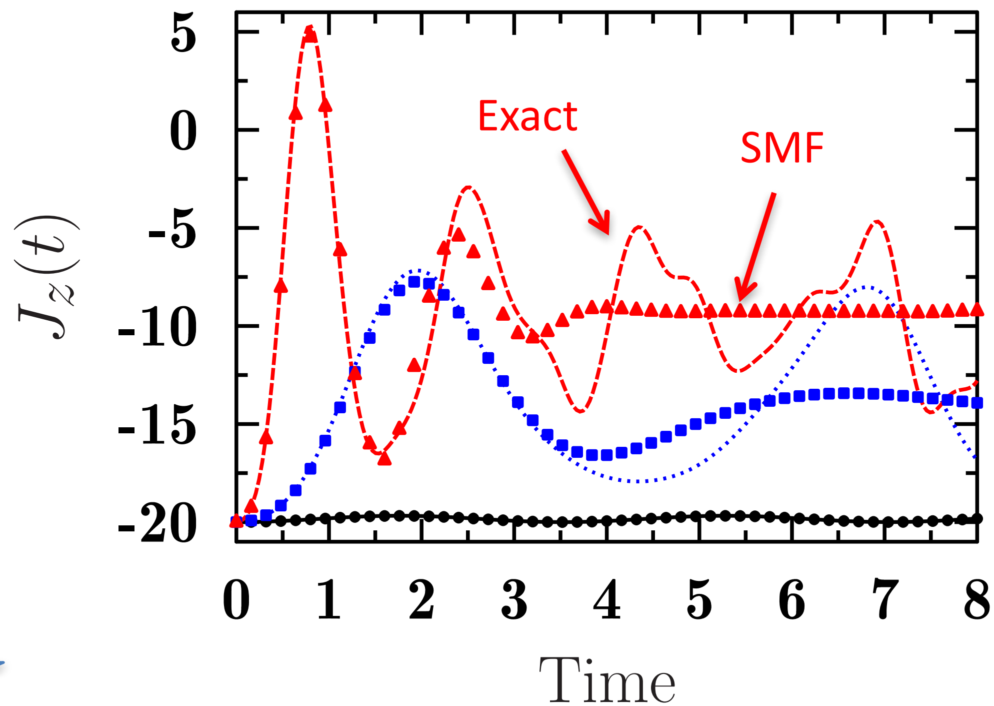
$$j_i \equiv \langle J_i \rangle / N \quad \Rightarrow \quad j_i^{\lambda}$$

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

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

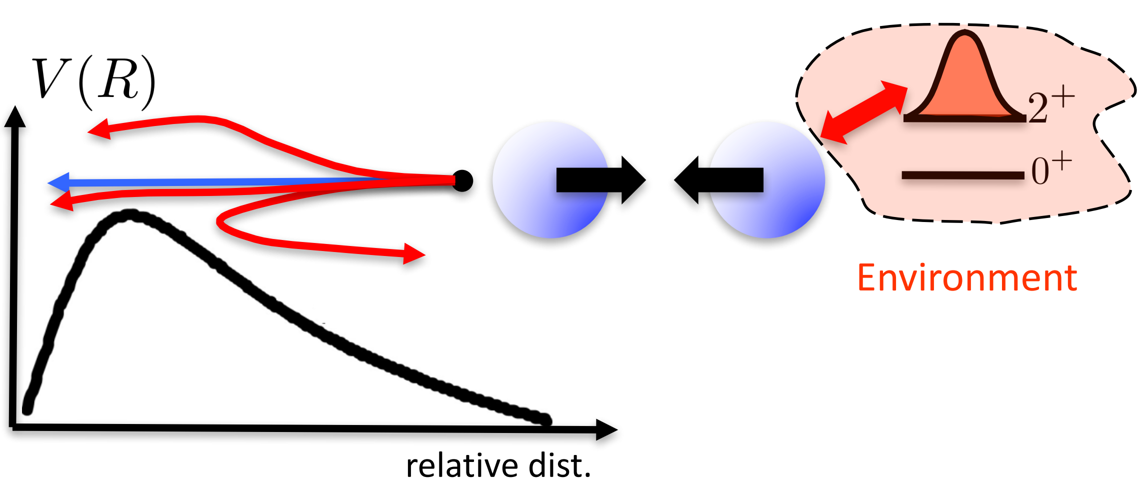
Initial condition

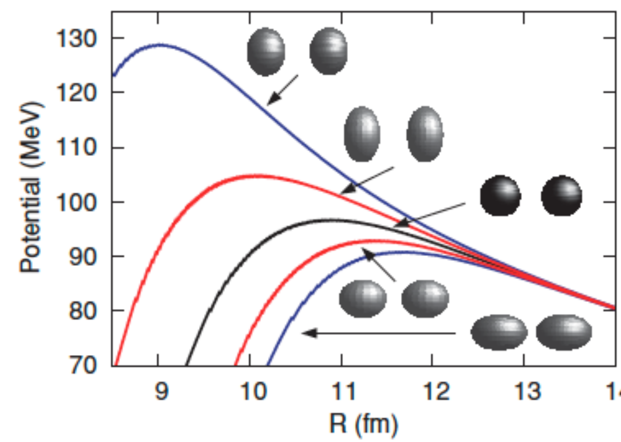




Lacroix, Ayik, Yilmaz, PRC 85 (2012)

Stochastic semi-classical treatment of discrete channels



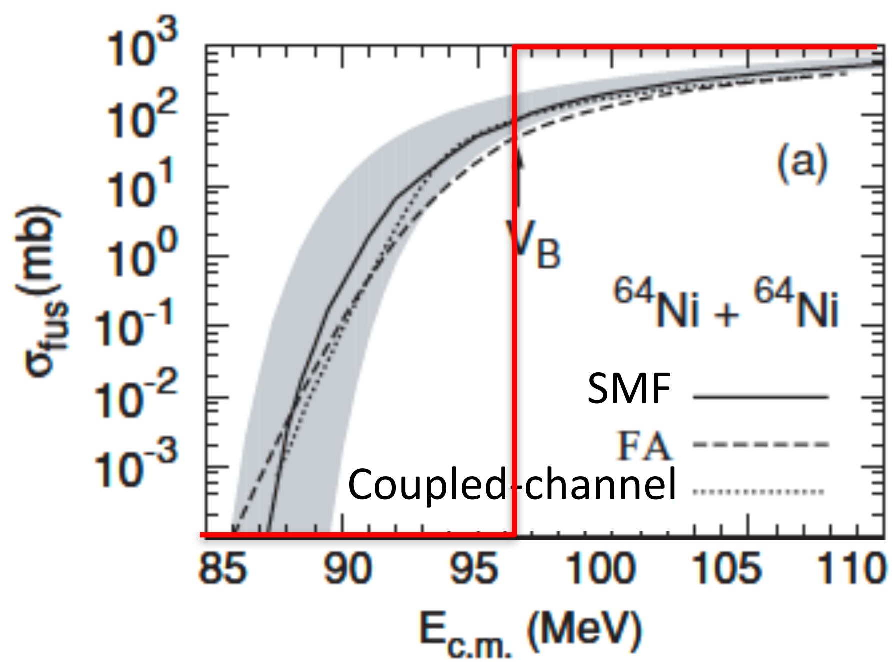


Collective Motion + Coupling

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

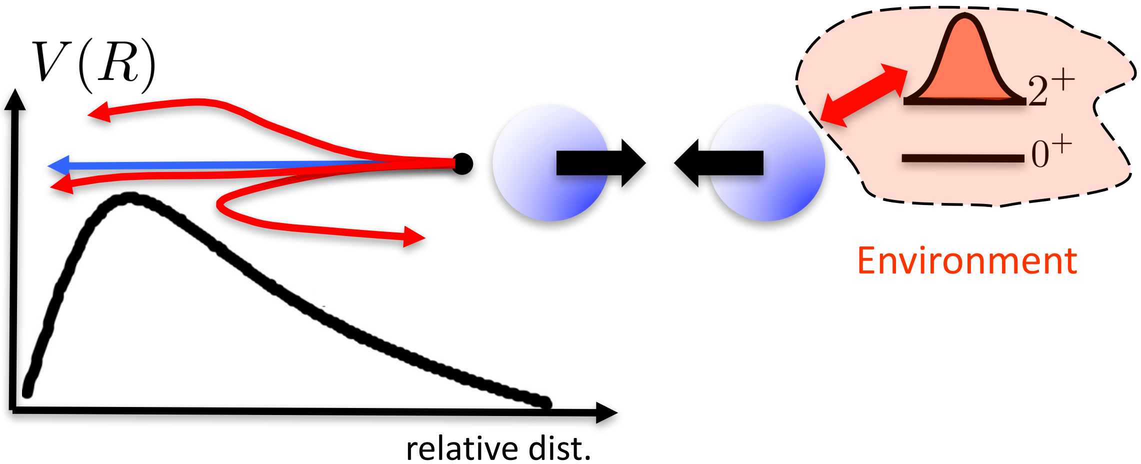
Discrete Channels

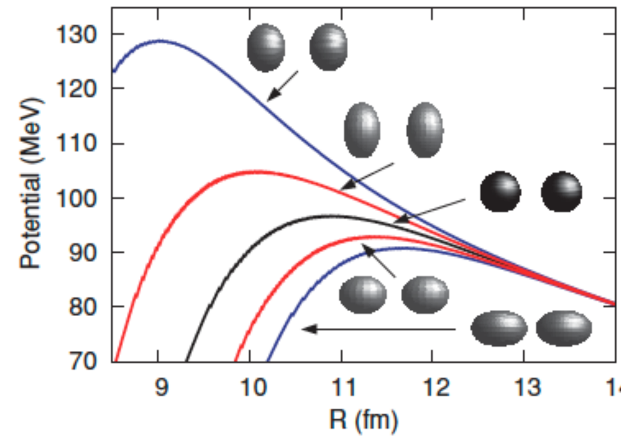
Esbensen et al, PRL 41 (1978)



Ayik, Yilmaz, Lacroix, PRC81 (2010)

Stochastic semi-classical treatment of discrete channels





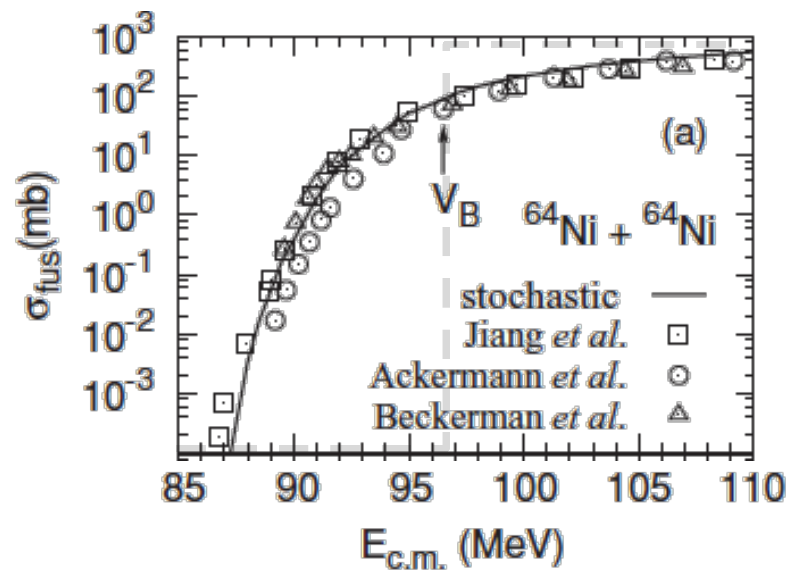
Collective Motion + Coupling

$$H = \frac{P^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu R^2} + V_C(R) + V_N(R, \Omega, \alpha_{i\lambda})$$

$$+ \sum_{i=1}^{2} \sum_{\lambda=0}^{N-1} \left[\frac{\Pi_{i\lambda}^2}{2D_{i\lambda}} + \frac{1}{2} C_{i\lambda} \alpha_{i\lambda}^2 \right],$$

Discrete Channels

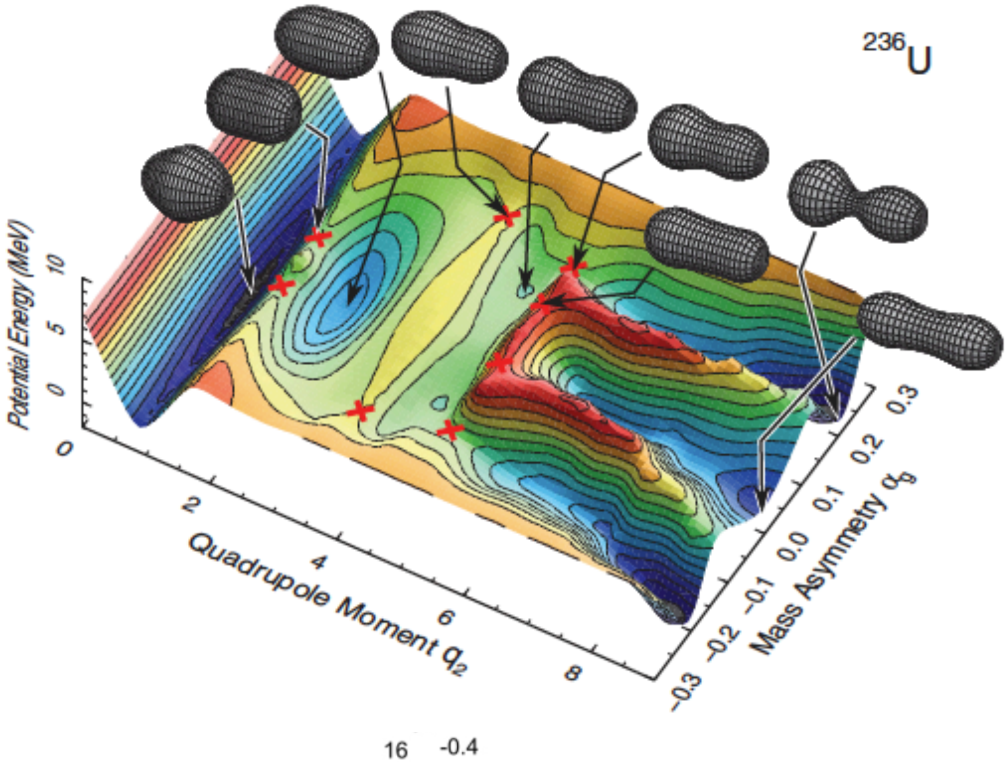
Esbensen et al, PRL 41 (1978)



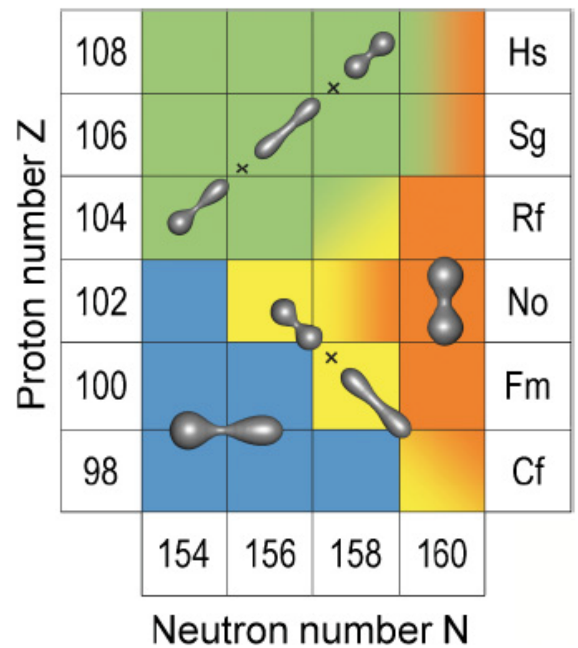
Ayik, Yilmaz, Lacroix, PRC81 (2010)

Application to fission: current quasi-static picture

Fission as a multi-dimensional process



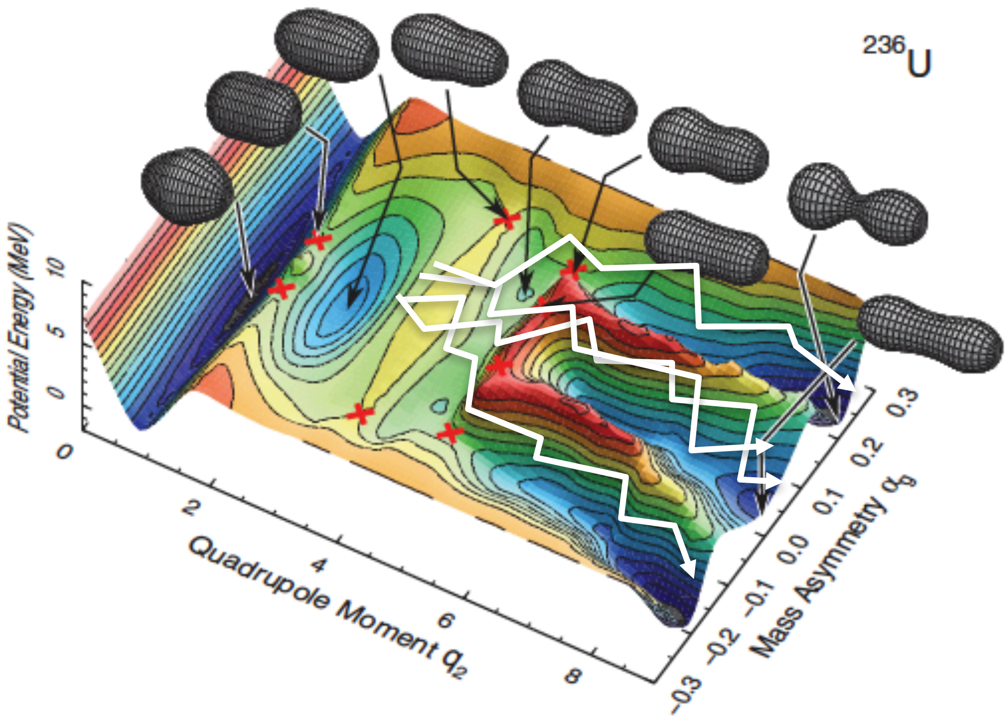
T. Ichikawa, Iwamoto, Möller, and Sierk, Phys. Rev. C 86 (2012)



Staszczak, Baran, Dobaczewski, and Nazarewicz Phys. Rev. C 80, 014309 (2009)

- Several fission paths
- Emergence of the notion of fission modes (multimodal fission)
- Beyond the quasi-static picture?

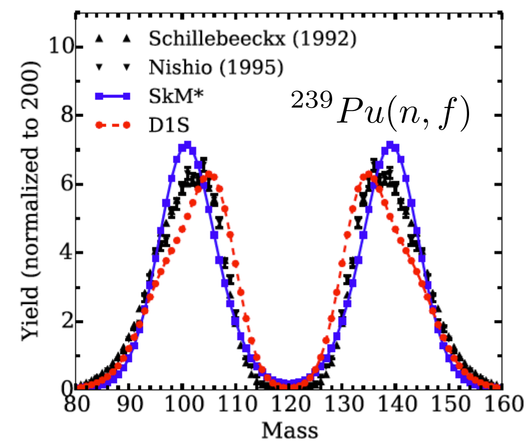
How modes are populated-role of dynamics?

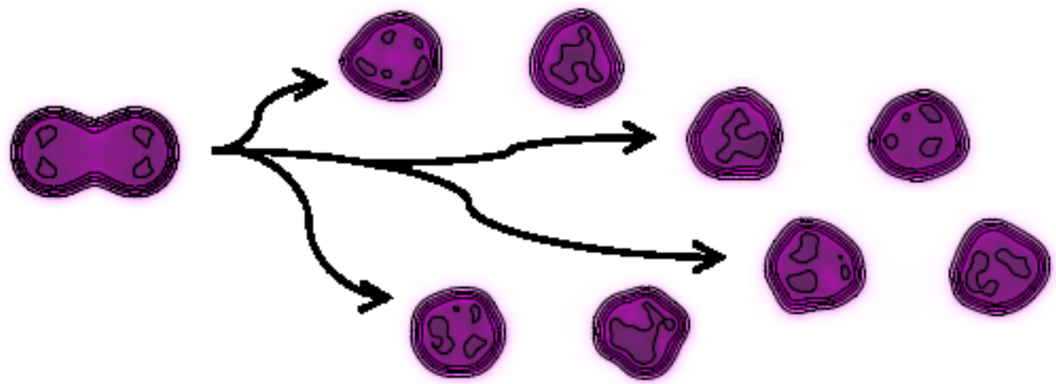


➡ Fission is a quantum dynamical Process (quantum tunneling, Entanglement…)

$$i\hbar\frac{\partial g(\mathbf{q},t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q})g(\mathbf{q},t).$$

Regnier, et al, Phys. Rev. C 93 (2016)

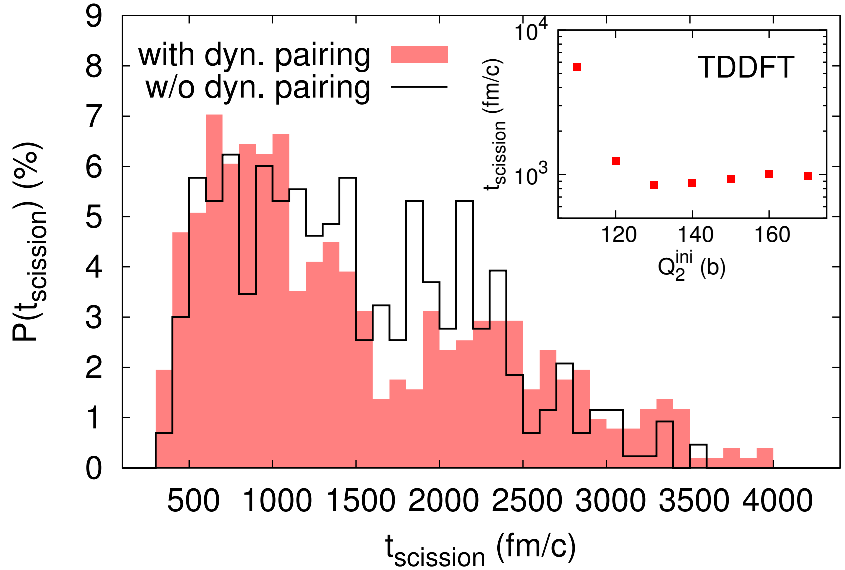




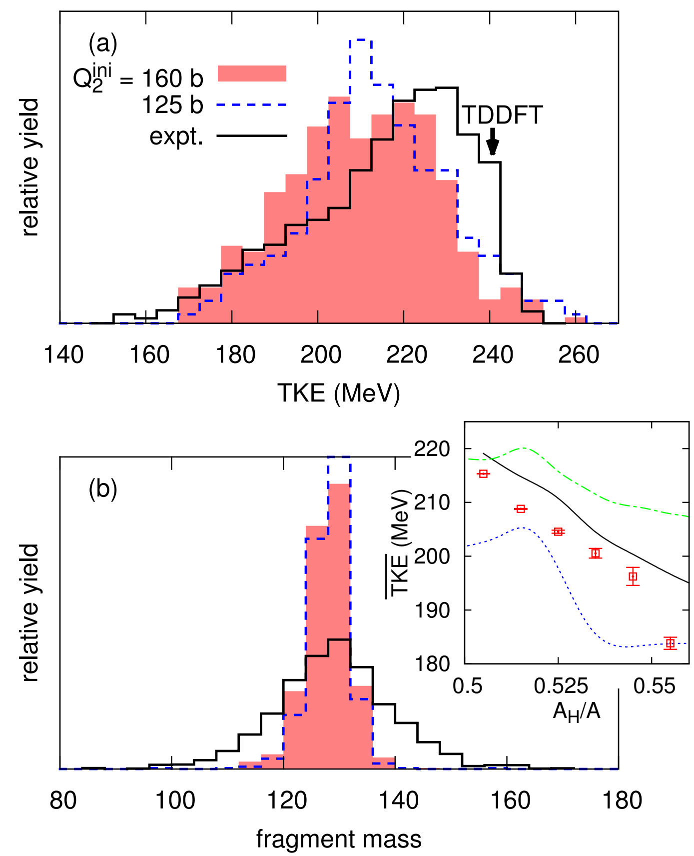
Tanimura, Lacroix, Ayik, PRL (2017)

From deterministic to statistical approach

Distribution des temps de fission



Experience vs Theory



Including binary collisions
The Stochastic TDHF method

GOAL: Restarting from an uncorrelated 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

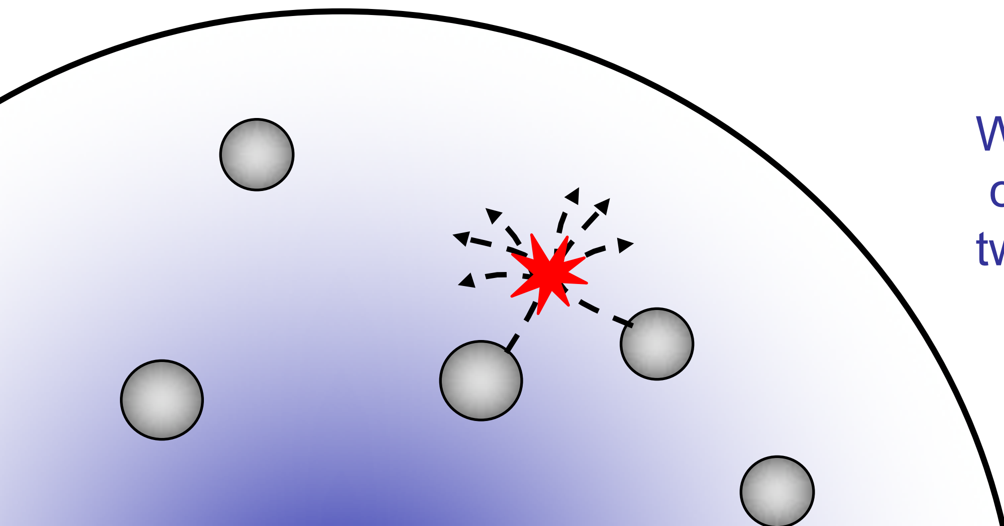
Weak coupling approximation : perturbative treatment

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

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

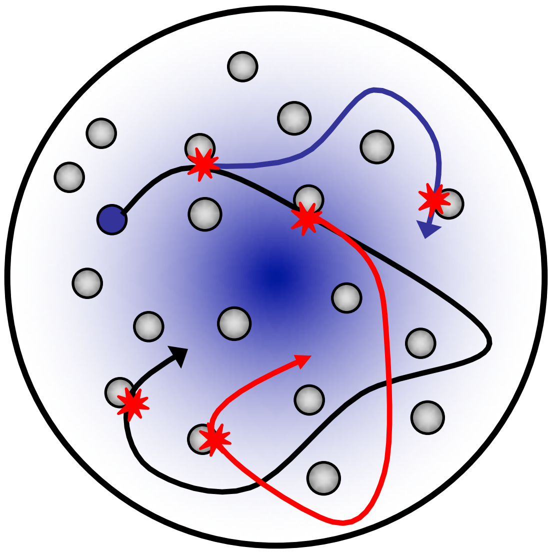
Residual interaction in the mean-field interaction picture

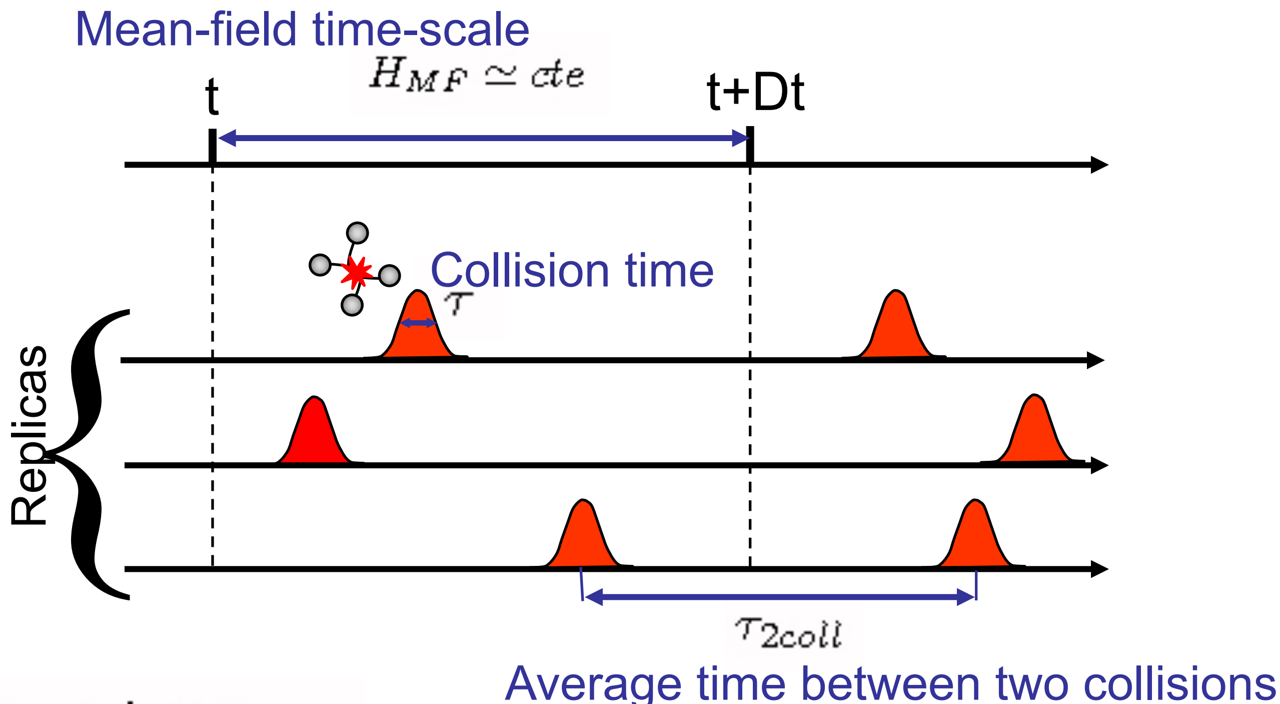
Statistical assumption in the Markovian limit :



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:

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

Dissipation: link between Extended TDHF and Lindblad Eq.

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

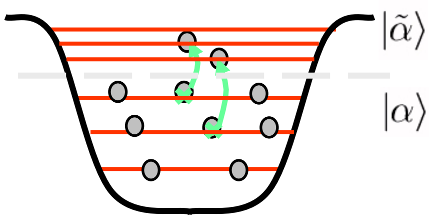
$$D = |\Phi\rangle\langle\Phi|$$

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

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

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

2p-2h nature
of the interaction



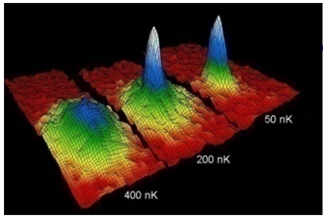
$$\mathcal{D}(\rho) = Tr_2[v_{12}, C_{12}]$$

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)*



1D bose condensate with gaussian two-body interaction

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

SSE on single-particle state :

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

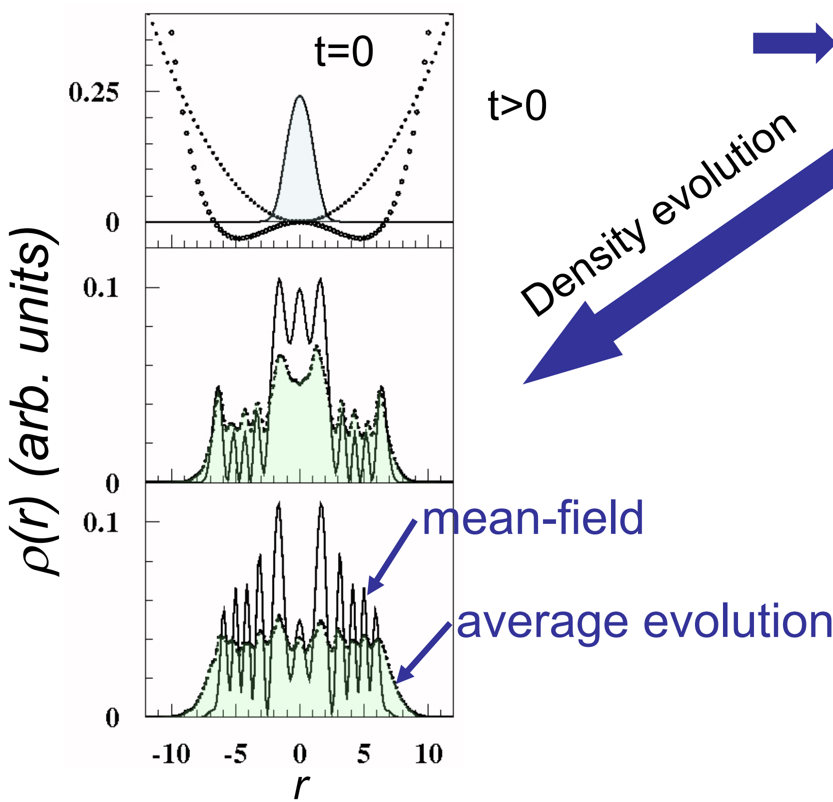
with $dW_k dW_{k'} = -\frac{dt\tau}{\hbar^2}\gamma_k \delta_{kk'}$

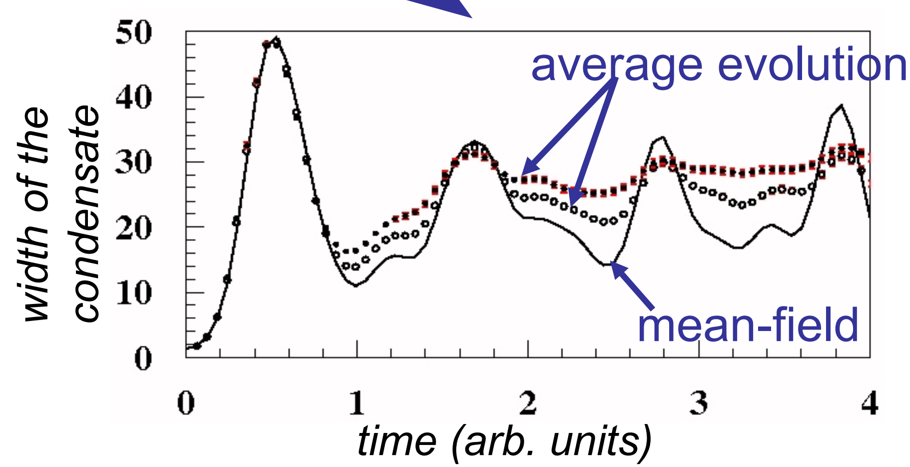
→ The numerical effort is fixed by the number of A_k

t>0

Density evolution

Condensate size

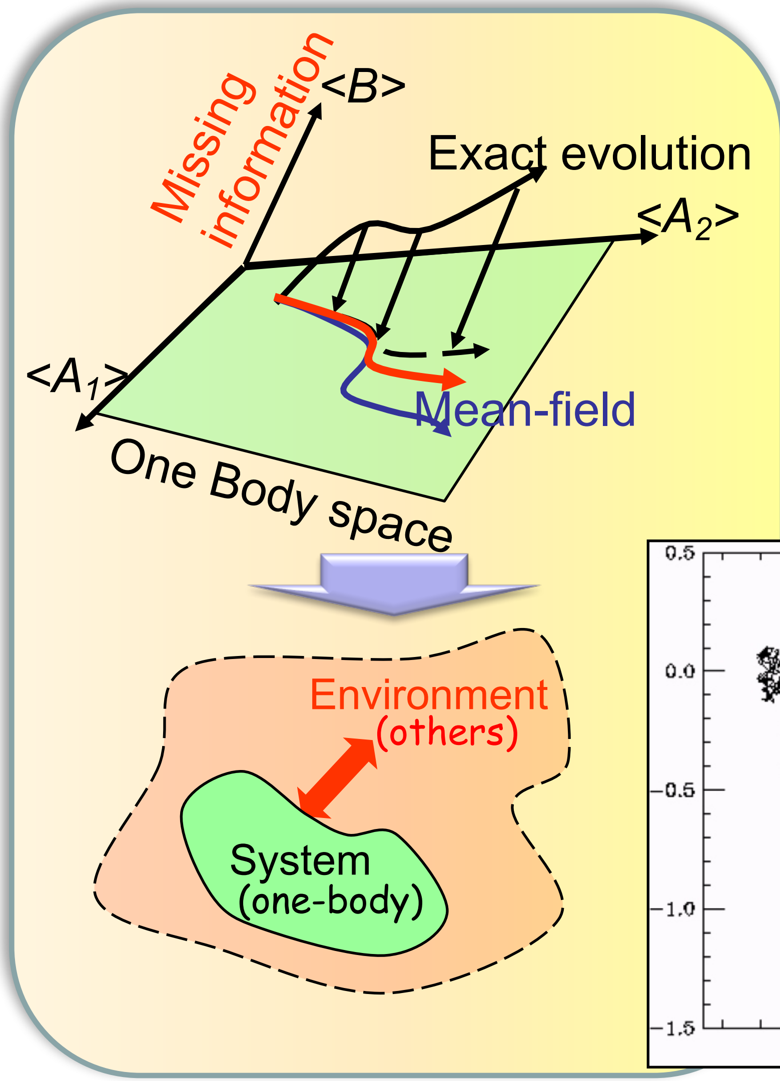




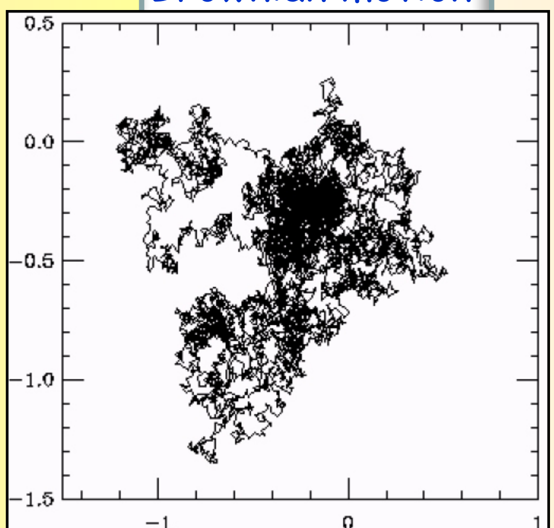
Including all correlations
The Quantum Monte-Carlo approach

Self-interacting vs Open Quantum systems

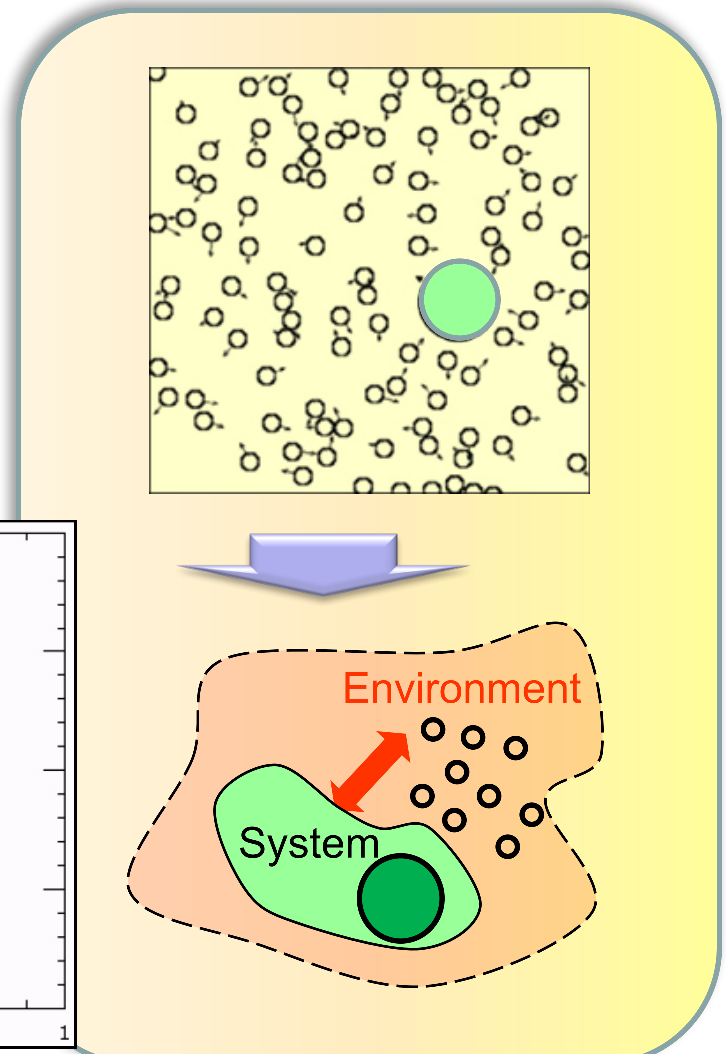
N-body



Brownian motion



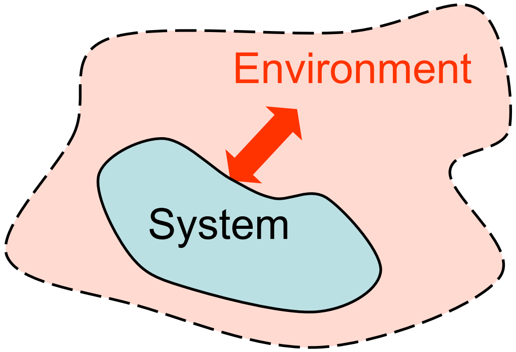
Open systems



Towards Exact stochastic methods for N-body and Open systems

Self-interacting vs Open Quantum systems

Approximate and exact Quantum jump



$$H = H_{\rm S} + H_{\rm E} + H_{\rm Coup}$$

$$H = H_{\rm MF} + H_{\rm Corr}$$

Projection

Lindblad master Eq.
+quantum Diffusion

$$\rho_S = \overline{|\phi\rangle\langle\phi|}$$

Lindblad master Eq.
+quantum Diffusion

$$\rho_S = \overline{|\phi\rangle\langle\phi|}$$

Gardiner and Zoller, *Quantum noise* (2000)
Breuer and Petruccione, *The Theory of Open Quant. Syst.(2002)*.

Quantum Monte-Carlo (Exact)

Stoch. master Eq.
+ quantum Diff.

$$D = \overline{\rho_S \otimes \rho_E}$$

$$\rho_S = \overline{|\phi_1\rangle\langle\phi_2|}$$

Stoch. master Eq.
+ quantum Diff.

$$D = \overline{\prod \rho_i}$$

$$D = \overline{|\phi_1\rangle\langle\phi_2|}$$

More insight in mean-field dynamics:

Exact state: $|\Psi(t)\rangle$

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

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

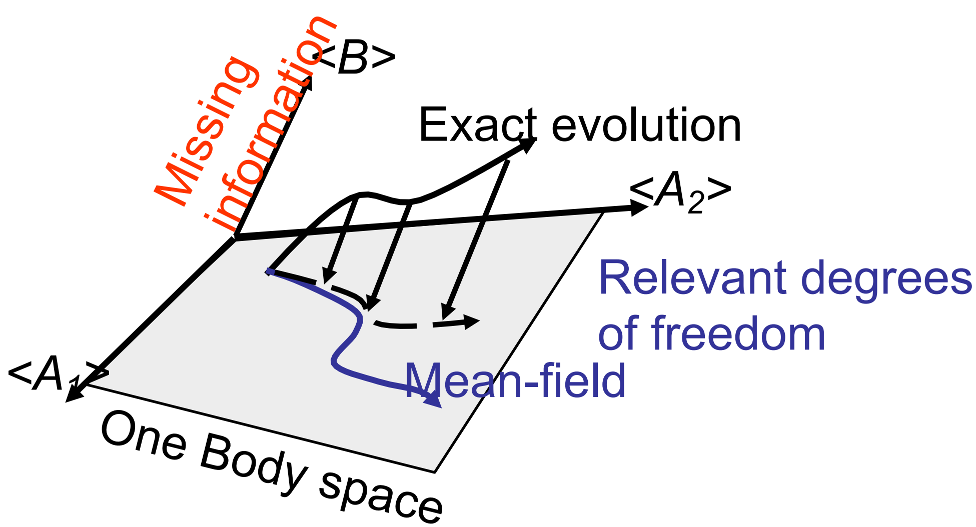
$$i\hbar \frac{d\langle A_\alpha\rangle}{dt} = \langle [A_\alpha, H]\rangle$$
→ exact Ehrenfest evolution

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

Missing part: correlations

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

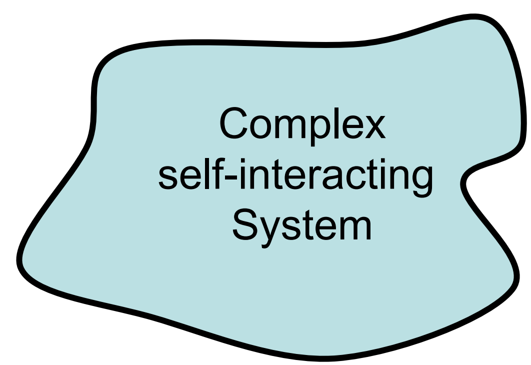
$$\rightarrow \quad i\hbar \frac{d\langle A_\alpha A_\beta\rangle}{dt} \neq \langle [A_\alpha A_\beta, H]\rangle$$



Hamiltonian splitting

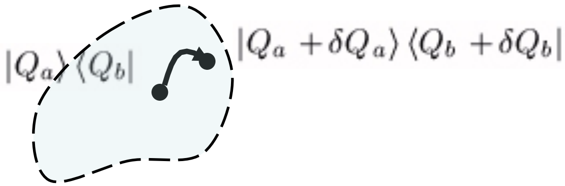
$$H = \mathcal{P}_1 H + (1-\mathcal{P}_1)H$$

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

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

Mean-field + noise

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

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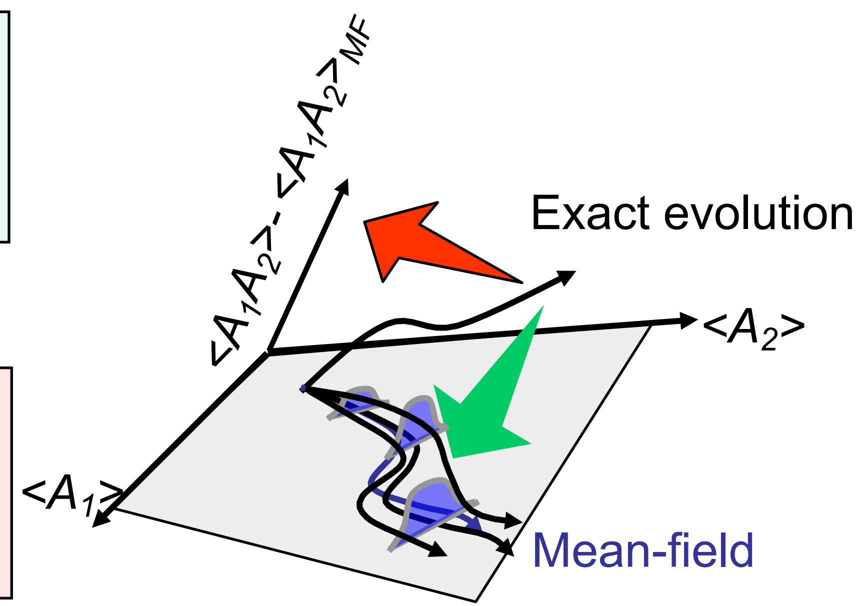
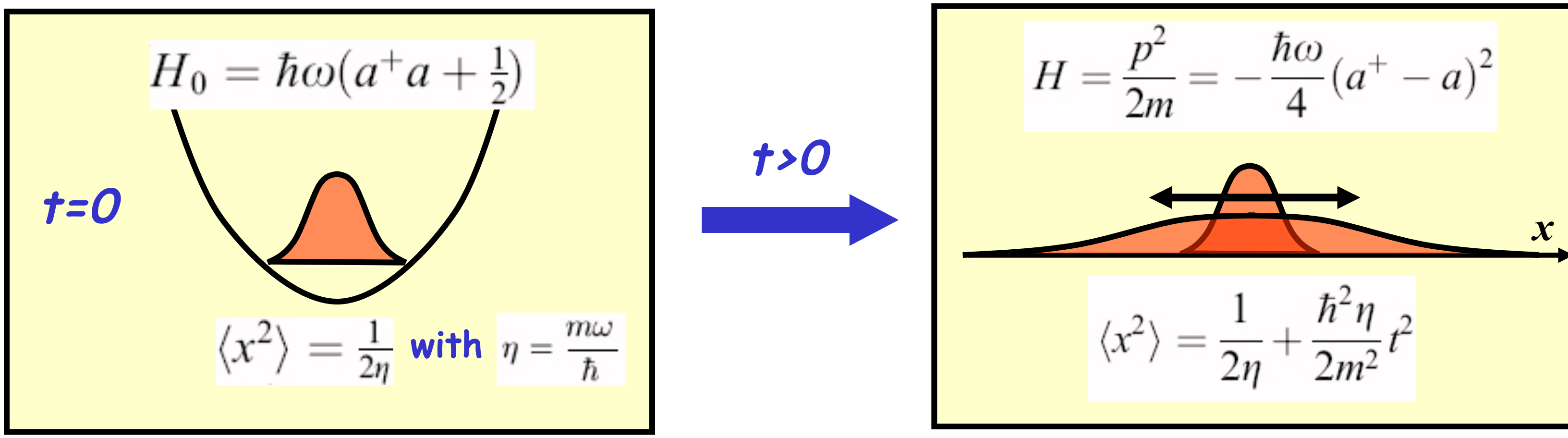
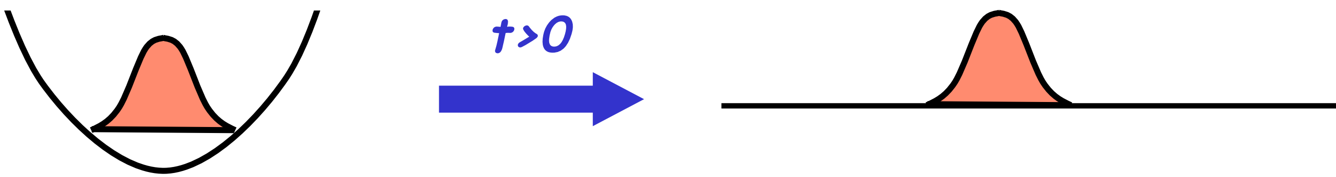




Reduction of the information: I want to simulate the expansion with Gaussian wave-function having fixed widths. $\langle x^2 \rangle = cte, \quad \langle p^2 \rangle = cte$

Mean-field evolution:



Relevant/Missing information:

Relevant degrees of freedom	Missing information	Trial states
$\langle x \rangle, \quad \langle p \rangle$	$\langle x^2 \rangle, \quad \langle p^2 \rangle, \quad \langle xp \rangle$	$\vert Q + \delta Q \rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha} \vert Q \rangle$
		↓ Coherent states
$\langle a^+ \rangle, \quad \langle a \rangle$	$\langle a^{+2} \rangle, \quad \langle a^2 \rangle, \quad \langle a^+ a \rangle$	$\vert \alpha + d\alpha \rangle = e^{d\alpha a^+} \vert \alpha \rangle$

Densities

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

Stochastic c-number evolution from Ehrenfest theorem

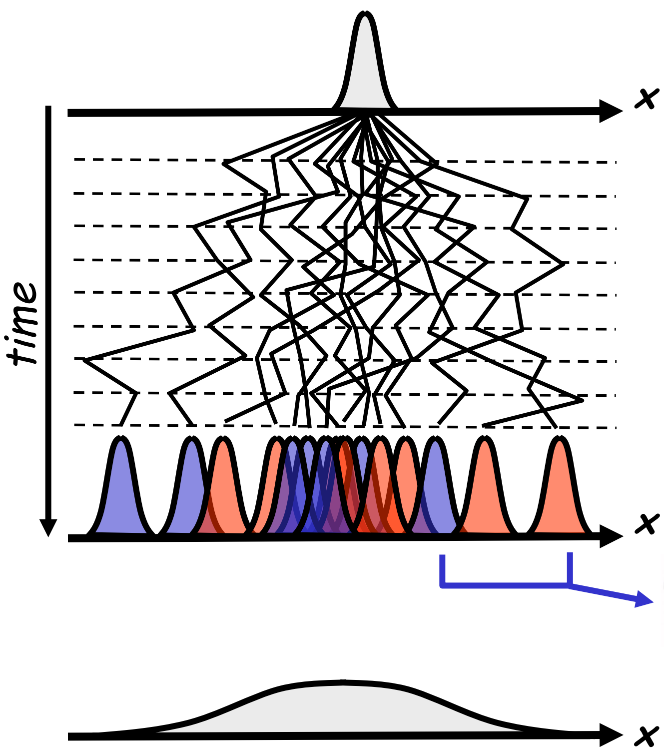
$$\begin{cases} \mathrm{d}\alpha = \overline{\mathrm{d}\alpha} + \mathrm{d}\xi^{[2]}, \\ \mathrm{d}\beta^* = \overline{\mathrm{d}\beta^*} + \mathrm{d}\eta^{[2]} \end{cases}$$

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

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

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. Phys. 322 (2007)

Starting point:

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

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

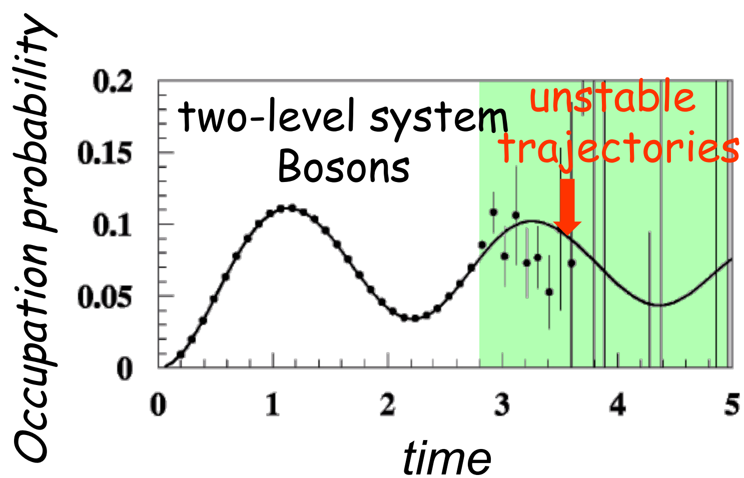
$$d\rho_1 = [h_{MF}, \rho_1] + \sum_\lambda d\xi_\lambda^{[2]}(1-\rho_1)O_\lambda\rho_1 + \sum_\lambda d\eta_\lambda^{[2]}(1-\rho_1)O_\lambda\rho_1$$

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…



Summary, stochastic methods for Many-Body Fermionic and bosonic systems

Approximate evolution

Mean-field

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

~~Fluctuation~~
~~Dissipation~~

Simplified QD

$$D = \overline{|\Phi_1\rangle\langle\Phi_2|}$$

Fluctuation ✓
~~Dissipation~~

Generalized QD

$$D = \overline{|\Phi\rangle\langle\Phi|}$$

Fluctuation ✓
Dissipation ✓

Exact QD

$$D = \overline{|\Phi_1\rangle\langle\Phi_2|}$$

Everything ✓

variational QD

$$D = \overline{|Q_1\rangle\langle Q_2|}$$

$$|Q_1\rangle = |q_1, \cdots, q_N\rangle$$

Partially everything ✓

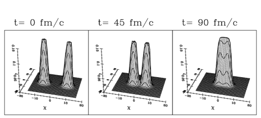
Numerical issues

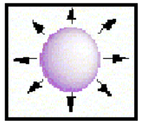
Simplified QD: Flexible

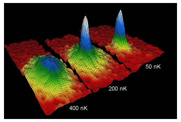
Generalized QD: Fixed

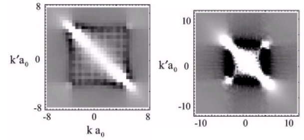
Exact QD: Fixed

variational QD: Flexible









Numerical instabilities