Time-dependent Green's Functions description of nuclear mean-field dynamics

Spatial off-diagonal structure

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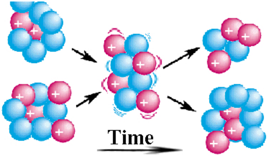
Outline

Time matters!

Nuclear reactions are time-dependent processes!

- Nuclei are self-bound, correlated, many-body systems
- "Scattering" approaches are limited to reaction type & energy...
- Advancements of time-dependent many-body techniques are needed for:
  - Central collisions of heavy isotopes ⇒ many participants, rearrangement
  - Low-energy fusion reactions ⇒ sub-barrier fusion, neck formation
  - Response of finite nuclei ⇒ collective phenomena, deexcitation



Existing time-dependent approaches

- "Transport" theory
  - Boltzmann equation with NN collisions and Pauli principle
  - Semiclassical "limit" of quantum transport
  - Sampling relevant regions of phase-space $\Rightarrow$ large simulations
  - Include fluctuations, no quantum correlations
  - Loose connection with nuclear structure

A. Bonasera, F. Guminelli and J. Molitoris, Phys. Rep. 243, 1 (1994).

- Time-dependent Hartree Fock
  - Fully quantal, but mean-field only
  - Based on TD variational principle
  - Available for 1D, 2D and 3D
  - No fluctuations, no quantum correlations
  - Same interactions than static calculations, connected to structure

J. W. Negele, Rev. Mod. Phys. 54, 913 (1982).

TDGF for nuclear reactions

Our goal:

Simulate time evolution of correlated nuclear systems in 3D

- Time-Dependent Green's Functions formalism
  - Fully quantal
  - GF's relatively well-understood in static case
  - Beyond mean-field correlations in initial state and in dynamics
  - Microscopic conservation laws are preserved

- Peculiarities of our approach:
  - So far, only mean-field evolution...
  - Initial states from adiabatic theorem
  - Calculations in a box: mesh of equidistant N_x points, $L = 25$ fm
  - Use of FFT $\Rightarrow$ periodic boundary conditions

Kadanoff-Baym equations

Eventually:

$$i\rho(\mathbf{x}_1 t_1, \mathbf{x}_{1'} t_{1'}) = \mathcal{G}^{<}(\mathbf{1}\mathbf{1}') = i\left\langle \Phi_0 \middle| \hat{a}^\dagger(\mathbf{1}')\hat{a}(\mathbf{1}) \middle| \Phi_0 \right\rangle = \sum_\alpha n_\alpha \phi^*_\alpha(\mathbf{1}')\phi_\alpha(\mathbf{1})$$

$$\mathcal{G}^{>}(\mathbf{1}\mathbf{1}') = -i\left\langle \Phi_0 \middle| \hat{a}(\mathbf{1})\hat{a}^\dagger(\mathbf{1}') \middle| \Phi_0 \right\rangle$$

$$\left\{ i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} \right\} \mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}') = \int \mathrm{d}\bar{\mathbf{r}}_1 \Sigma_{HF}(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}')$$
$$+ \int_{t_0}^{t_1} \mathrm{d}\bar{\mathbf{1}} \left[\Sigma^{>}(\mathbf{1}\bar{\mathbf{1}}) - \Sigma^{<}(\mathbf{1}\bar{\mathbf{1}}) \right] \mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}') - \int_{t_0}^{t_{1'}} \mathrm{d}\bar{\mathbf{1}}\, \Sigma^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}}) \left[\mathcal{G}^{>}(\bar{\mathbf{1}}\mathbf{1}') - \mathcal{G}^{<}(\bar{\mathbf{1}}\mathbf{1}') \right]$$

$$\left\{ -i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} \right\} \mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}') = \int \mathrm{d}\bar{\mathbf{r}}_1 \mathcal{G}^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}})\Sigma_{HF}(\bar{\mathbf{1}}\mathbf{1}')$$
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- Conserving evolution for non-equilibrium systems, derived from general principles
- Include correlation and memory effects
- Already implemented in other fields: nanostructures, atomic, quantum dots
- Difficult numerics: $\mathcal{G}^{\lessgtr}(\mathbf{x}_1, t_1; \mathbf{x}_{1'}, t_{1'}) \rightarrow 3 \times 1 \times 3 \times 1 \Rightarrow$ 8D!

Kadanoff & Baym, *Quantum Statistical Mechanics* (1962).

Kadanoff-Baym equations

Right now:

$$i\rho(\mathbf{x}_1 t_1, \mathbf{x}_{1'} t_{1'}) = \mathcal{G}^{<}(\mathbf{1}\mathbf{1}') = i\left\langle \Phi_0 \middle| \hat{a}^\dagger(\mathbf{1}')\hat{a}(\mathbf{1}) \middle| \Phi_0 \right\rangle = \sum_{\alpha<F} \phi^*_\alpha(\mathbf{1}')\phi_\alpha(\mathbf{1})$$

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Mean-field TDGF vs. TDHF

- MF-TDGF and TDHF are numerically equivalent...
- but are expressed in different terms!

Time Dependent Green's Functions

$$i\frac{\partial}{\partial t}\mathcal{G}^<(x,x';t)=\left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right\}\mathcal{G}^<(x,x';t)-\left\{-\frac{1}{2m}\frac{\partial^2}{\partial x'^2}+U(x')\right\}\mathcal{G}^<(x,x';t)$$

- 1 equation ... $N_x \times N_x$ matrix
- Testing ground
- Natural extension to correlated case via KB

Time Dependent Hartree-Fock

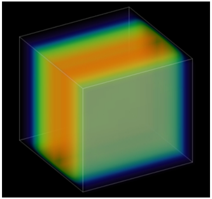
for $\alpha = 1, \ldots, N_\alpha$

$$i\frac{\partial}{\partial t}\phi_\alpha(x,t)=\left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2}+U(x)\right\}\phi_\alpha(x,t)$$

end

- N_α equations ... vectors of size N_x
- Limited to mean-field!
- Extension needs additional assumptions

Collisions of 1D slabs



- Frozen & extended y, z coordinates, dynamics in x
- Simple zero-range mean field (1D-3D connection)

$$U(x) = \frac{3}{4} t_0 \, n(x) + \frac{2+\sigma}{16} t_3 \left[n(x) \right]^{(\sigma+1)}$$

- Attemp to understand nuclear Green's functions
- 1D provide a simple visualization
- Insight into familiar quantum mechanics problems
- Learning before correlations & higher D's

Practical implementation

- KB equations reduce to:

$$i\frac{\partial}{\partial t}\mathcal{G}^<(x,x';t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x,t)\right\}\mathcal{G}^<(x,x';t)$$
$$-\left\{-\frac{1}{2m}\frac{\partial^2}{\partial x'^2} + U(x',t)\right\}\mathcal{G}^<(x,x';t)$$

- Implemented via the Split Operator Method:

$$\text{Small } \Delta t \Rightarrow \mathcal{G}^<(t+\Delta t) \sim e^{-i\left\{\frac{\nabla_1^2}{2m}+U(x_1,t_1)\right\}\frac{\Delta t}{\hbar}}\mathcal{G}^<(t)e^{+i\left\{\frac{\nabla_{1'}^2}{2m}+U(x_{1'},t_{1'})\right\}\frac{\Delta t}{\hbar}}$$

$$e^{i(\hat{T}+\hat{U})\Delta t} \sim e^{i\frac{\hat{U}}{2}\Delta t}e^{i\hat{T}\Delta t}e^{i\frac{\hat{U}}{2}\Delta t} + O[\Delta t^3]$$

- Baker-Campbell-Hausdorff formula
- FFT to switch representations

Initial state and adiabatic switching

- Initial state should be ground state of the Hamiltonian
    - Mean-field approx. $\Rightarrow$ solve static Hartree-Fock equations
    - Correlated case $\Rightarrow$???
- Possible solution: use adiabatic theorem!

$$H(t) = f(t)H_0 + [1 - f(t)]\, H_1$$

$$f(t) = \begin{cases} 1, & t \to -\infty \\ 0, & t \to t_0 \end{cases}$$

- Advantage: a single code for everything!
- For practical applications:
    - H_0 & H_1 with similar spectra to avoid crossing
    - $H_0 = \frac{1}{2}kx^2$
    - $H_1 = U_{\mathrm{mf}}$
    - Adiabatic transient: $f(t) = \frac{1}{1+\mathrm{e}^{(t-\tau_0)/\tau}}, \qquad \tau \to \infty$

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Adiabatic switching: practical examples

$$N_\alpha = 2 \qquad \Longleftrightarrow \qquad A = 8$$

$$U(t) = f(t)\frac{1}{2}kx^2 + [1 - f(t)]\, U_{\mathsf{mf}}(x,t) \qquad \Longleftrightarrow \qquad f(t) = \frac{1}{1 + \mathrm{e}^{(t-\tau_0)/\tau}}$$

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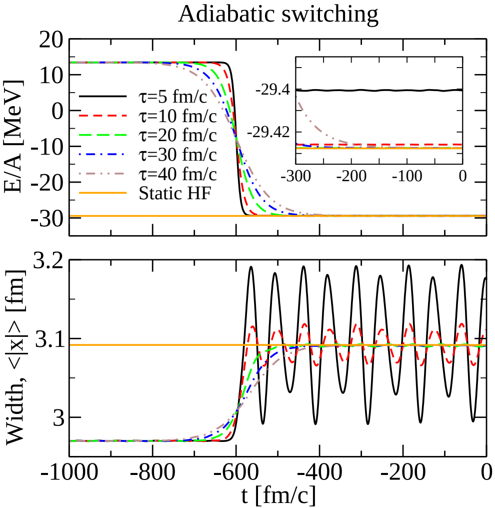
Adiabatic switching & observables



Collisions of 1D slabs: fusion

$$\mathcal{G}^{<}(x,x',P) = e^{iPx}\mathcal{G}^{<}(x,x',P=0)e^{-iPx'}$$
$$\mathcal{G}^{<}(x,x') = \sum_{\alpha<F}\phi_\alpha(x)\phi_\alpha(x')$$

$$E_{CM}/A = 0.1\,\mathrm{MeV}$$

Collisions of 1D slabs: break-up

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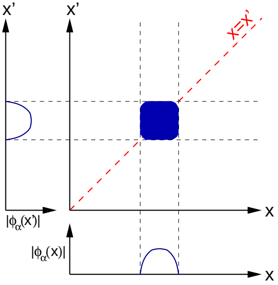
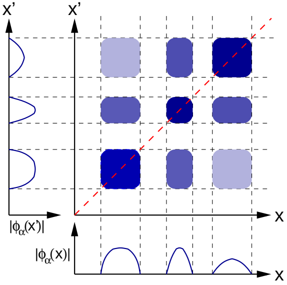
$$\mathcal{G}^{<}(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi_\alpha(x')$$

$$E_{CM}/A = 4\,\mathrm{MeV}$$

Off-diagonal elements: origin





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Correlation of single-particle states that are far away!

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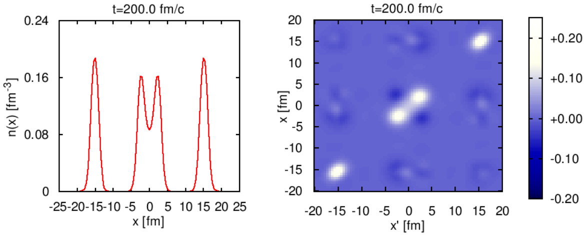

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Correlation of single-particle states that are far away!

Collisions of 1D slabs: multifragment.

$$\mathcal{G}^<(x,x',P) = e^{iPx}\mathcal{G}^<(x,x',P=0)e^{-iPx'}$$

$$\mathcal{G}^<(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi_\alpha(x')$$

$$E_{CM}/A = 25\,\mathrm{MeV}$$

Off-diagonal elements: issues

Diagonal vs off-diagonal

$$n(x) = \mathcal{G}^<(x, x' = x) = \sum_{\alpha < F} |\phi_\alpha(x)|^2 \qquad K = \sum_{k < k_F} \frac{k^2}{2m} \mathcal{G}^<(k, k' = k)$$

Conceptual issues

- Should far away sp states be connected in a nuclear reaction?
- Decoherence and dissipation will dominate late times...
- Are $x \neq x'$ elements really necessary for the time evolution?

Practical issues

- Green's functions are $N_x^D \times N_t \times N_x^D \times N_t$ matrices
- Eliminating off-diagonalities drastically reduces numerical cost

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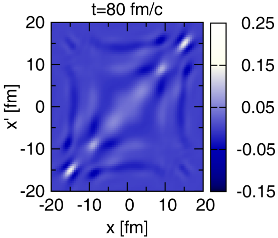
Off-diagonal elements: cutting procedure



- How can we delete off-diag. without perturbing diagonal evolution?
- Super-operator: act in two places instantaneously (nonlocal)
- Use a damping imaginary potential off the diagonal

$$\mathcal{G}^<(x,x',t+\Delta t) \sim e^{i(\varepsilon(x)+iW(x,x'))\Delta t}\mathcal{G}^<(x,x',t)e^{-i(\varepsilon(x')-iW(x,x'))\Delta t}$$

- Properties chosen to preserve: norm, FFT, periodicity, symmetries
- Other choices do not yield good results!

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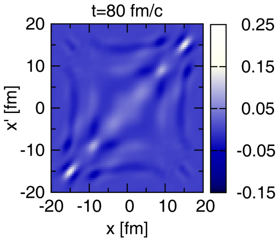

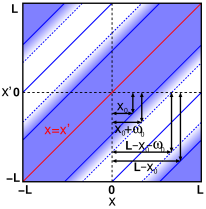

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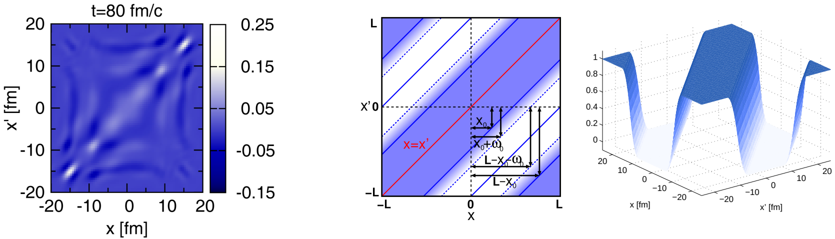

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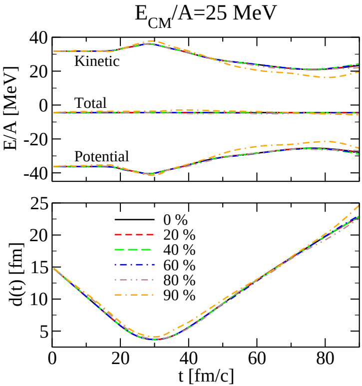
Off-diagonally cut evolution

$$E_{CM}/A = 25\,\mathrm{MeV}$$

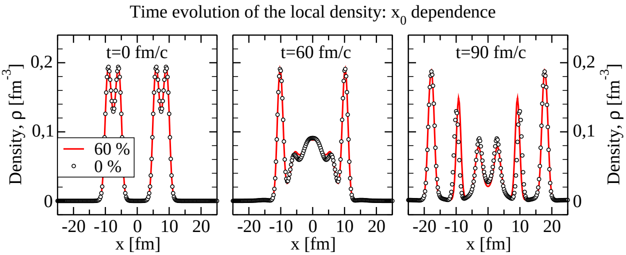
Cutting off-diagonal elements

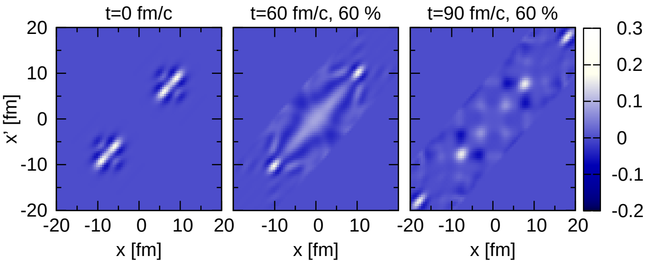


- Total energy and different components are unaffected!
- Integrated quantities appear to be cut-independent

Cutting off-diagonal elements

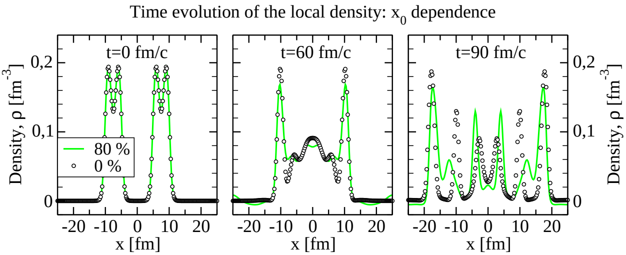
$$E_{CM}/A = 25\,\mathrm{MeV}, |x - x'| \lesssim 10\,\mathrm{fm} \rightarrow 60\%$$

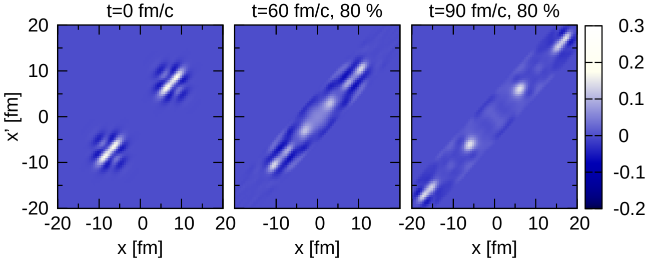




Cutting off-diagonal elements

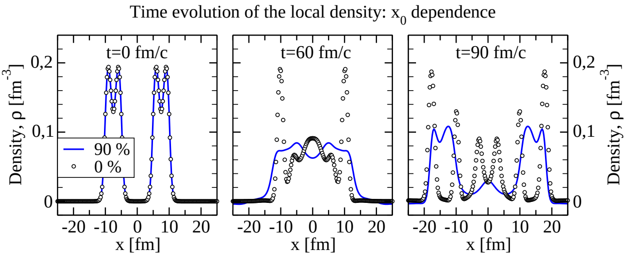
$$E_{CM}/A = 25\,\mathrm{MeV}, |x - x'| \lesssim 5\,\mathrm{fm} \rightarrow 80\%$$

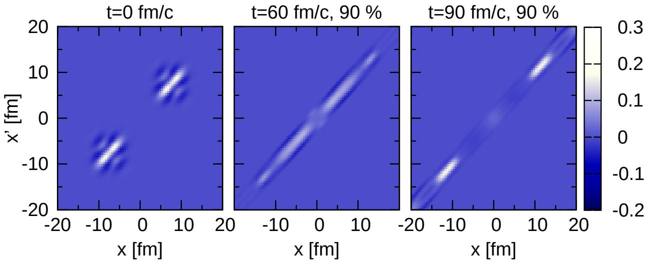




Cutting off-diagonal elements

$$E_{CM}/A = 25\,\mathrm{MeV}, |x - x'| \lesssim 2.5\,\mathrm{fm} \rightarrow 90\%$$





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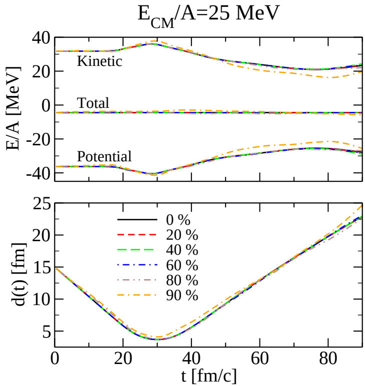


- 60% off-diagonal elements can be neglected safely!
- Small effect of erasure for observables in high energy reactions...
- Observables are not sensitive to unphysical cuts!

Consequences of cuts: irreversibility

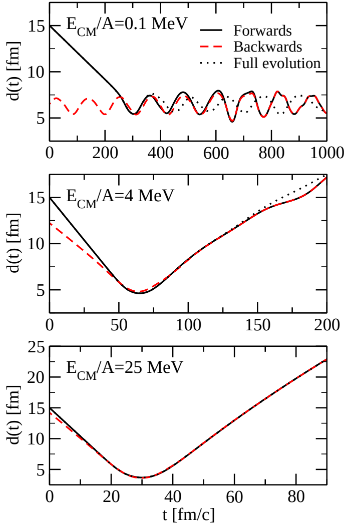
What processes are sensitive to cuts?

$$E_{CM}/A = 25\,\mathrm{MeV}$$

Uncut evolution, forward & backwards

Cut evolution forward $|x - x'| < 10\ \mathrm{fm}$, uncut backwards

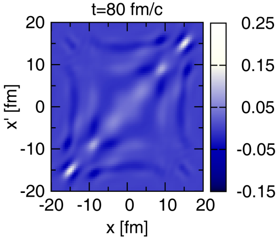
Irreversibility & observables



Off-diagonal elements contain information...
Relevant for coming back to the past!

- Solid: forward cut evolution, with $|x - x'| < 5 \text{ fm} \rightarrow 80\%$
- Dashed: backwards evolution after cut
- Dotted: forward & backward full evolution

Wigner distribution



- Fourier transform along relative variable (Wigner transform)

$$f_W(x,p) = \int \frac{\mathrm{d}y}{2\pi}\, e^{-ipy}\, \mathcal{G}^<\left(x+\frac{y}{2}, x-\frac{y}{2}\right)$$

- Simultaneous information on real and momentum space!
- Quantum analog of phase-space density → connected to transport

Wigner distribution

- Fourier transform along relative variable (Wigner transform)

$$f_W(x,p) = \int \frac{\mathrm{d}y}{2\pi}\, e^{-ipy}\, \mathcal{G}^< \left(x + \frac{y}{2}, x - \frac{y}{2} \right)$$

- Simultaneous information on real and momentum space!
- Quantum analog of phase-space density $\rightarrow$ connected to transport

Smearing out the distribution

Wigner transform $\mathcal{G}^<$ with gaussian cut off the diagonal...

$$f_\sigma(x,p) = \int \mathrm{d}y \, e^{-ipy} e^{-\frac{y^2}{2\sigma^2}} \, \mathcal{G}^< \left(x + \frac{y}{2}, x - \frac{y}{2} \right)$$

is equivalent to momentum average of $f_W(x,P)$!

Smearing out the distribution

Wigner transform $\mathcal{G}^<$ with gaussian cut off the diagonal...

$$
\begin{aligned}
f_\sigma(x,p) &= \int \mathrm{d}y \, e^{-ipy} e^{-\frac{y^2}{2\sigma^2}} \, \mathcal{G}^< \left(x + \frac{y}{2}, x - \frac{y}{2} \right) \\
&= \int \mathrm{d}q \, e^{-\frac{\sigma^2 (p-q)^2}{2}} \int \mathrm{d}y \, e^{-ipy} \mathcal{G}^< \left(x + \frac{y}{2}, x - \frac{y}{2} \right) \\
&= \int \mathrm{d}q \, e^{-\frac{\sigma^2 (p-q)^2}{2}} \, f_W(x,q)
\end{aligned}
$$

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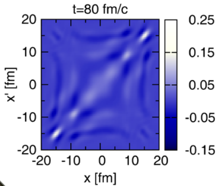
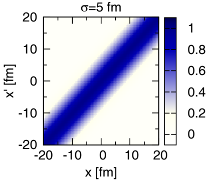
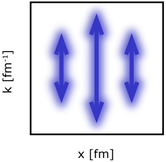


X

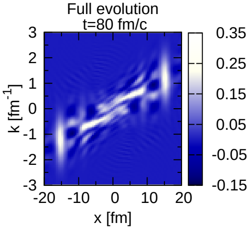


Wigner Tr.

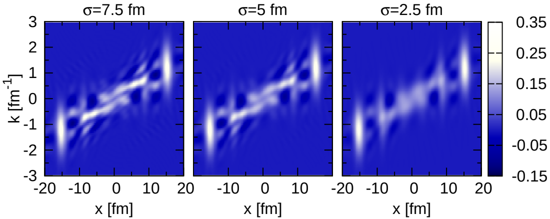


Smearing out the distribution

Full evolution Wigner distribution

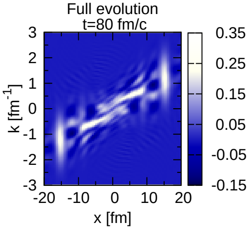


Gaussian average off the diagonal

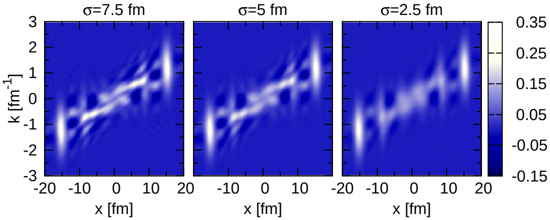


Smearing out the distribution

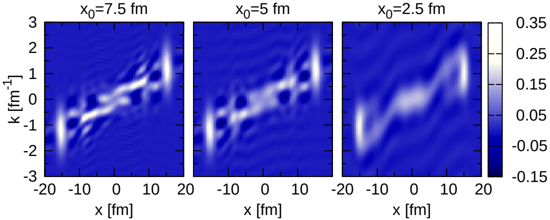
Full evolution Wigner distribution



Gaussian average off the diagonal



Superoperator cut off the diagonal



Conclusions & Outline

- KB equations are promising for nuclear reactions
- Time evolution of 1D slabs in the mean-field via SOM, FFT
- $60 - 80\%$ off-diagonal elements are unimportant...
- Off-diagonal elements can be detected by reversibility
- Wigner functions give insight on lack of NN collisions
- Off diagonal cut in real space $\sim$ blur in momentum space

- Beyond mean-field calculations are being implemented
- Extension to 3D in progress

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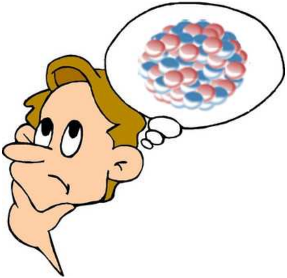
Thank you!



MARIE CURIE ACTIONS

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Limitations of TDHF: diagrams

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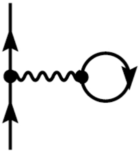
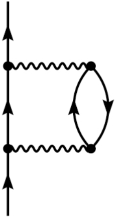
TDHF



- Collision with mean-field wall
- Energy independent ⇒ "elastic"
- Instantaneous process ...
- but scape & ... widths included!

2nd order



- Excitation of particle-hole pair
- Energy transfer ⇒ "inelastic"
- NN collisions, source of dissipation
- Time-dependent process in time evolution?