Towards Application of Nonequilibrium Green's Functions to Processes in Nuclear Systems

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Solving Kadanoff-Baym Equations
Status and Open Problems

Christian-Albrechts-Universität Kiel

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Outline

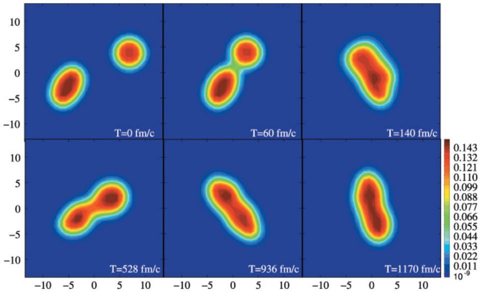
Time-Dependent Hartree-Fock

Sensible for degenerate low-energy reacting systems.

Time-dependent Slater determinant

$$\Phi\left(\{\boldsymbol{r}_i\}_{j=1}^{A}, t\right) = \frac{1}{A!}\sum_{\sigma}\prod_{k=1}^{A}(-1)^{\mathrm{sgn}\,\sigma}\phi_k\left(\boldsymbol{r}_{\sigma(k)}, t\right)$$

$$\Rightarrow \qquad i\frac{\partial}{\partial t}\phi_j = -\frac{\nabla^2}{2m}\phi_j + U(\{\phi_k\})\,\phi_j$$



semicentral

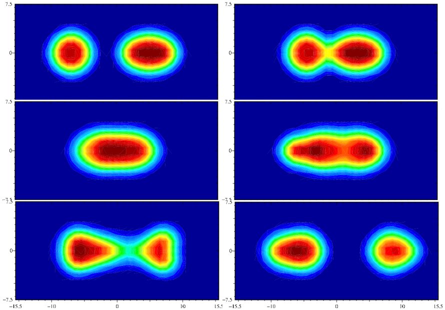
$^{22}Ne + ^{16}O$

$E_{cm} = 95\,\text{MeV}$

Umar & Oberacker
Phys. Rev. C 74 (2006) 024606

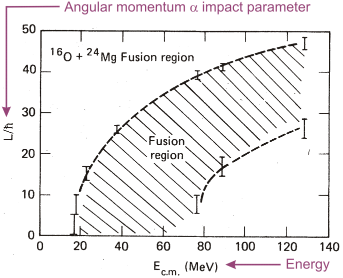
Time-Dependent Hartree-Fock in Practice

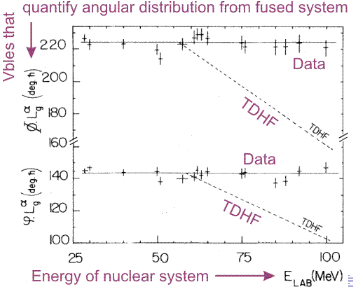
Theory predicts a low-ℓ fusion window developing at higher energies in reactions.



head-on ^{16}O+^{22}Ne at $E_{cm} = 95\,$MeV
Umar & Oberacker '07

Data: NO low-ℓ fusion window!





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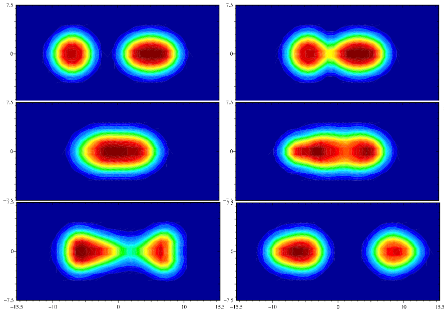

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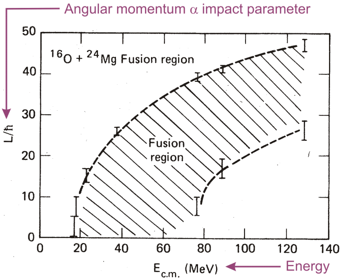
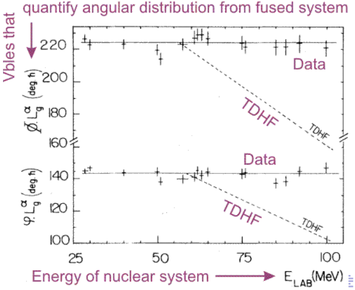
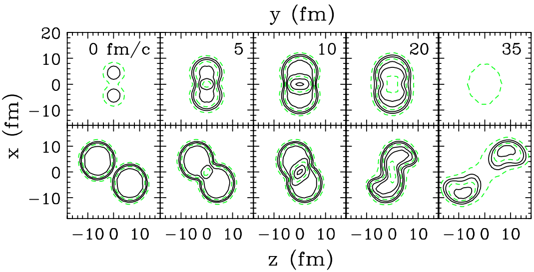




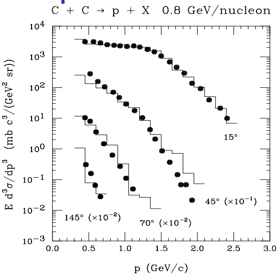
High Energies: Boltzmann Equation

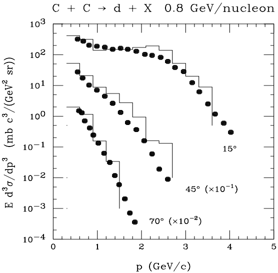
$$\frac{\partial f}{\partial t} + \frac{\partial \omega_{\boldsymbol{p}}}{\partial \boldsymbol{p}} \frac{\partial f}{\partial \boldsymbol{r}} - \frac{\partial \omega_{\boldsymbol{p}}}{\partial \boldsymbol{p}} \frac{\partial f}{\partial \boldsymbol{p}} = I\{f\}$$



Au+Au at 400 MeV/nucleon

P.D. Nucl Phys A673 (2000) 375





$$f(\boldsymbol{r}, \boldsymbol{p}, t) \simeq \sum_i \delta(\boldsymbol{r} - \boldsymbol{r}_i(t))\, \delta(\boldsymbol{p} - \boldsymbol{p}_i(t))$$

Test particles: $\dot{\boldsymbol{r}}_i = \frac{\partial \omega_{\boldsymbol{p}}}{\partial \boldsymbol{p}} \qquad \dot{\boldsymbol{p}}_i = -\frac{\partial \omega_{\boldsymbol{p}}}{\partial \boldsymbol{r}}$

system gasifies symbols - data, histograms - calcs

Quantum 1-Particle Dynamics

1-Ptcle Green's Function: $i\,G(1,1') = \langle\Phi|\,T\left\{\psi(1)\,\psi^{\dagger}(1')\right\}|\Phi\rangle$

T - generalized time-ordering operator: allows either order

Dyson Eq: $G = G_0 + G_0\,\Sigma\,G$ where

$i\,\Sigma(1,1') = \langle\Phi|\,T\left\{j(1)\,j^{\dagger}(1')\right\}|\Phi\rangle_{\text{irr}}$ and $\underbrace{\left(i\,\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)}_{G_0^{-1}}\psi(1) = \underbrace{j(1)}_{\text{source}}$

Kadanoff-Baym eqs - Dyson for a specific operator order, such as $-iG^{<}(1,1') = \langle\psi^{\dagger}(1')\,\psi(1)\rangle$,

$$\left(i\,\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)G^{\lessgtr}(1,1') = \int d1''\,\Sigma^{+}(1,1'')\,G^{\lessgtr}(1'',1')$$

$$+\int d1''\,\Sigma^{\lessgtr}(1,1'')\,G^{-}(1'',1')$$

Kadanoff-Baym Equations

$$\left(i\,\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right)\,G^{\lessgtr}(1,1')=\int \mathrm{d}1''\,\Sigma^{+}(1,1'')\,G^{\lessgtr}(1'',1') + \int \mathrm{d}1''\,\Sigma^{\lessgtr}(1,1'')\,G^{-}(1'',1')$$

Variety of physics in different situations, for a variety of Σ

E.g. when $\Sigma_{mf} >> \Sigma^{\lessgtr}$, as in a highly degenerate system, the mean-field (TDHF) approximation applies with

$$-i\,G(1,1') \approx \sum_{j=1}^{A} \phi_j(1)\,\phi_j^*(1')$$

If *scale*$_{(1+1')}$ $>>$ *scale*$_{(1-1')}$ in Green's functions, quasiparticle approximation with evolution governed by Boltzmann equation applies

$$-i\,G^{<}(1,1') \approx \int \mathrm{d}\boldsymbol{p}\, f(\boldsymbol{p},1)\, \mathrm{e}^{i\,\boldsymbol{p}(\boldsymbol{x}_1-\boldsymbol{x}_{1'})-i\,\omega_{\boldsymbol{p}}(t_1-t_{1'})}$$

Direct solution of KB??: 4+4=8D calculation! TDHF - 4D ($\times$ 1D)

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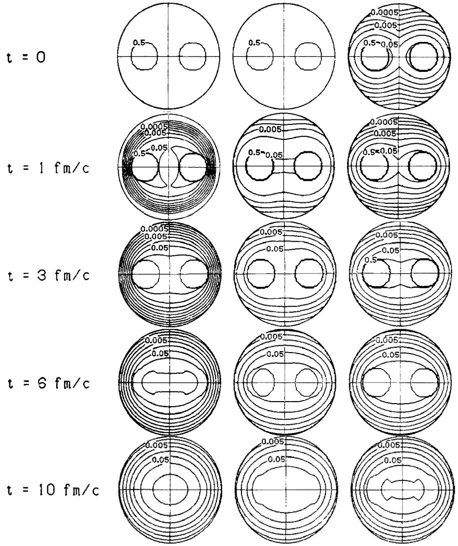
Direct solution of KB??: 4+4=8D calculation! TDHF - 4D ($\times$ 1D)

Equilibration in Uniform Matter

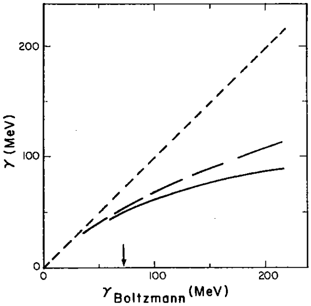


400 MeV/nucleon model of early reaction dynamics test of Boltzmann eq

G, Σ diagonal in $\boldsymbol{p}$

$\boxed{8\text{D} \rightarrow 5\text{D}} - 1D = 4D$ (like TDHF)

Rate comparison



PD '84 (Thesis)

Towards Reaction Simulations: Collisions in 1D

Issues to consider for nonuniform matter:

- matrix rather than wavefunction dynamics
- preparation of initial state
- abundance of mtx elements $(50)^8 = 4 \times 10^{13}$!

START W/MF:

$$\left(i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - \Sigma_{\rm mf}\left(-iG^<(1,1)\right)\right)(-i)G^<(1,1') = 0$$

$$G^<(x_1\, t_1\, x_{1'}\, t_{1'}) \overset{FFT}{\leftrightarrow} G^<(p_1\, t_1\, p_{1'}\, t_{1'})$$

$$G^<(t_1+\Delta t, t_{1'}) = e^{-i\Delta t(K+\Sigma)}\, G^<(t_1, t_{1'})$$
$$= \left(e^{-i\Delta t\,\Sigma/2}\, e^{-i\Delta t\,K}\, e^{-i\Delta t\,\Sigma/2} + \mathcal{O}\left((\Delta t)^3\right)\right) G^<(t_1, t_{1'})$$

So far, just altering mtx-element phase; full unitarity

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$$G^<(x_1\,t_1\,x_{1'}\,t_{1'}) \overset{FFT}{\leftrightarrow} G^<(p_1\,t_1\,p_{1'}\,t_{1'})$$

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So far, just altering mtx-element phase; full unitarity

Initial State Through Adiabatic Evolution

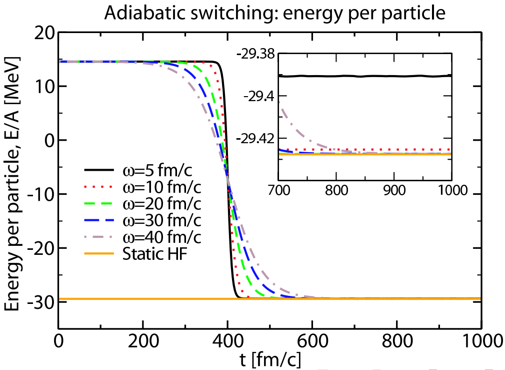
Optimally, the same code for reaction dynamics and initial-state preparation. Adiabatic switching, from harmonic oscillator to self-consistent mean-field solution:

$$\mathcal{H}(t) = \mathcal{H}_{\rm HO}\, f(t) + \mathcal{H}_{\rm mf}(t)\, (1 - f(t))$$

$$f \rightarrow \begin{cases} 1\,, & t \rightarrow -\infty \\ 0\,, & t \rightarrow +\infty \end{cases}$$

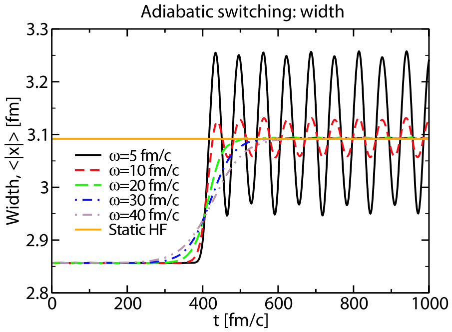
E.g.

$$f(t) = \frac{1}{1 + \exp\frac{t - t_0}{w}}$$

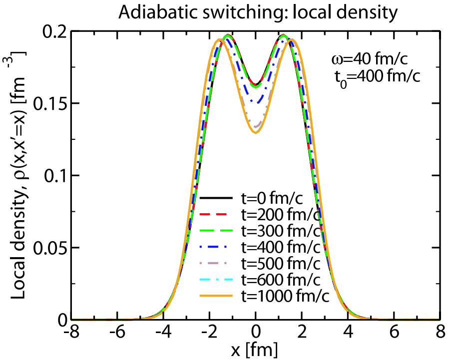


Adiabatic Switching of Interaction

Width of density distribution

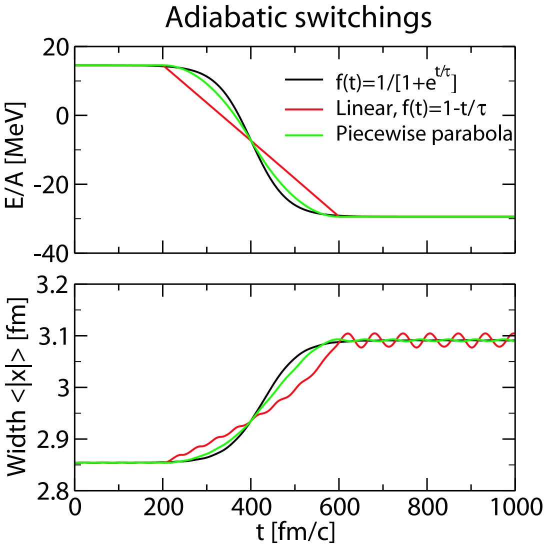


Density



from HO to self-consistent solution

Dependence on Transition Function



paradox: slower change yields inferior results than smoother

Collisions at $E_{\rm cm}/A = 0.1$ MeV

Boost: $G(x,x',t=0) \rightarrow e^{ipx}\, G(x,x',t=0)\, e^{-ipx'}$

Without Coulomb force, fusion takes place at the low energy.

Density $n(x,t)$ and real part of density matrix $G^<(x,x',t)$

x

density $n(x) = G^<(x,x)$ (diagonal), $G^<(x,x') = \sum_\alpha n_\alpha\, \varphi_\alpha(x)\, \varphi^*_\alpha(x')$

Collisions at $E_{cm}/A = 4\,\text{MeV}$

Break-up

Density $n(x,t)$ and real part of density matrix $G^{<}(x,x',t)$

X

density $n(x) = G^{<}(x,x)$ (diagonal), $G^{<}(x,x') = \sum_{\alpha} n_{\alpha}\,\varphi_{\alpha}(x)\,\varphi_{\alpha}^{*}(x')$

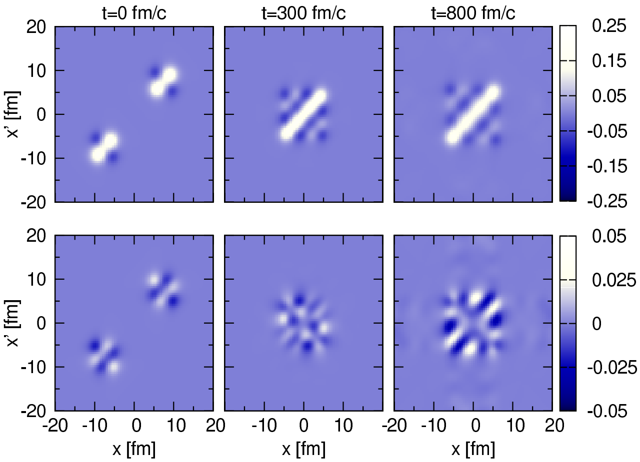
Collisions at $E_{\mathrm{cm}}/A = 25\,\mathrm{MeV}$

Multifragmentation

Density $n(x,t)$ and <u>real</u> part of density matrix $G^<(x,x',t)$

Density is identical with the diagonal: $n(x,t) = G^<(x,x,t)$.

Re & Im of $G^<$ at $E_{cm}/A = 0.1$ MeV



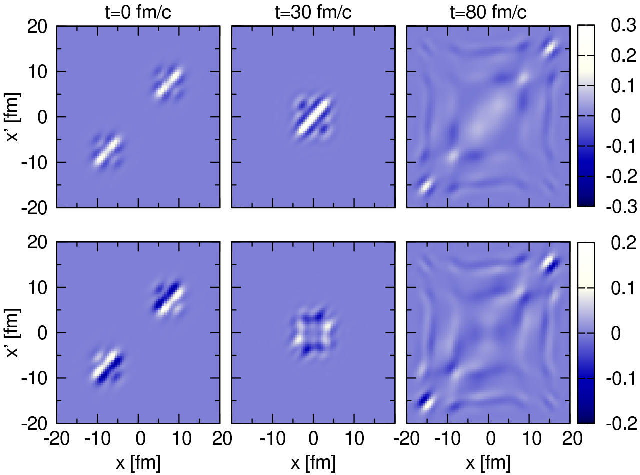
Re

symmetric

Im

antisymmetric

Re & Im of $G^<$ at $E_{cm}/A = 25\,\text{MeV}$



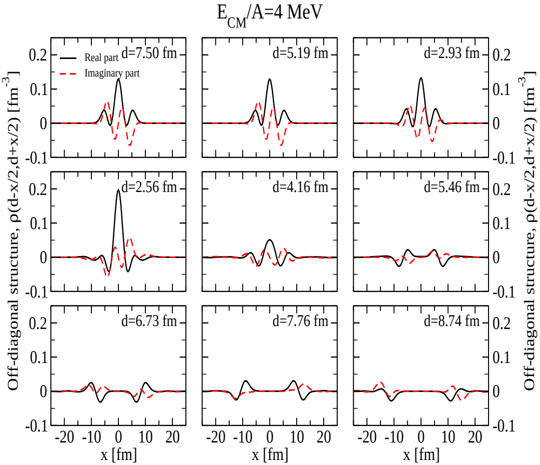
Re

symmetric

Im

antisymmetric

Cuts of $G^<(x_1, x_2, t)$, across the Diagonal

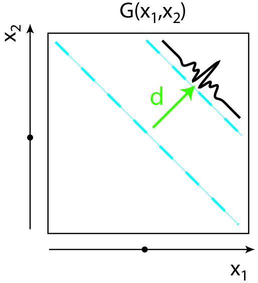


$E_{cm}/A = 4\,\mathrm{MeV}$

each panel another t

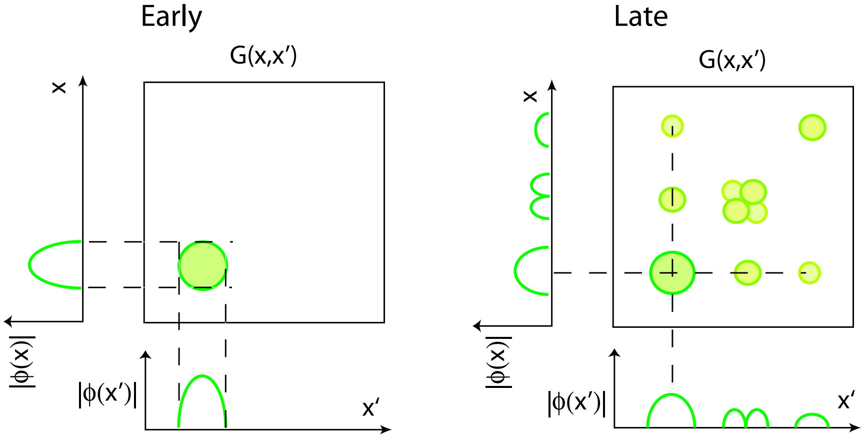
Real part
- symmetric

Imaginary part
- antisymmetric



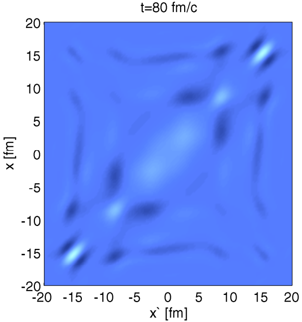
Origin of Far-Off Terms in $G^<(x, x', t)$

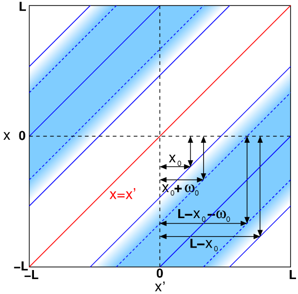
$$G^<(x, x', t) = \sum_\alpha n_\alpha \, \varphi_\alpha(x, t) \, \varphi^*_\alpha(x', t)$$



Suppressing the Off-Diagonal Elements

Following far off-diagonal elements of the density matrix $G^<(x,x',t)$ or of generalized density matrix $G^<(x,t,x',t')$ impossible in 3D. How important are those elements? They account for a phase relation between separating fragments.

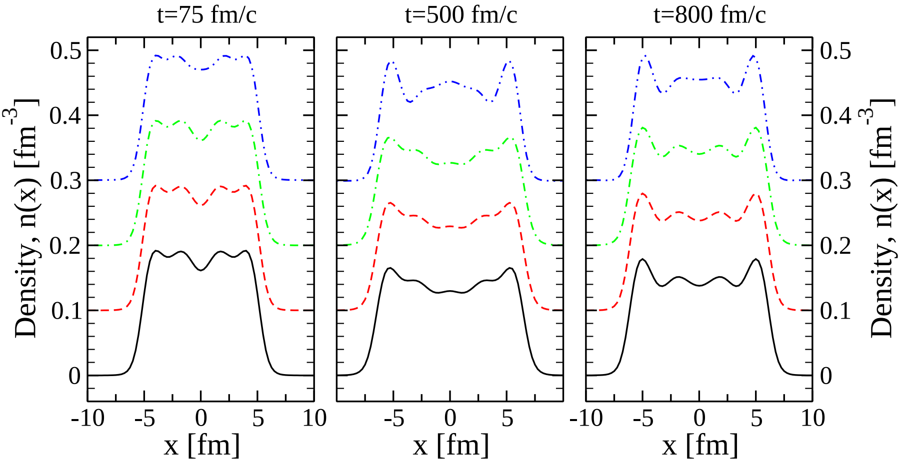




Evolution using imaginary superoperator suppressing large $|x-x'|$

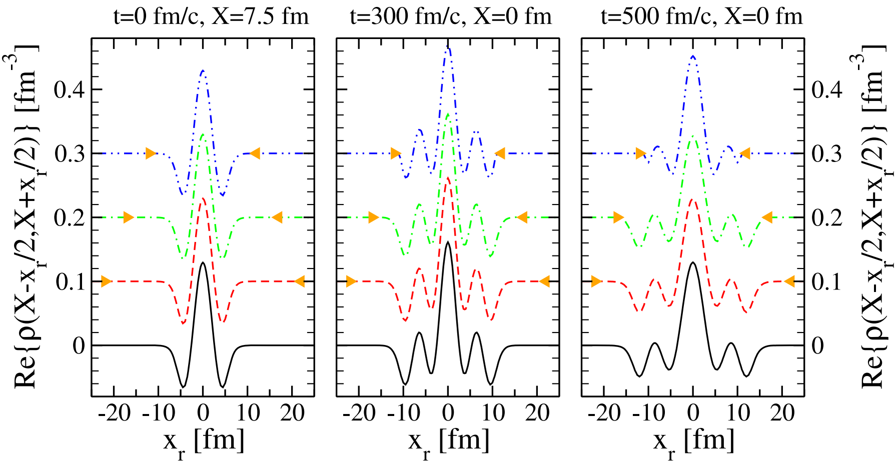
$$G^<(x,x',t+\Delta t) \sim e^{-i(\epsilon(x)+iW(x,x'))\Delta t}\, G^<(x,x',t)\, e^{+i(\epsilon(x)-iW(x,x'))\Delta t}$$

Evolution with Erased Elements at $E_{cm}/A = 0.1$ MeV



Lines: all elements there, only $|x - x'| < 20$ fm, 15 fm, 10 fm

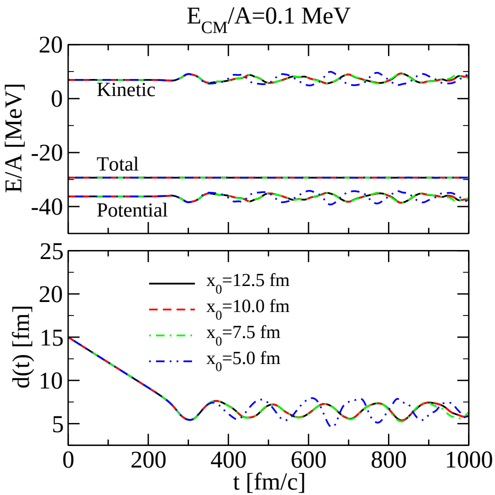
Evolution with Erased Elements at $E_{cm}/A = 0.1$ MeV



Different cuts across the diagonal

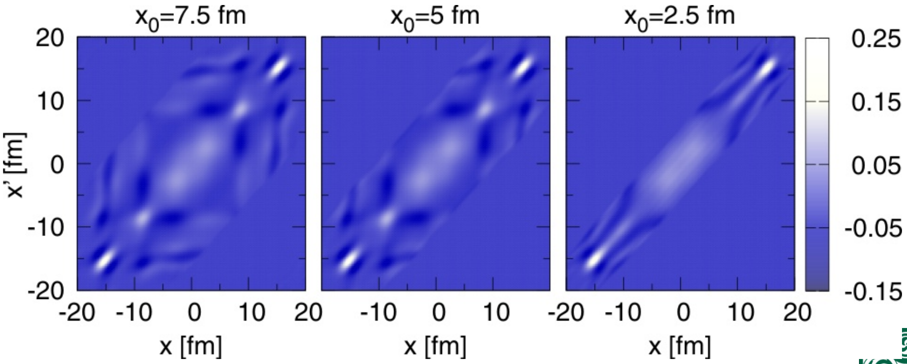
Evolution with Erased Elements at $E_{cm}/A = 0.1$ MeV

Energy and System Size for Different Suppressions

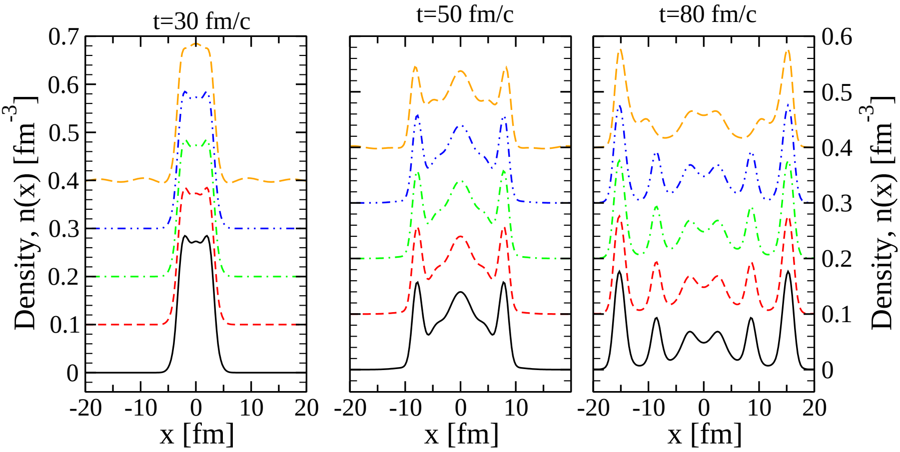


Evolution with Erased Elements at $E_{cm}/A = 25\,\text{MeV}$

Real Part of Density Matrix $G(x, x', t)$
for Different Suppressions at $t = 80\,\text{fm}/c$

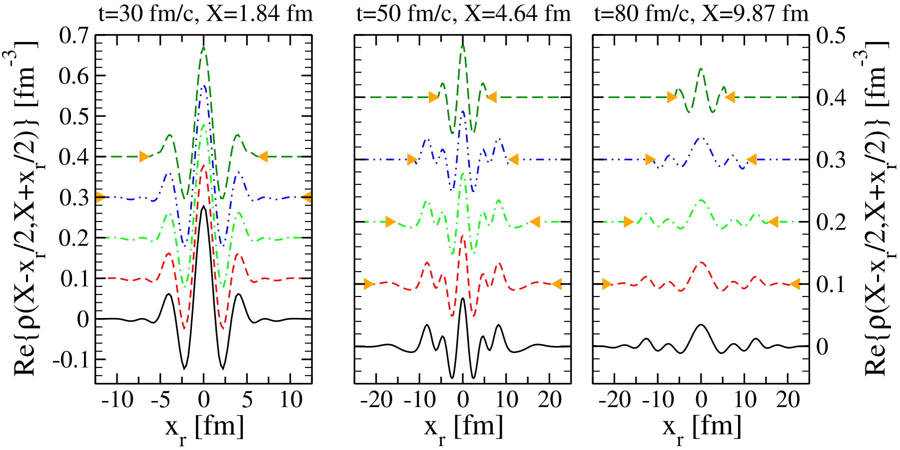


Evolution with Erased Elements at $E_{cm}/A = 25\,\mathrm{MeV}$



Lines: all elements there, only $|x - x'| < 20\,\mathrm{fm}$, $15\,\mathrm{fm}$, $10\,\mathrm{fm}$, $5\,\mathrm{fm}$

Evolution with Erased Elements at $E_{cm}/A = 25\,\text{MeV}$



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Evolution with Erased Elements at $E_{cm}/A = 25\,\text{MeV}$

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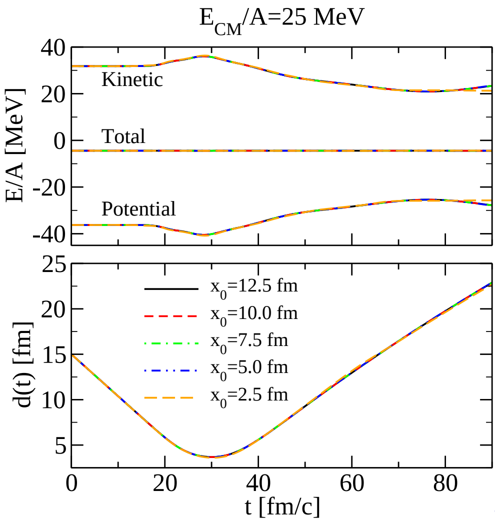


Wigner-Function Evolution

Wigner function: $f(p,x) = \int \mathrm{d}y\, \mathrm{e}^{-ipy}\, G^{<}\left(x + \frac{y}{2}, x - \frac{y}{2}\right)$

- quantum analog of phase-space occupation
- in semiclassical limit satisfies Vlasov eq
- alternate definition $f(p,x) \equiv G^{<}(p,x) = \sum_{\alpha} n_{\alpha}\, \varphi_{\alpha}(p)\, \varphi^{*}_{\alpha}(x)$

$E_{\mathrm{cm}}/A = 25\,\mathrm{MeV}$ (multifragmentation)

Cutting Elements $\leftrightarrow$ Averaging Momenta

Wigner function $f(p,x) = \int dy\, e^{-ipy}\, G^<\left(x+\frac{y}{2}, x-\frac{y}{2}\right)$

Wigner f. from $G^<$ with far-off elements cut-off by $e^{-y^2/2\sigma^2}$:

$$\bar{f}(p,x) = \int dy\, e^{-ipy}\, e^{-y^2/2\sigma^2}\, G^<\left(x+\frac{y}{2}, x-\frac{y}{2}\right)$$
$$= \int dq\, e^{-(p-q)^2\,\sigma^2/2} \int dy\, e^{-iqy}\, G^<\left(x+\frac{y}{2}, x-\frac{y}{2}\right)$$
$$\equiv \int dq\, e^{-(p-q)^2\,\sigma^2/2}\, f(q,x)$$

Suppressing of far-off matrix elements in the density matrix $G^<$ is equivalent to averaging out details in the Wigner function!

Cutting Elements $\leftrightarrow$ Averaging Momenta

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

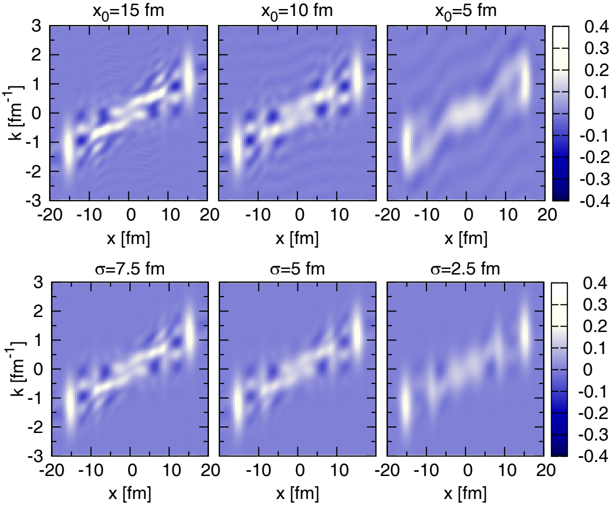
Wigner f. from $G^{<}$ with far-off elements cut-off by $\mathrm{e}^{-y^2/2\sigma^2}$:

$$\begin{aligned}
\overline{f}(p,x) &= \int \mathrm{d}y \, \mathrm{e}^{-ipy} \, \mathrm{e}^{-y^2/2\sigma^2} \, G^{<}\left(x+\frac{y}{2}, x-\frac{y}{2}\right) \\
&= \int \mathrm{d}q \, \mathrm{e}^{-(p-q)^2\,\sigma^2/2} \int \mathrm{d}y \, \mathrm{e}^{-iqy} \, G^{<}\left(x+\frac{y}{2}, x-\frac{y}{2}\right) \\
&\equiv \int \mathrm{d}q \, \mathrm{e}^{-(p-q)^2\,\sigma^2/2} \, f(q,x)
\end{aligned}$$

Suppressing of far-off matrix elements in the density matrix $G^{<}$ is equivalent to averaging out details in the Wigner function!

Wigner-Function Comparison ($E_{cm}/A = 25\,\text{MeV}$)

Top: Wigner f from $G^<$ with elements cut off (late stage)



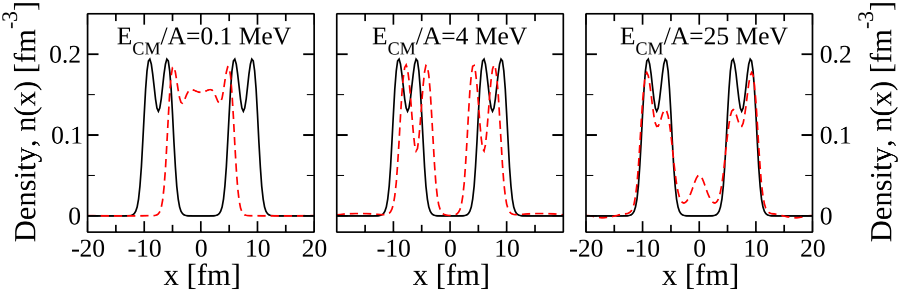
Bottom: Wigner function from Gaussian averaging

Forward and Backward in Time!

Red: systems evolved forward in time, with elements at $|x - x'| > 10\,\mathrm{fm}$ suppressed. After reaction completion, evolved back to $t = 0$, still with the far-off elements suppressed.

Black: actual initial state

$t = 0$:



Far off-diagonal elements are important for coming back to the initial state! Without the elements, remote past reminds remote future.

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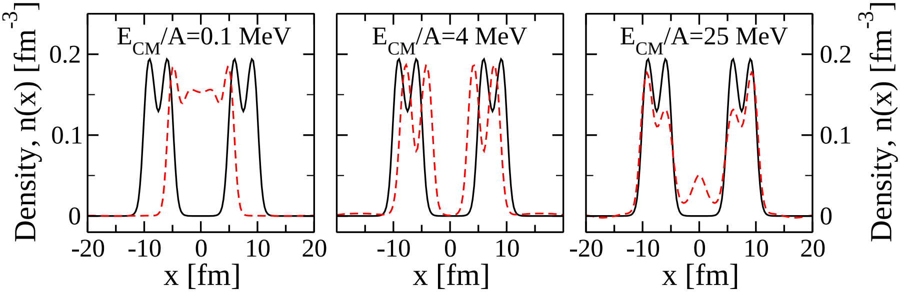

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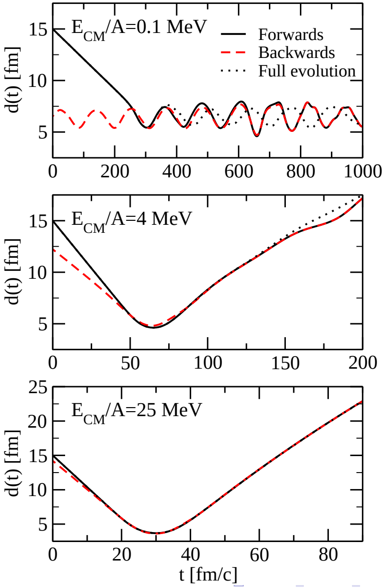
Forward and Backward in Time!

System Size

Dotted: complete evolution, time-reversible

Solid: forward when only $|x - x'| < 10\,\text{fm}$ retained

Dashed: backward when only $|x - x'| < 10\,\text{fm}$ retained



Conclusions

- Low-energy approach to central nuclear reactions: TDHF
- High energy: kinetic *Both Deficient*
- Kadanoff-Baym equations attractive as generalizing either of the existing approaches.
- Findings so far: It should be possible to switch on the self-consistent interactions adiabatically.
- Even for the coherent mean-field evolution, forward in time, only a limited range ($\lesssim \hbar/p_F$) of the Green's function matrix elements matters.
- Discarding far-off spatial elements corresponds to an averaging over a short scale in momenta.
- The far-off elements important for temporal reversibility.

Currently: correlations in 1D. Next: mean-field in 3D

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