Towards Quantum Transport for Central Nuclear Reactions

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Hot & Cold Baryonic Matter 2010

Budapest - Hungary

15-20 August, 2010

Coming from US, hard acts to follow include Kelly Pickler

X

American Idol finalist, recipient of Country Music TV awards

Outline

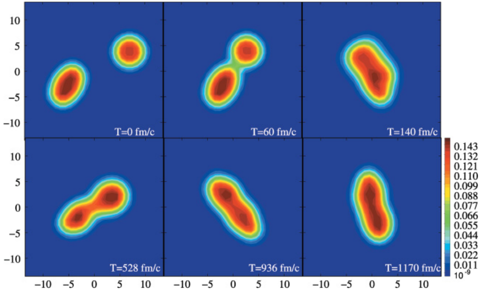
Time-Dependent Hartree-Fock

Sensible for degenerate low-energy reacting systems.

Time-dependent Slater determinant

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

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



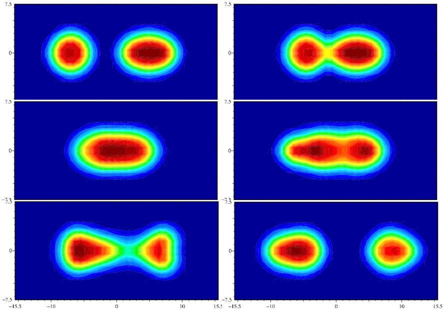
semicentral ^{22}Ne + ^{16}O

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

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

Time-Dependent Hartree-Fock in Practice

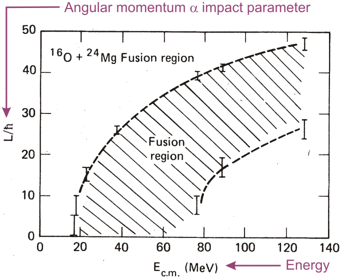
Theory predicts a low-ℓ fusion window developing at higher energies in reactions.

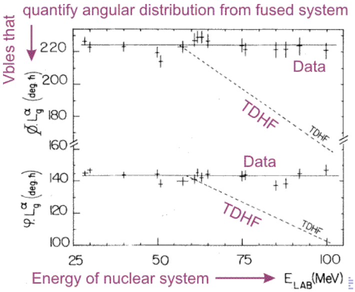


head-on ^{16}O+^{22}Ne at $E_{cm} = 95\,$MeV

Umar & Oberacker '07

Data: NO low-ℓ fusion window!





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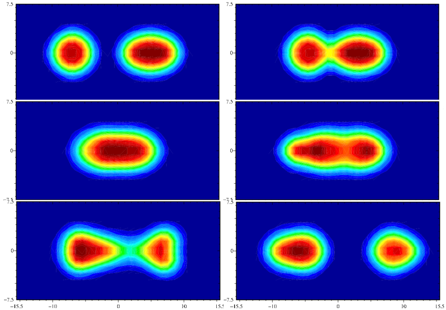

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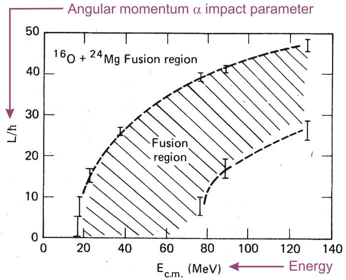
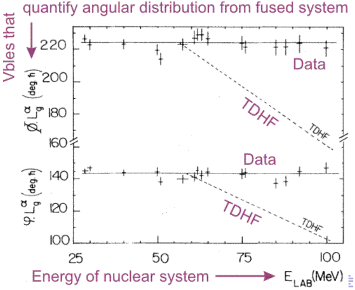
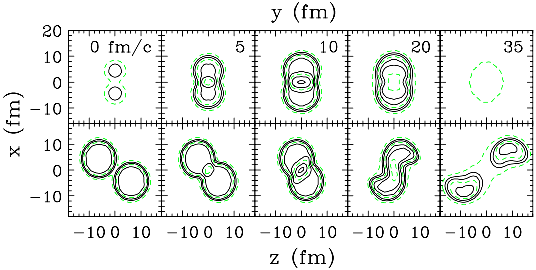




High Energies: Boltzmann Equation

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



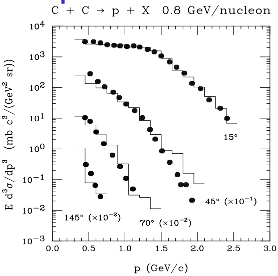
Au+Au at 400 MeV/nucleon

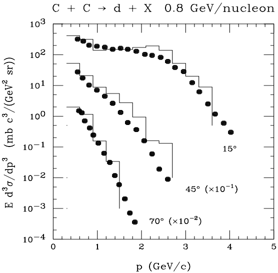
P.D. Nucl Phys A673 (2000) 375

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

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

$i\,\Sigma(1,1') = \langle\Phi|\,T\left\{j(1)\,j^\dagger(1')\right\}|\Phi\rangle_{\rm irr}$ 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 $-iG^<(1,1') = \langle\psi^\dagger(1')\,\psi(1)\rangle$,

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

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

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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

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

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

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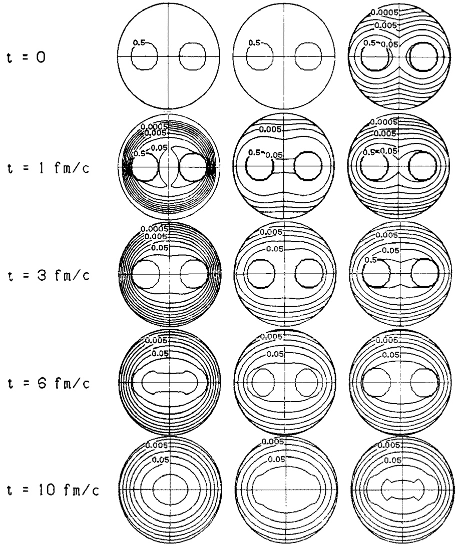
Equilibration in Uniform Matter

Boltzmann GF GF+ini corr

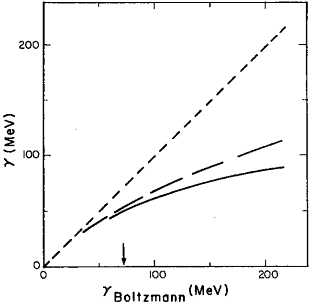


400 MeV/nucleon model of early reaction dynamics test of Boltzmann eq

G, Σ diagonal in $\boldsymbol{p}$

$\boxed{\text{8D} \rightarrow \text{5D}} - 1D = 4D$ (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:

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

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

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

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

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

Initial State Through Adiabatic Evolution

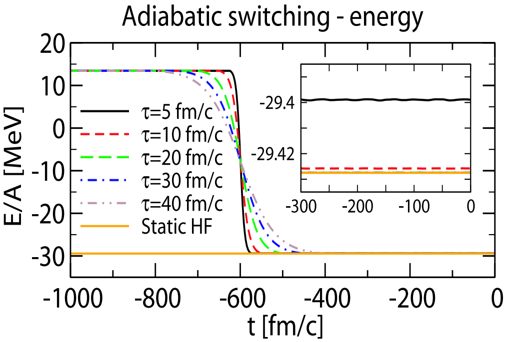
Optimally, the same code for reaction dynamics and initial-state preparation. Adiabatic switching, from harmonic oscillator to self-consistent mean-field solution:

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

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

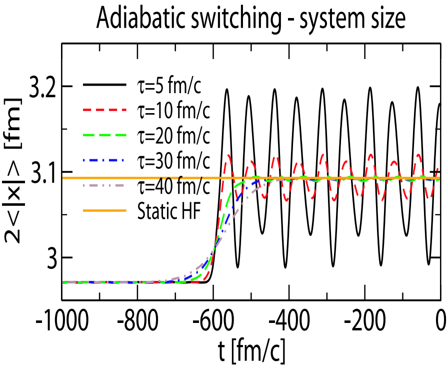
E.g.

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

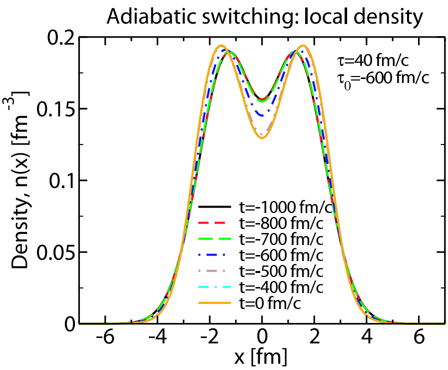


Adiabatic Switching of Interaction

System Size

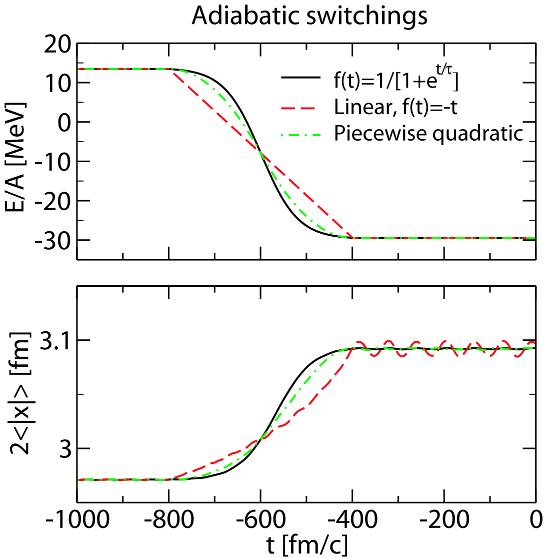


Density



from HO to self-consistent solution

Dependence on Transition Function



paradox: slower change yields inferior results than smoother

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

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

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

Break-up

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

X

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

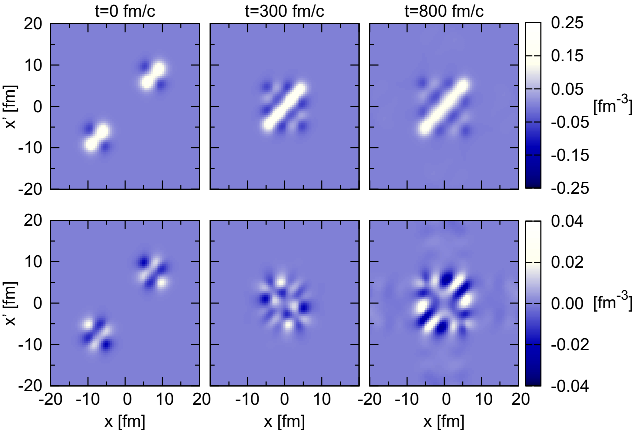
Collisions at $E_{\rm cm}/A = 25\,{\rm MeV}$

Multifragmentation

Density $n(x,t)$ and real 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



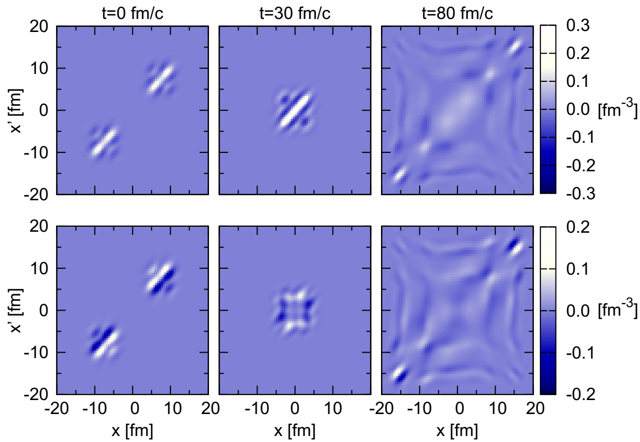
Re

symmetric

Im

antisymmetric

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



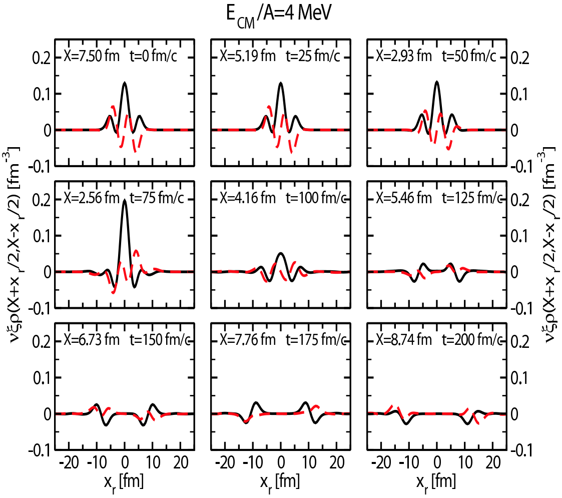
Re

symmetric

Im

antisymmetric

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

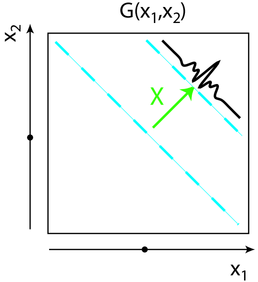


$E_{cm}/A = 4\,\mathrm{MeV}$

each panel another t

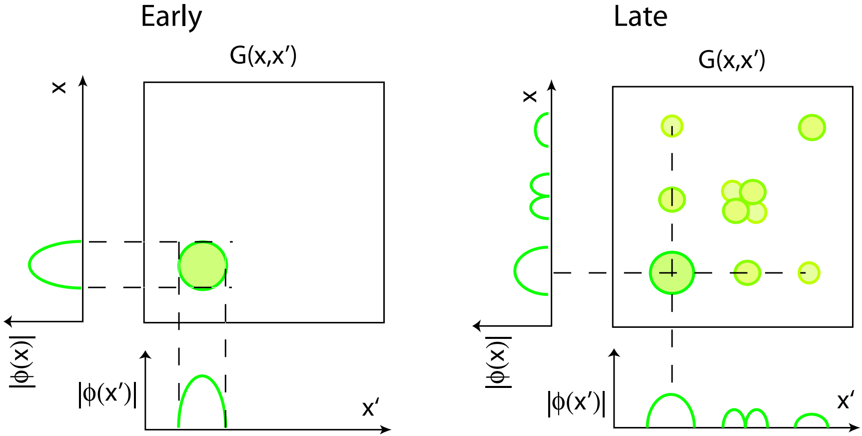
Real part
- symmetric

Imaginary part
- antisymmetric



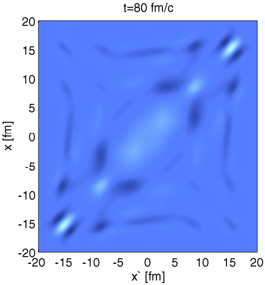
Origin of Far-Off Terms in $G^<(x, x', t)$

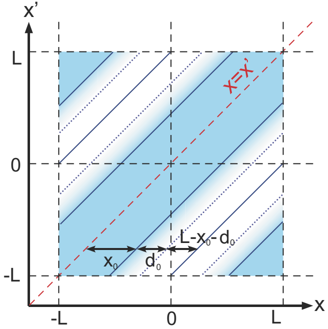
$$G^<(x, x', t) = \sum_\alpha n_\alpha \, \varphi_\alpha(x, t) \, \varphi^*_\alpha(x', t)$$



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.

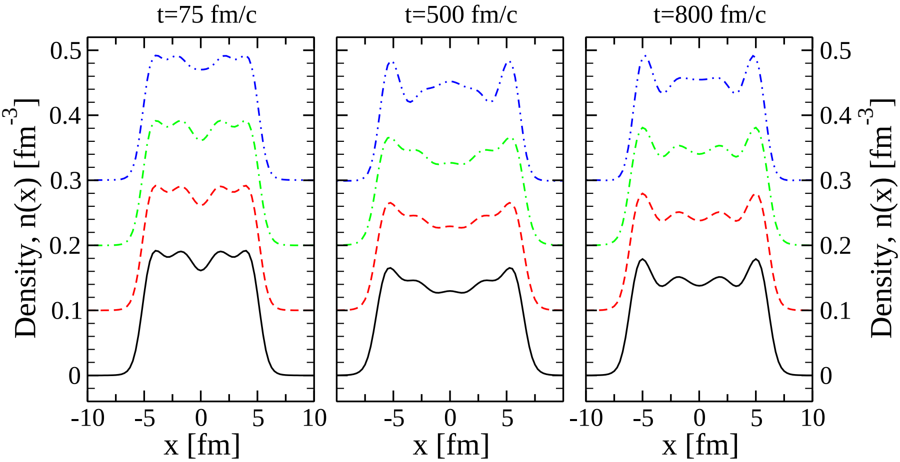




Evolution using imaginary superoperator suppressing large $|x - x'|$

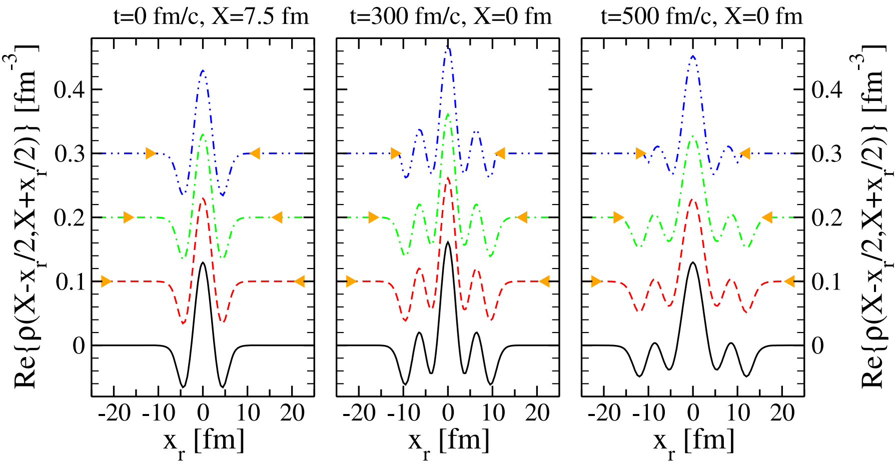
$$G^<(x, x', t+\Delta t) \sim e^{-i(\epsilon(x)+iW(x,x'))\Delta t}\, G^<(x, x', t)\, e^{+i(\epsilon(x)-iW(x,x'))\Delta t}$$

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



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

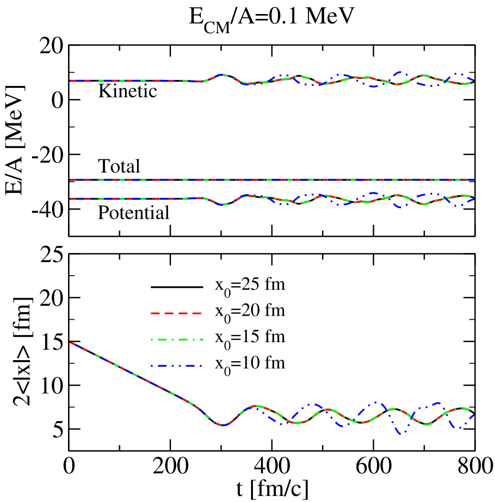
Evolution with Erased Elements at $E_{cm}/A = 0.1$ MeV



Different cuts across the diagonal of the density matrix

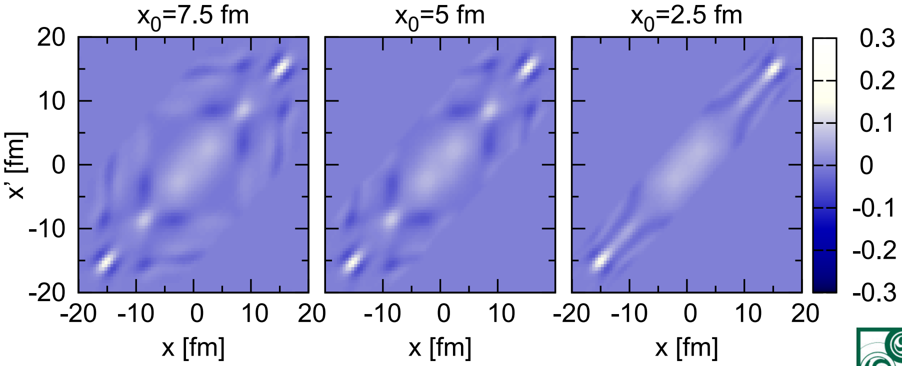
Evolution with Erased Elements at $E_{cm}/A = 0.1$ MeV

Energy and System Size for Different Suppressions

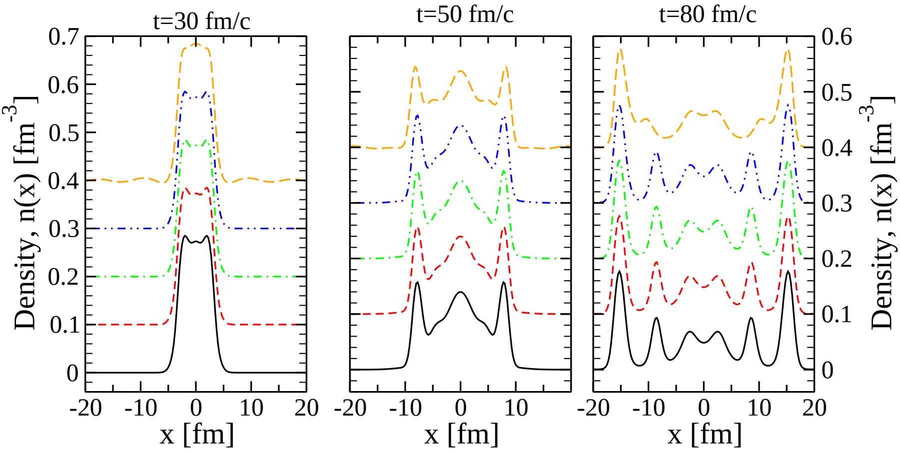


Evolution with Erased Elements at $E_{cm}/A = 25\,\mathrm{MeV}$

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

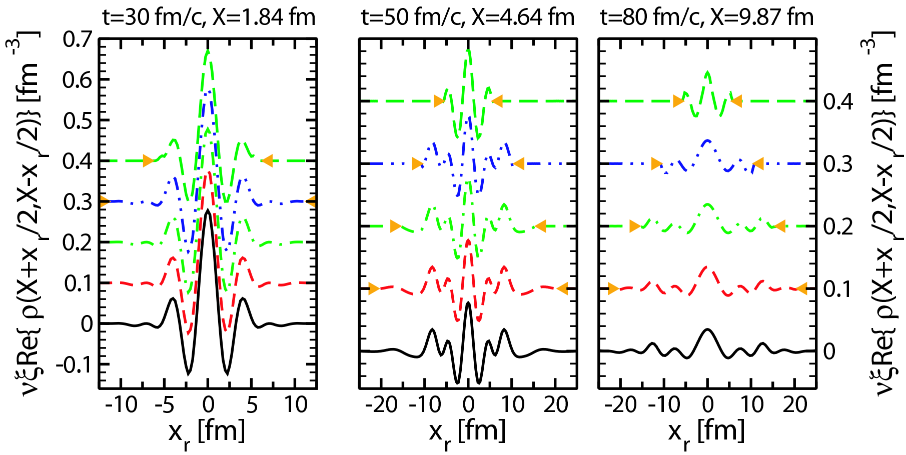


Evolution with Erased Elements at $E_{cm}/A = 25\,\text{MeV}$



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

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



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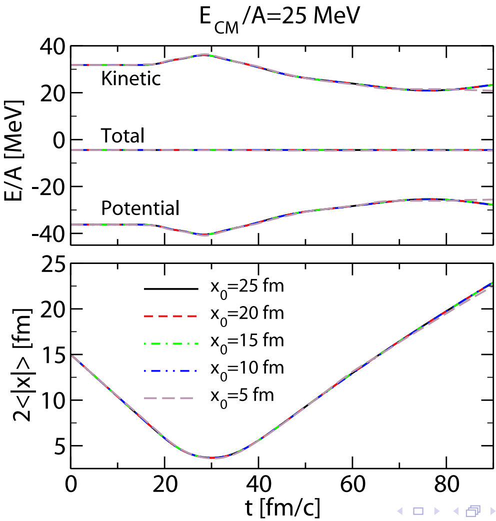

Wigner-Function Evolution

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

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

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

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

Cutting Elements $\leftrightarrow$ Averaging Momenta

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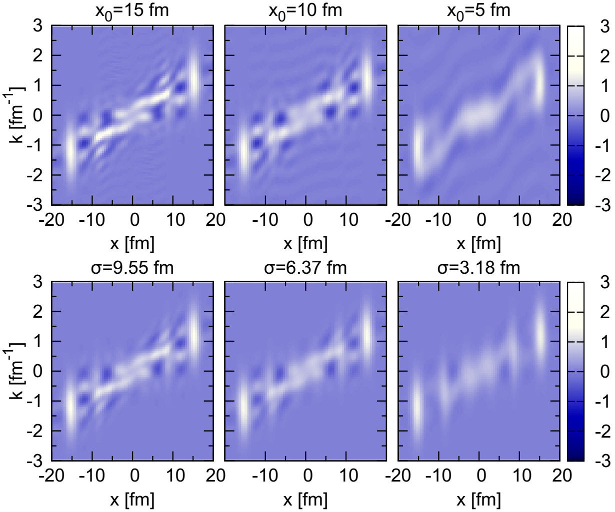
&= \int \mathrm{d}q\, \mathrm{e}^{-(p-q)^2\,\sigma^2/2} \int \mathrm{d}y\, \mathrm{e}^{-iqy}\, G^<\left(x+\frac{y}{2}, x-\frac{y}{2}\right) \\
&\equiv \int \mathrm{d}q\, \mathrm{e}^{-(p-q)^2\,\sigma^2/2}\, f(q,x)
\end{aligned}$$

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

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

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



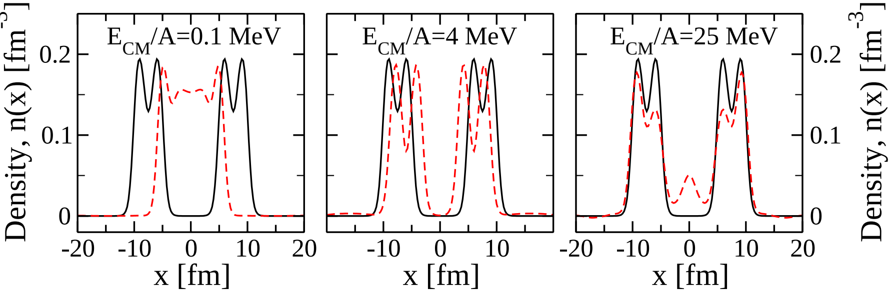
Bottom: Wigner function from Gaussian averaging

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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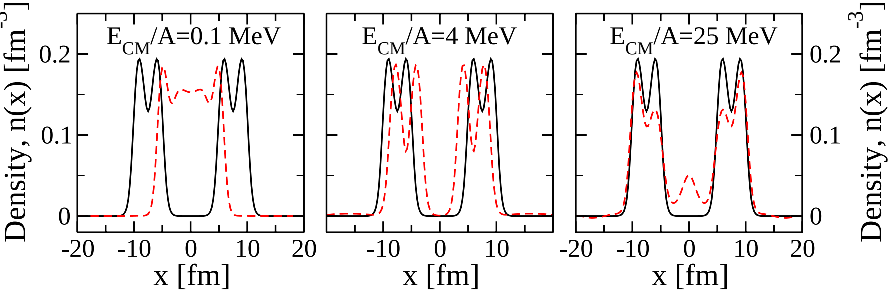

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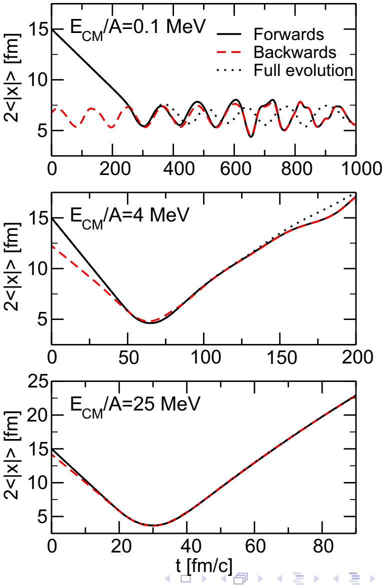
Forward and Backward in Time!

System Size

Dotted: complete evolution, time-reversible

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

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



Switching-On Correlations

Slab placed in external harmonic-oscillator potential.

At time $t = 0$ collisions/correlations switched on.

Shown: density in p, scattering-in rate in p, density in x occupations, slab size, energy breakdown

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.
- System expansion $\Rightarrow$ Growing redundancy of info
- The far-off elements important for temporal reversibility.

Currently: correlations in 1D. Next: mean-field in 2/3D

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