# Quantum Transport for Nuclear Reactions: From Basics to Perspective on Irreversibility

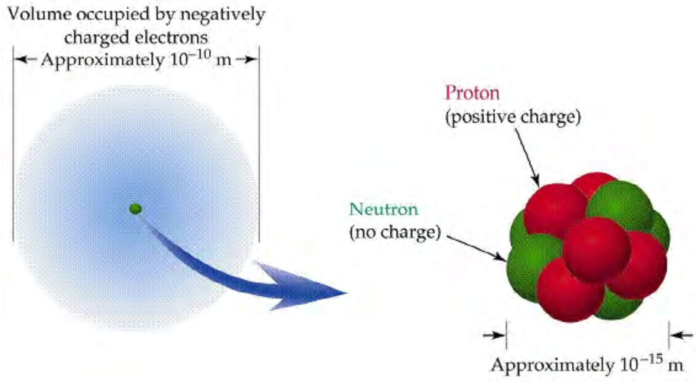
Pawel Danielewicz

Isolated Quantum Many-Body systems out of Equilibrium: From Unitary Time Evolution to Quantum Kinetic Equations

Physikzentrum Bad Honnef

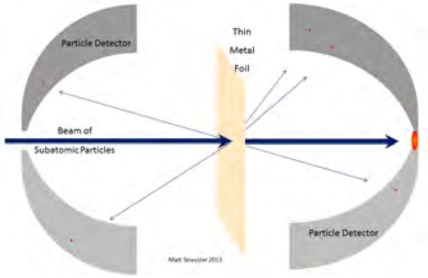
November 30-December 3, 2015

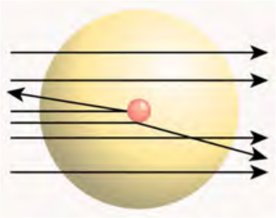
# Nuclei: Best Isolated Systems

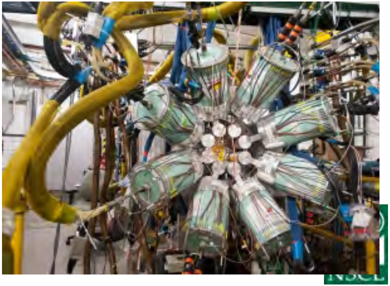


# Nuclear Reactions

Accelerated ions directed
onto foil or gas target



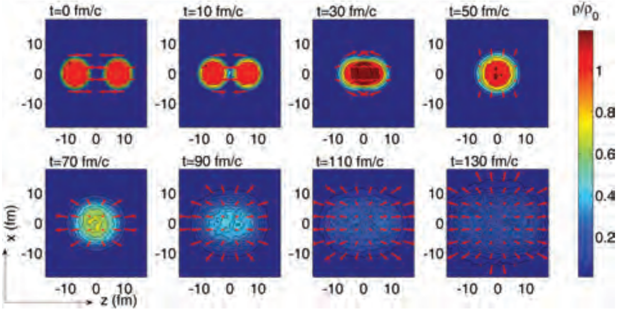





# Reaction Dynamics

E.g. head-on $^{129}$Xe + $^{120}$Sn at 50 MeV/nucleon

Su *et al* PRC89(14)014619




Conclusions ⇒

# Reaction Phenomenology

Dynamic quantities: Wigner functions of different particles $X$

$$f(\boldsymbol{p}, \boldsymbol{R}, t) = \int \mathrm{d}\boldsymbol{r}\, \mathrm{e}^{-i\boldsymbol{p}\boldsymbol{r}} \langle \hat{\phi}_X^{\dagger}(\boldsymbol{R} - \boldsymbol{r}/2, t)\, \hat{\phi}_X(\boldsymbol{R} + \boldsymbol{r}/2, t) \rangle$$

Relativistic energy functional $\mathcal{E}$ following Landau Fermi-liquid theory

$$\mathcal{E} = \mathcal{E}\{f_X\}$$

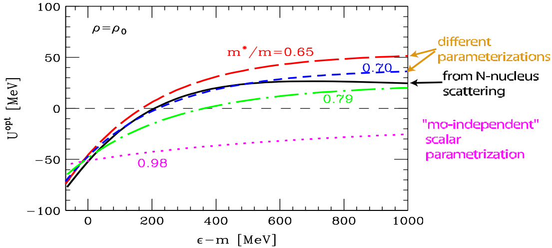
Single-particle energies $\epsilon_X(\boldsymbol{p}, \boldsymbol{r}, t)$ and optical potentials $U_X$

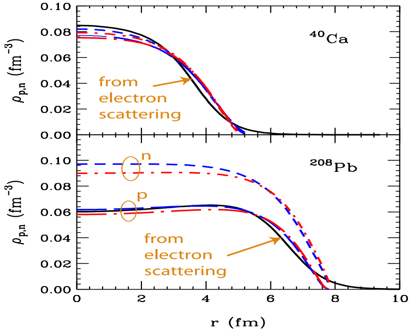
$$\epsilon_X(\boldsymbol{p}, \boldsymbol{r}, t) = \frac{\delta \mathcal{E}}{\delta f_X(\boldsymbol{p}, \boldsymbol{r}, t)} \qquad U_X = \epsilon_X - \sqrt{p^2 + m_X^2}$$

Energy functional constrained by ground-state measurements.
*Minimization yields Thomas-Fermi theory.*

# Ground-State Constraints

Potential from p-scattering (Hama *et al.* PRC41(90)2737) & parameterizations




Ground-state densities from electron scattering and from functional minimization.

From $E\{f\} = min$ :

$$0 = \epsilon\left(p^F(\rho)\right) - 2\,a_{gr}\,\nabla^2\left(\frac{\rho}{\rho_0}\right) - \mu$$

$\Rightarrow$ $\boxed{\text{Thomas-Fermi eq.}}$

# Transport Theory

Wigner functions satisfy Boltzmann equations:

$$\boxed{\frac{\partial f}{\partial t} + \frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{p}} \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{r}} \frac{\partial f}{\partial \mathbf{p}} = I}$$

Particle species $X$: nucleons, pions, $\Delta$ resonances, $N^*$ resonances, deuterons, tritons...

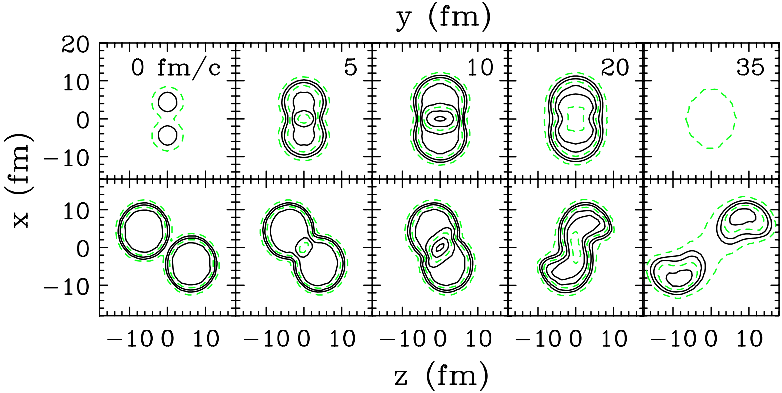
Important: Collision integral $I$ is *local*, consistently with Landau Fermi-liquid theory. Those nonlocal lead to problems relativistically.

Entropy then is such as for ideal gas:

$$S(t) = -\int d\mathbf{r} \int d\boldsymbol{p} \sum_X \left[ f_X \log f_X \mp (1 \mp f_X) \log (1 \mp f_X) \right]$$

# Reaction Simulations

Contour plots for spatial density



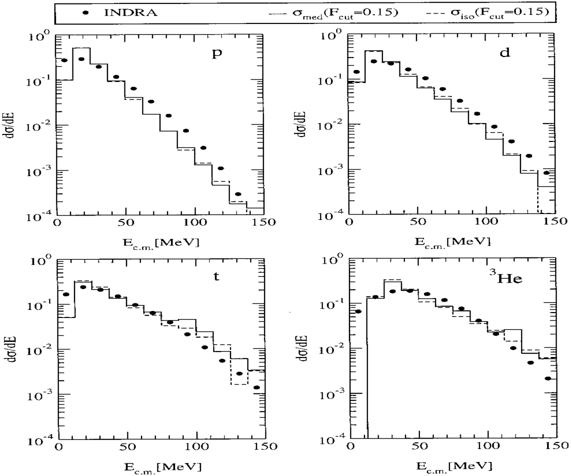

Au + Au at 400 MeV/nucl (PD)

# Low-Energy Comparison to INDRA

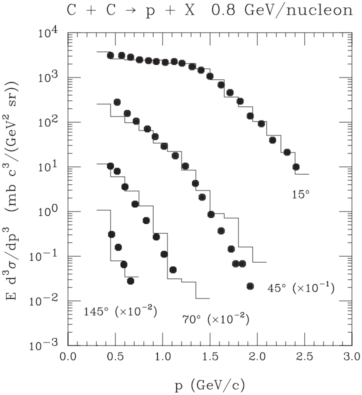
$^{129}$Xe+$^{119}$Sn at 50 MeV/nucleon

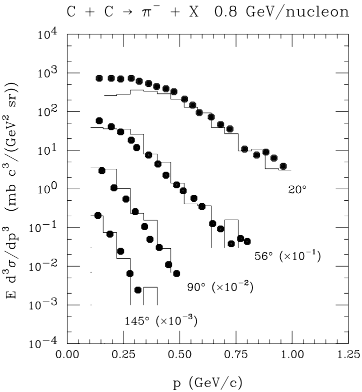
points - data
Gorio *et al*
EPJA7(00)245

histograms - calculations
Kuhrts, Beyer *et al*
PRC63(01)034605



# High-Energy Inclusive Data



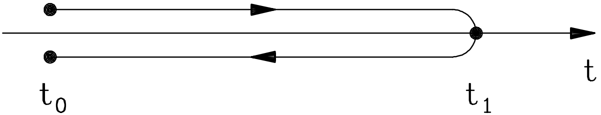




proton & pion spectra

points - data Nagamiya *et al* PRC24(81)971
histograms - calculations

# Evolution Contour

$$
\begin{aligned}
\langle \hat{O}_H(t_1) \rangle &= \langle T^a \left[ \exp \left( -i \int_{t_1}^{t_0} dt' \, \hat{H}_I^1(t') \right) \right] \hat{O}_I(t_1) \\
&\quad \times T^c \left[ \exp \left( -i \int_{t_0}^{t_1} dt' \, \hat{H}_I^1(t') \right) \right] \rangle \\
&= \langle T \left[ \exp \left( -i \, \fint_{t_0}^{t_0} dt' \, \hat{H}_I^1(t') \right) \hat{O}_I(t_1) \right] \rangle \, ,
\end{aligned}
$$

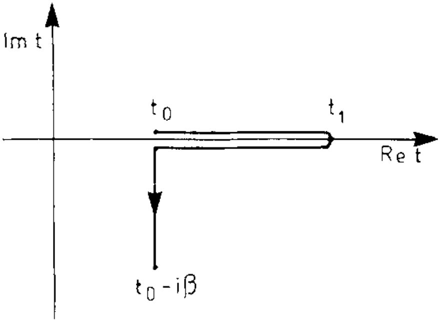



If initial state admits Wick decomposition, expectation value expanded perturbatively in terms of $V$ and noninteracting 1-ptcle Green's functions on contour; *$T$ orders on contour*

$$
iG_0(\mathbf{x}, t, \mathbf{x}', t') = \langle T \left[ \hat{\psi}_I(\mathbf{x}, t) \hat{\psi}_I^\dagger(\mathbf{x}', t') \right] \rangle
$$

# Contour for Equilibrium Initial State

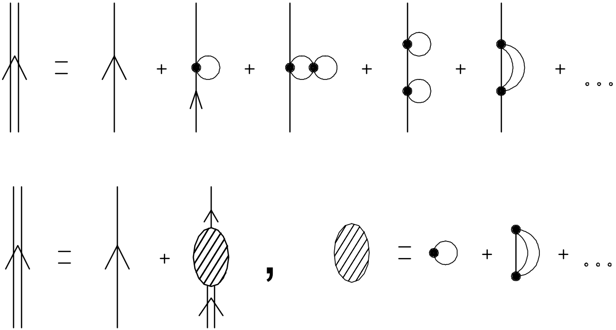
$$\hat{\rho} = \mathrm{e}^{-\beta \hat{H}} \qquad \langle \hat{O}_H(t_1) \rangle = \mathrm{Tr}\left[ \hat{\rho}\, \hat{O}_H(t_1) \right]$$



# Dyson Equation

Towards intrinsically closed description: resummation of perturbation expansion for Green's function *on contour*

$$G = G_0 + G_0\,\Sigma\,G$$



# Formal Solution

Outcome of evolution:

$$\mp i G^{<}(x,t;x',t') = \int \mathrm{d}x_1\,\mathrm{d}t_1\,\mathrm{d}x_1'\,\mathrm{d}t_1'\; G^{+}(x,t;x_1,t_1) \times(\mp i)\Sigma^{<}(x_1,t_1;x_1',t_1')\,G^{-}(x,t;x_1,t_1)$$

and

$$\mp i\Sigma^{<}(x,t;x',t') = \langle \hat{j}^{\dagger}(x',t')\,\hat{j}(x,t)\rangle_{irred}$$

where the source $j$ is

$$\hat{j}(x,t) = \left[\hat{\psi}(\mathbf{x},t),\hat{H}^{1}\right]$$

Finite memory time...

Uniform limit w/stationary functions: thermal Green's functions $G^{>}(\boldsymbol{p},\omega) = \mathrm{e}^{\beta(\omega - \boldsymbol{v}\boldsymbol{p} - \mu)}\,G^{<}(\boldsymbol{p},\omega)$

# Differential Kadanoff-Baym Eqs

Integral Dyson Eq

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

with

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

$j \equiv [\psi, H^1]$; converted to differential eq of motion on contour:

$$G_0^{-1} \, G = \not{1} + \Sigma \, G$$

For specific order on the contour, such as yielding $-iG^<(1,1') = \langle \psi^\dagger(1') \, \psi(1) \rangle$, Kadanoff-Baym eqs:

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

# Quasiparticle Limit

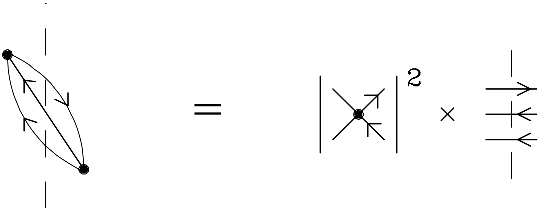
Under slow spatial and temporal changes in the system, the Green's function expressible in terms of the Wigner function $f$ and 1-ptcle energy $\epsilon_p$

$$\mp i G^<(x,t;x',t') \approx \int \mathrm{d}p\, f\Big(p; \frac{x+x'}{2}, \frac{t+t'}{2}\Big)\, \mathrm{e}^{i(p(x-x')-\epsilon_p(t-t'))}$$

Then also Boltzmann eq from Kadanoff-Baym eqs:

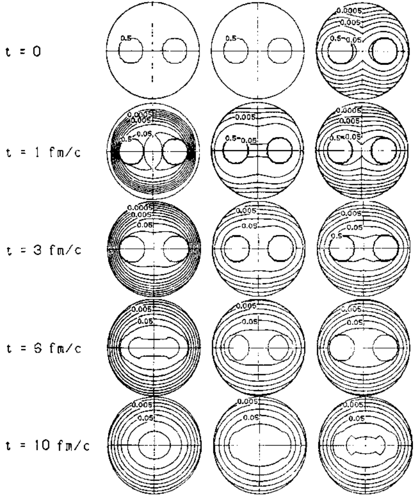
$$\frac{\partial f}{\partial t} + \frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{p}} \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial \epsilon_{\mathbf{p}}}{\partial \mathbf{r}} \frac{\partial f}{\partial \mathbf{p}} = -i\Sigma^< (1-f) - i\Sigma^> f$$

$\mp i\Sigma^<$ :



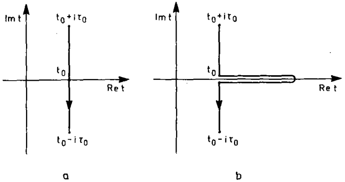
# Kadanoff-Baym in Uniform Matter: Personal Prehistory

Boltzmann GF GF+ini corr

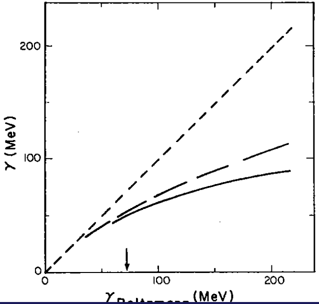



*Bourgeois gentilhomme* →quench

PD '84




Rate comparison



# Towards Reaction Simulations

Issues to consider for nonuniform matter:

- matrix (space-time) form of dynamics
- preparation of initial state
- abundance of mtx elements $(50)^8 = 4 \times 10^{13}$ ! $\sim 100\,\mathrm{TB}$

START W/MF: Ann Phys 326(11)1274

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

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

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

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

Only $t = t'$ matters for MF, so $G \leftarrow \rho$! 1D

# Towards Reaction Simulations

Issues to consider for nonuniform matter:

- matrix (space-time) form of dynamics
- preparation of initial state
- abundance of mtx elements $(50)^8 = 4 \times 10^{13}\,!$ $\sim 100\,\mathrm{TB}$

START W/MF: Ann Phys 326(11)1274

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

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

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

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

Only $t = t'$ matters for MF, so $G \leftarrow \rho$! 1D

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

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

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

Density $n(x,t)$ and real part of density matrix $\rho(x, x', t)$

x

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

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

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 $E_{\text{cm}}/A = 25\,\text{MeV}$

Multifragmentation

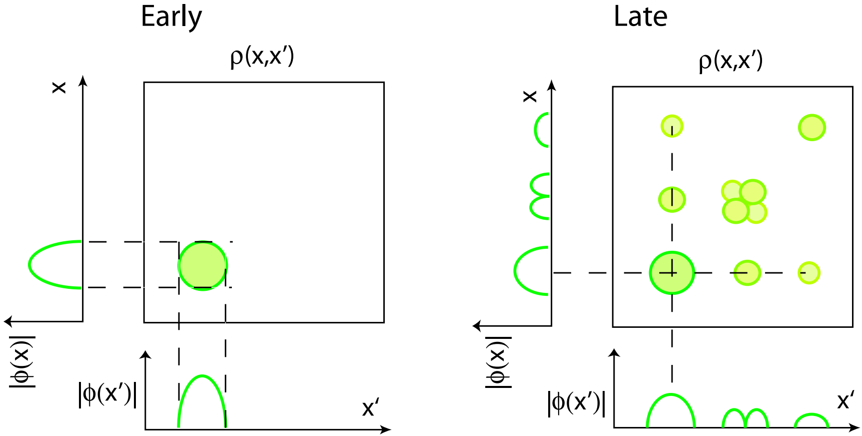
Density $n(x,t)$ and real part of density matrix $\rho(x,x',t)$

X

Density is identical with the diagonal: $n(x,t) = \rho(x,x,t)$.

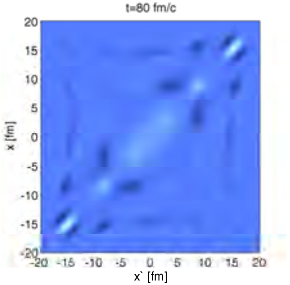
# Origin of Far-Off Terms in $\rho(x, x', t)$

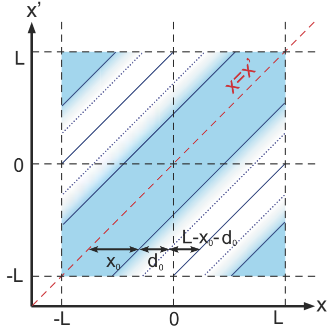
$$\rho(x, x', t) = \sum_\alpha n_\alpha \, \varphi_\alpha(x, t) \, \varphi^*_\alpha(x', t)$$



# Suppressing the Off-Diagonal Elements

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

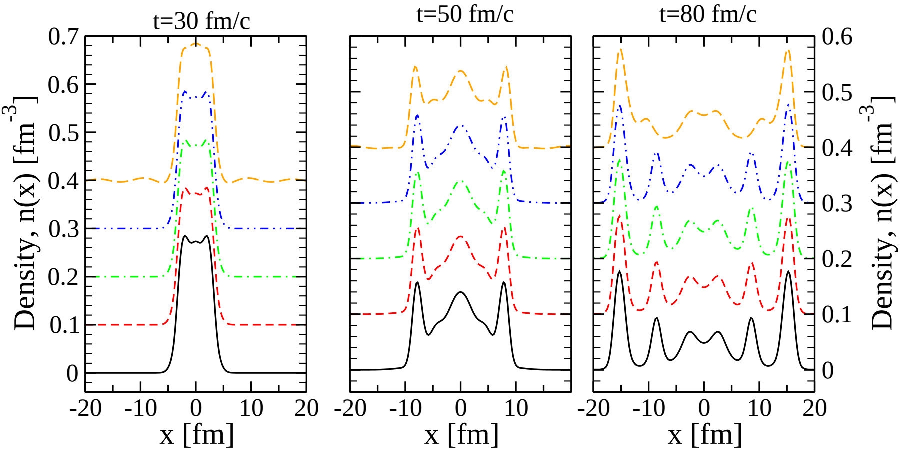



Evolution using imaginary superoperator suppressing large $|x - x'|$

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

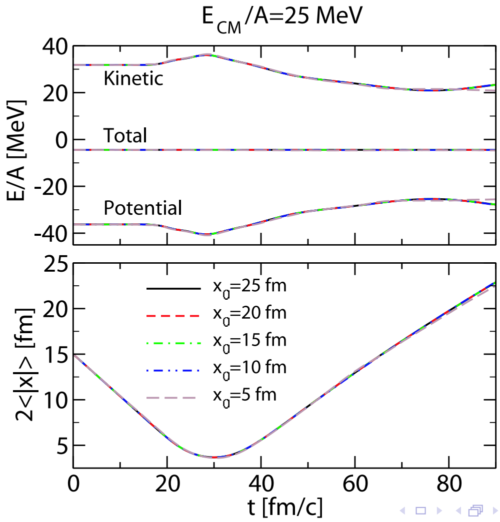
# Evolution with Erased Elements at $E_{\rm cm}/A = 25\,\rm MeV$




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

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

Energy and System Size for Different Suppressions



# Wigner-Function Evolution

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

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

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

# Cutting Elements $\leftrightarrow$ Averaging Momenta

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

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

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

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

# Cutting Elements $\leftrightarrow$ Averaging Momenta

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

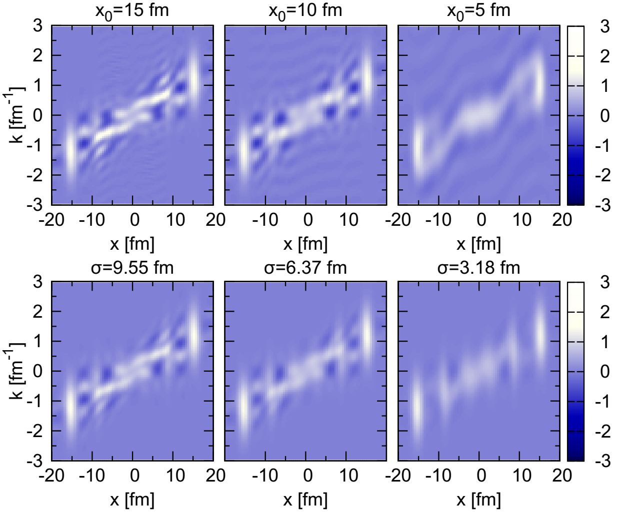
Wigner f. from $\rho$ with far-off elements cut-off by $\mathrm{e}^{-y^2/2\sigma^2}$:

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

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

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

Top: Wigner f from $\rho$ with elements cut off (late stage)

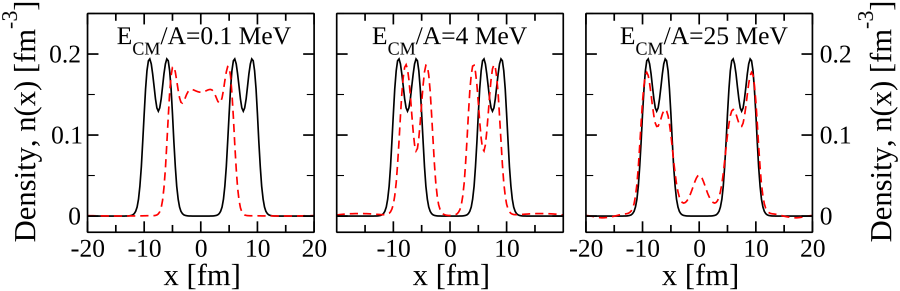



Bottom: Wigner function from Gaussian averaging

# Forward and Backward in Time!

Systems evolved forward in time, with elements at $|x - x'| > 10$ fm suppressed. After reaction completion, evolved back to $t = 0$, still with the far-off elements suppressed.

$t = 0$:

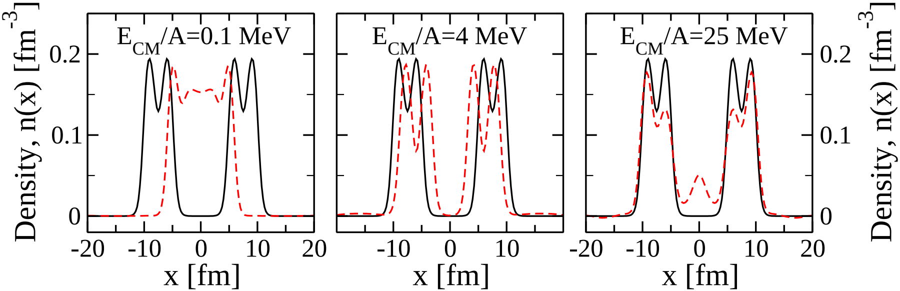



Far off-diagonal elements are important for coming back to the initial state! Without the elements, remote past looks like remote future.

# Forward and Backward in Time!

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.

$t = 0$:




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

# Correlated Evolution: A=16 Finite System

Uncorrelated initial state in HO trap: density mo/conf space, self-energy, net energy…

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion...

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion…

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion...

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion. . .

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion...

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion…

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion. . .

*Thanks: NSF PHY-1520971*

# Conclusions

- Semiclassical phenomenology, with roots in Landau Fermi-liquid theory, dominates central-reaction simulations
- Kadanoff-Baym eqs attractive as generalizing the transport and integrating well with practice for nuclear structure
- Findings so far: Even for coherent mean-field evolution only limited range ($\lesssim \hbar/p_F$) of GF matrix elements matters
- Discarding far-off spatial elements corresponds to averaging over short scale in momenta
- Discarding will be facilitated by coordinate rotation and allow to approach classical limit with impunity
- 2/3D Outlook: Systems locally close to isotropy - expansion in spherical cartesian harmonics
- Time-arrow for irreversibility $\Leftrightarrow$ Arrow for Universe expansion…

*Thanks: NSF PHY-1520971*