Time-dependent Green's Functions method for nuclear reactions

Mean-field & correlated 1D evolution

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Non-Equilibrium Dynamics Workshop
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Collaborators
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B. Barker (MSU, NSCL)
M. Buchler

Ann. Phys. **326**, 1274 (2011)

Outline

First principles in nuclear physics

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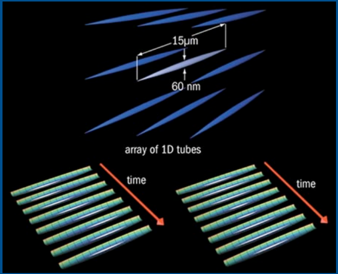
	Nuclear structure	Nuclear reactions
Phenomenological	• Fit effective interactions to stable nuclei • Rely on Hartree-Fock approximation • Extrapolate exotic nuclei • Fastest way to objective	Time Dependent Hartree-Fock
First principles	• Microscopic NN force • Use many-body theory to describe nuclear medium • Build exotic nuclei • Safest way to objective	?

Research program

Kadanoff-Baym

- *Full 1D simulations*
- *Test numerical propagation schemes*
- *Assessment of many-body approximations*

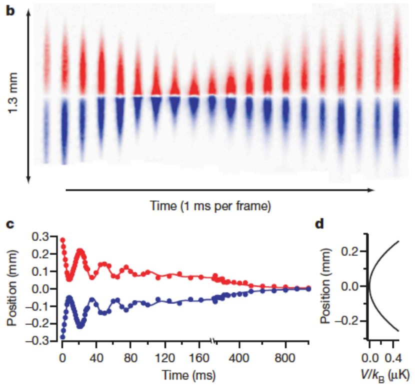
1D ultracold gases



- Why start with 1D systems?
- 1D correlated evolution for dynamics of ultracold atoms
- Progressive understanding of higher D
- Ultimately: correlated nuclear 3D evolution

Research program

Collisions of spin ↑ & ↓ ^{6}Li atom clouds



Sommer *et al.*, Nature 472, 201 (2011)

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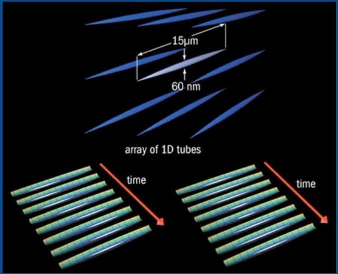

Nuclear physics

- Why start with 1D systems?
- 1D correlated evolution for dynamics of ultracold atoms
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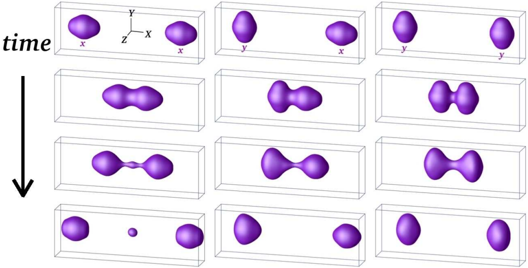
Research program

$^{238}U + ^{238}U$ TDHF simulation (Saclay)



Golabek & Simenel, PRL **103**, 042701 (2009)

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Nuclear time-dependent correlations

- Experience already gathered in:
  - Uniform systems

Wong & Tang, PRL 40, 1070 (1978)
Danielewicz, Ann. Phys. 152, 239 (1984)
H. S. Köhler, PRC 51 3232 (1995)

  - Nuclei

J. Aichelin & G. Bertsch, PRC 31, 1730 (1985)
Tohyama, PRC 36, 187 (1987)
C. Greiner & S. Leupold, Ann. Phys. 270, 328 (1998)
W. Cassing et al., Nucl. Phys. A 665, 377 (2000)

- Expected physical effects
  - Thermalization ($0 < n_\alpha < 1$)
  - Damping of collective modes
- Correlations in the initial state
  - Adiabatic switching on of correlations?
  - Imaginary time evolution
- Testing ground calculations: 1D fermions
  - Do 1D fermions inhomogeneous actually thermalize?
  - Test with mock gaussian NN force

Kadanoff-Baym equations

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

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

$$\left\{ -i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} \right\} \mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}') = \int \mathrm{d}\bar{\mathbf{r}}_1 \mathcal{G}^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}})\Sigma_{HF}(\bar{\mathbf{1}}\mathbf{1}')$$
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- Evolution of non-equilibrium systems from general principles
- Include correlation and memory effects, via self-energies
- Complicated numerical solution, but very universal framework

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

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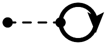
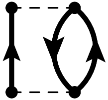
$\Sigma_{HF} \Rightarrow$  $\Sigma^{\lessgtr} \Rightarrow$ 

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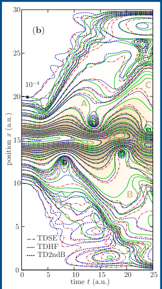
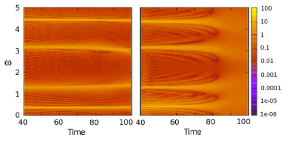
Kadanoff-Baym equations

Atoms & molecules



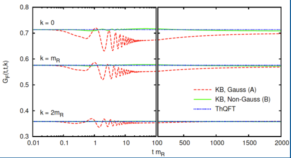
Dahlen, van Leeuwen, PRL **98**, 153004 (2007)
Balzer, Bonitz et al., PRA **81**, 022510 (2010)
Balzer, Bonitz et al., PRA **82**, 033427 (2010)

Transport in nanostructures



Stefanucci & Almbladh, JPG **35**, 17 (2006)
Myohanen, Stan, et al., PRB **80**, 115107 (2009)
von Friesen, et al., PRL **103**, 176404 (2009)
Perfetto & Stefanucci, EPL **95**, 10006 (2011)

Nonequilibrium QFT



Aarts & Berges, PRD 64, 105010 (2001)
Garny & Muller, PRD **80**, 085011 (2009)
Berges et al., PRL **100**, 085011 (2009)
Kronenwett & Gasenzer, APB **102**, 469 (2011)

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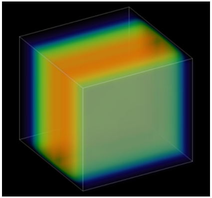
Collisions of 1D slabs

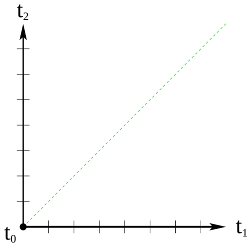


- Frozen & extended y, z coordinates, dynamics in x
- Simple zero-range mean field (1D-3D connection)

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

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

Mean-field evolution: implementation



- The mean-field is time-local & memory-less

$$\Sigma_{HF}(\mathbf{12}) = \delta(t_1 - t_2)\,\Sigma_{HF}(x_1, x_2) \Rightarrow \mathcal{G}^{\lessgtr}(t_1, t_2) \to \mathcal{G}^{\lessgtr}(t_1 = t_2 = t)$$

- KB equations reduce to single differential equation for $\mathcal{G}^<$

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

- Implemented via the Split Operator Method:

$$\mathcal{G}^<(t + \Delta t) \sim e^{-i\left\{\frac{k^2}{2m} + U(x)\right\}\frac{\Delta t}{\hbar}}\,\mathcal{G}^<(t)\,e^{+i\left\{\frac{k'^2}{2m} + U(x')\right\}\frac{\Delta t}{\hbar}}$$

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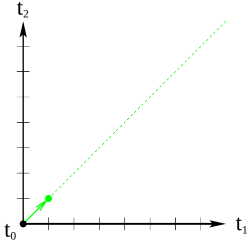
Mean-field evolution: implementation



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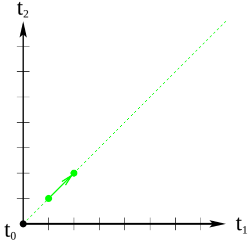

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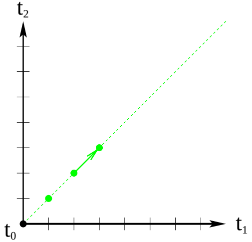

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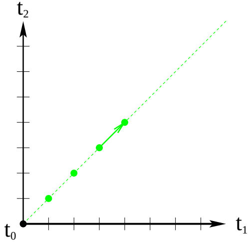

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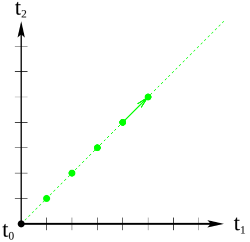

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Mean-field TDGF vs. TDHF

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Time-dependent Green's functions

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- A single equation for an N_x x N_x matrix
- Naturally extended to correlated case via KB
- Relatively unknown for nuclear systems

Time-dependent Hartree-Fock

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

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

end

- N_a equations for vectors of dim=N_x
- Limited to mean-field approximation
- Thoroughly studied for nuclear reactions

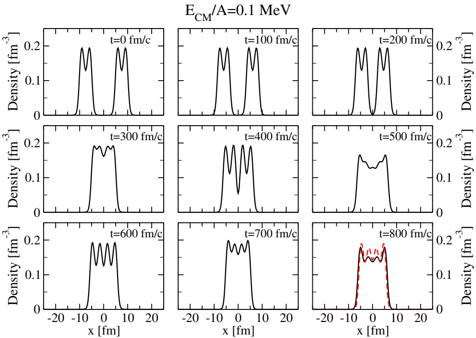
Equivalent results if same initial state and mean-field are used

Collisions of 1D slabs: fusion

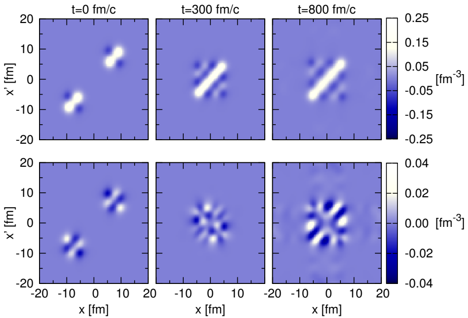
$$\mathcal{G}^{<}(x,x',P) = e^{iPx}\mathcal{G}^{<}(x,x',P=0)e^{-iPx'}$$

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

Time evolution of density profile



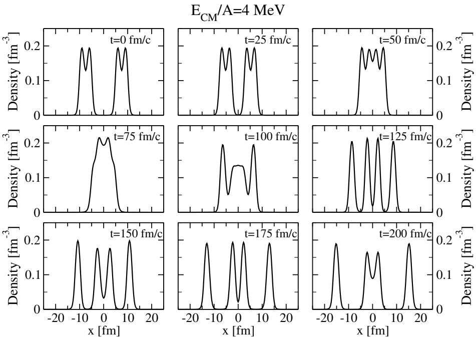
Time evolution of real part of density matrix



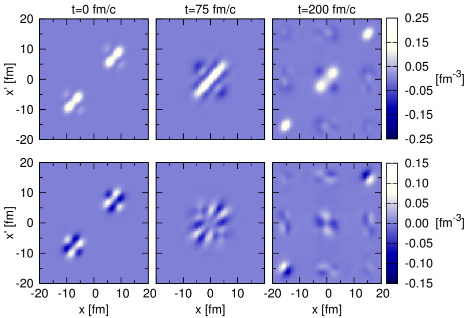
Collisions of 1D slabs: break-up

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

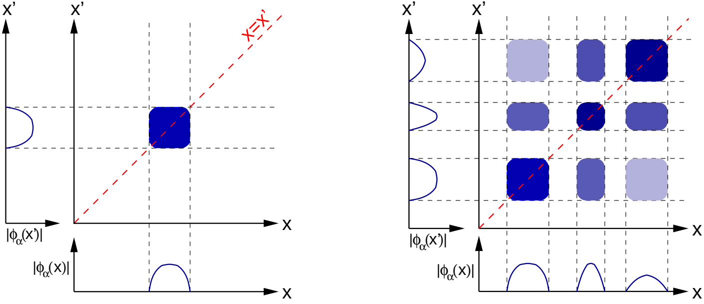
Time evolution of density profile



Time evolution of real part of density matrix



Off-diagonal elements: origin



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

Correlation between single-particle states that are far away

Collisions of 1D slabs: multifragment.

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

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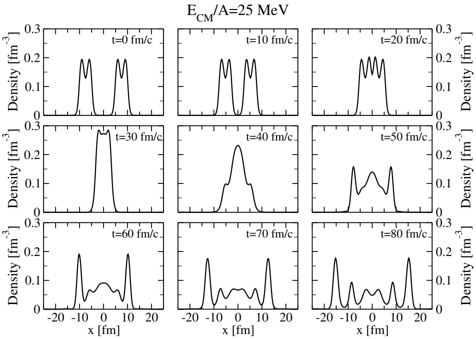
Time evolution of density profile



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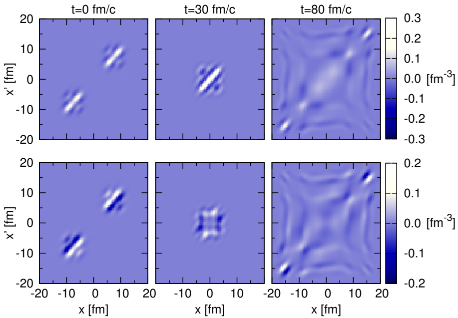
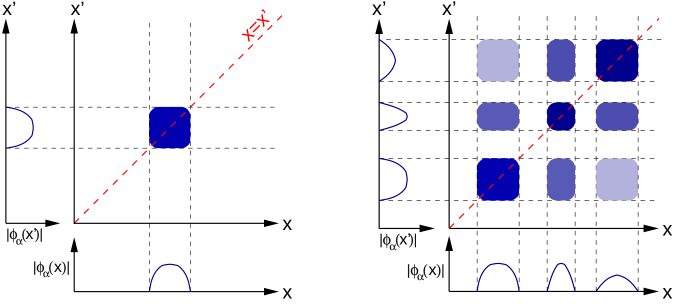


Off-diagonal elements: origin



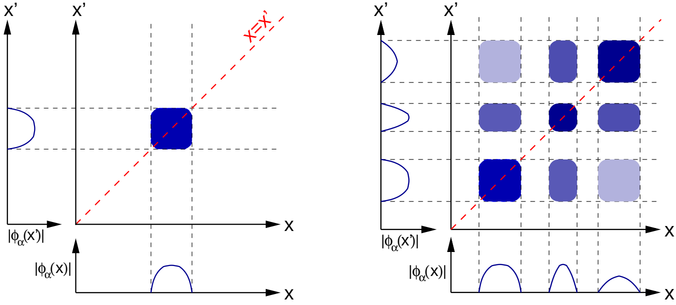
- Off-diagonal elements describe correlation of single-particle states

$$-i\mathcal{G}^<(x,x') = \sum_{\alpha=0}^{N_\alpha} \phi_\alpha(x)\phi^*_\alpha(x')$$

- Diagonal elements yield physical properties

$$n(x) = -i\mathcal{G}^<(x,x'=x) = \sum_{\alpha=0}^{N_\alpha} n_\alpha |\phi_\alpha(x)|^2 \qquad K = -i\sum_k \frac{k^2}{2m}\mathcal{G}^<(k,k'=k)$$

Off-diagonal elements: importance



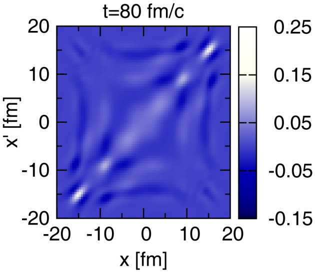
Conceptual issues:

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

Practical issues:

- Green's functions are $N_x^D \times N_x^D \times N_t^2$ matrices: $20^6 \sim 10^8$
- Eliminating off-diagonalities drastically reduces numerical cost

Off-diagonal elements: cutting procedure



- Can we delete off-diagonal elements without perturbing diagonal evolution?
- Super-operator: act in two positions of $\mathcal{G}^<$ instantaneously
- Use an imaginary super-operator 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

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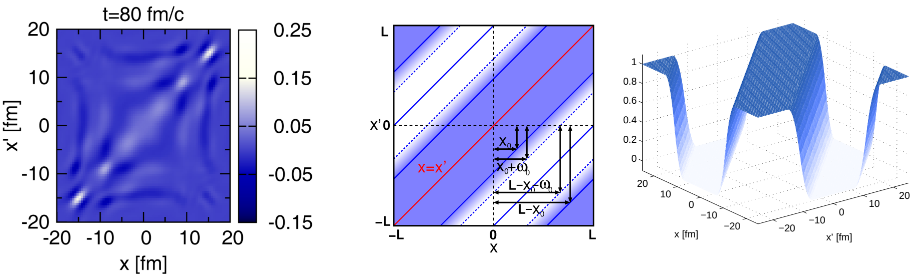

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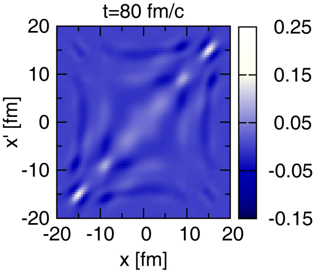

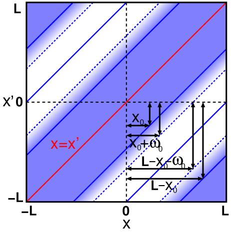

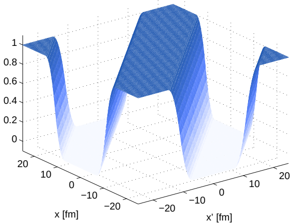

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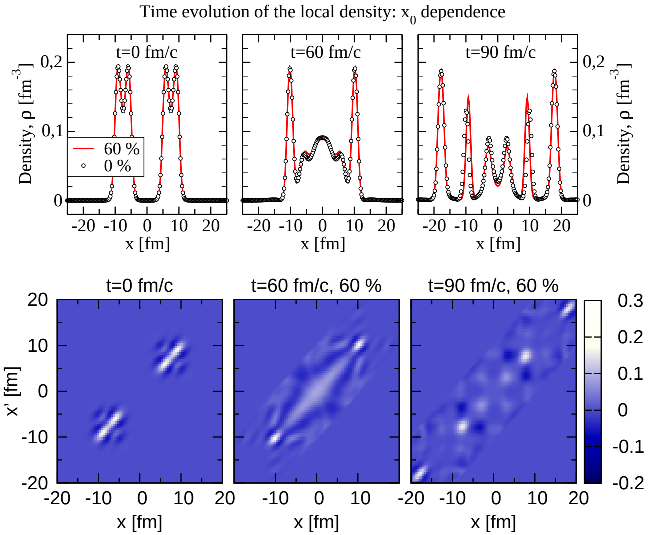
Cutting off-diagonal elements

Practicalities

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



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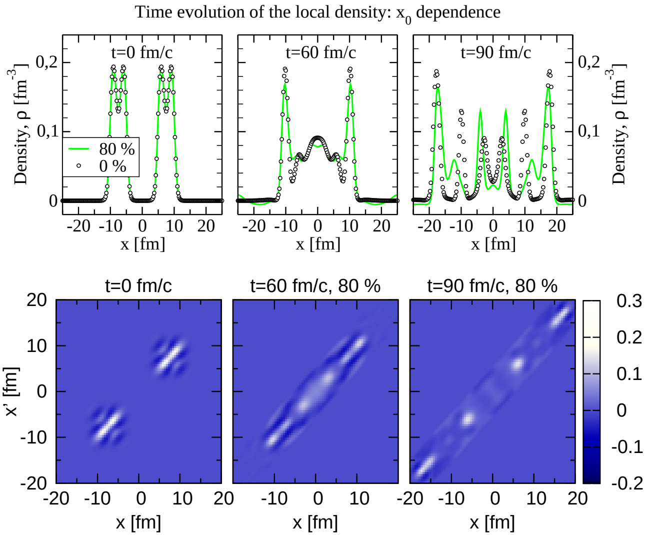
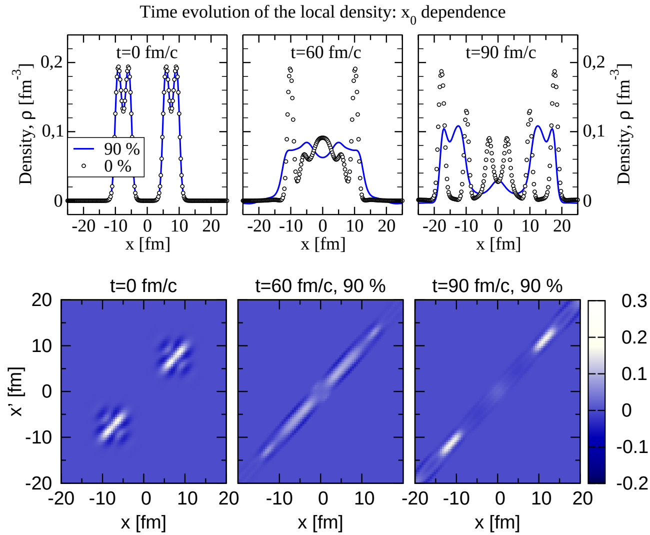
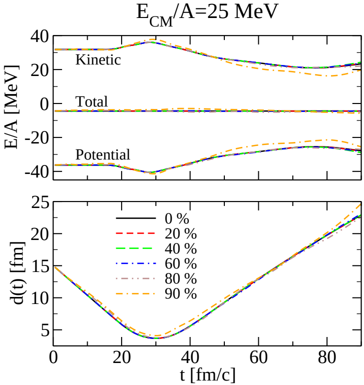
$$E_{CM}/A = 25\,\text{MeV}, |x - x'| \lesssim 5\,\text{fm} \rightarrow 80\%$$



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

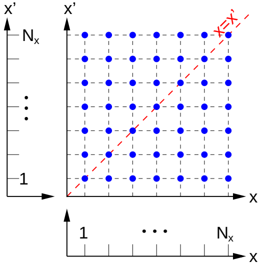


Cutting off-diagonal elements
Practicalities



- 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!

Rotated coordinate frame



- Traditional calculations performed on $N_x \times N_x$ mesh
- Periodic boundary conditions
- Rotated coordinate frame (aka Wigner space): $x_a = \frac{x+x'}{2}$, $x_r = x' - x$
- Control lengths and meshpoints $\Rightarrow$ $(L_a, N_a) \times (L_r, N_r)$
- Reduce numerical effort by factors of $2-10$

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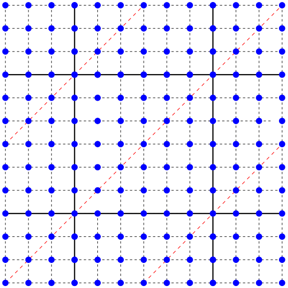

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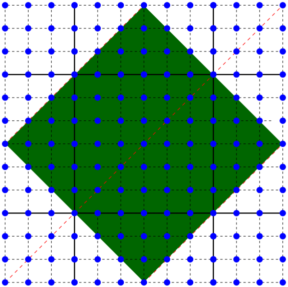

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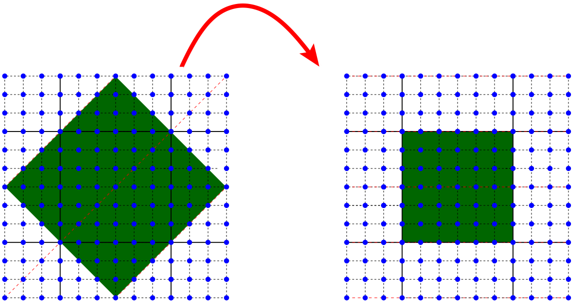

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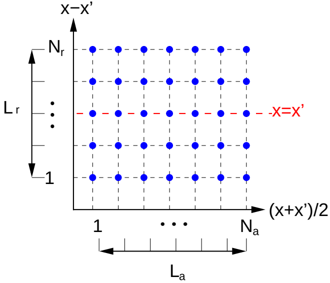

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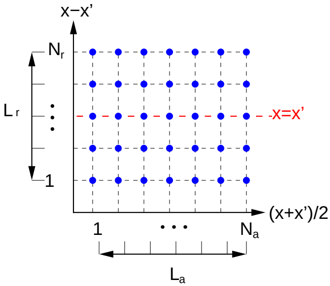

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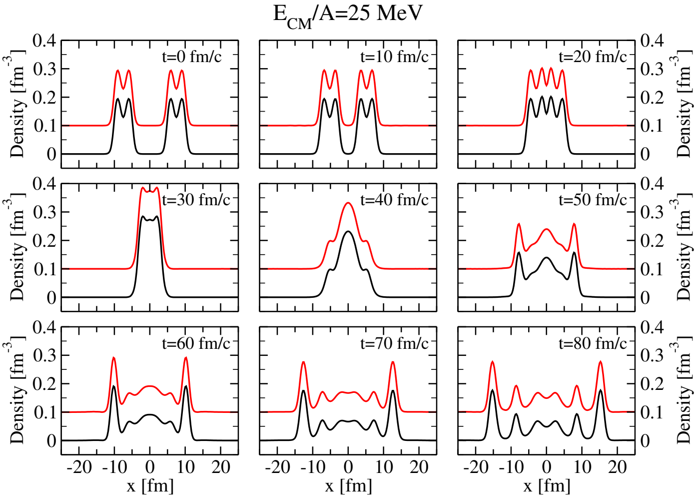
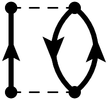
Traditional vs. rotated evolutions



Black line: full $N_x \times N_x$ calculation with $N_x = 200$
Red line: full $N_a \times N_r$ calculation with $N_a = 200$, $N_r = 50$

Time evolution beyond the mean-field

$$\left\{-i\frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \int d\bar{\mathbf{r}}_1 \Sigma_{HF}(\mathbf{1}\bar{\mathbf{1}})\right\} \mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}') = \underbrace{\int_{t_0}^{t_1} d\bar{\mathbf{1}}\, \Sigma^{R}(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}') + \int_{t_0}^{t_{1'}} d\bar{\mathbf{1}}\, \Sigma^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^{A}(\bar{\mathbf{1}}\mathbf{1}')}_{I_1^{\lessgtr}(\mathbf{1},\mathbf{1}';t_0)}$$



- Direct Born approximation $\Rightarrow$ simplest conserving approximation
- FFT to compute convolution integrals
- Collision integrals $\Rightarrow$ memory effects in 2D $\Rightarrow$ (t,t')
- First benchmark calculation to get acquainted with methodology

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$$\Sigma^{\lessgtr}(p,t;p',t') = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi} V(p-p_1)V(p'-p_2)\mathcal{G}^{\lessgtr}(p_1,t;p_2,t')\Pi^{\lessgtr}(p-p_1,t;p'-p_2,t')$$

$$\Pi^{\lessgtr}(p,t;p',t') = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi} \mathcal{G}^{\lessgtr}(p_1,t;p_2,t')\mathcal{G}^{\gtrless}(p_2-p',t';p_1-p,t)$$

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$$\begin{aligned} I_1^{>}(p_1,t_1;p_{1'},t_{1'}) = & \int_{t_0}^{t_1} \mathrm{d}\bar{t} \int \frac{\mathrm{d}\bar{p}}{2\pi} \left[\Sigma^{>}(p_1,t_1;\bar{p},\bar{t}) - \Sigma^{<}(p_1,t_1;\bar{p},\bar{t})\right] \mathcal{G}^{>}(\bar{p},\bar{t};p_{1'},t_{1'}) \\ & - \int_{t_0}^{t_{1'}} \mathrm{d}\bar{t} \int \frac{\mathrm{d}\bar{p}}{2\pi} \Sigma^{>}(p_1,t_1;\bar{p},\bar{t}) \left[\mathcal{G}^{<}(\bar{p},\bar{t};p_{1'},t_{1'}) - \mathcal{G}^{>}(\bar{p},\bar{t};p_{1'},t_{1'})\right] \end{aligned}$$

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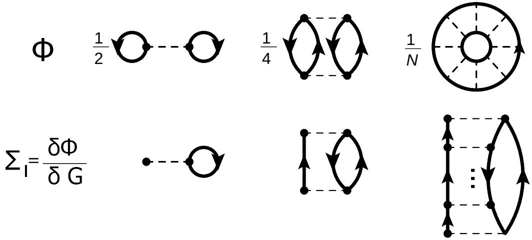
Time evolution beyond the mean-field



Puig von Friesen et al., PRL **103**, 176404 (2009)

- Direct Born approximation ⇒ simplest conserving approximation
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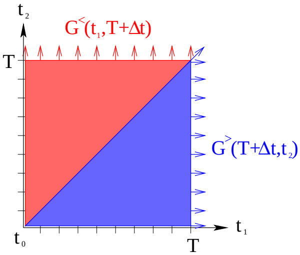
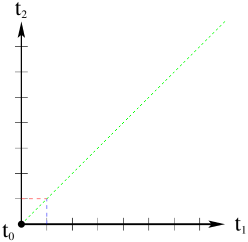
Two time Kadanoff-Baym equations



Köhler *et al*, Comp. Phys. Comm. 123, 123 (1999)
Stan, Dahlen, van Leeuwen, Jour. Chem. Phys. 130, 224101 (2009)
Balzer, Bauch, Bonitz, Phys. Rev. A 82, 033427 (2010)

- Strategy to deal with memory & two-times
- Use symmetries $\mathcal{G}^{\lessgtr}(\mathbf{1},\mathbf{2}) = -[\mathcal{G}^{\lessgtr}(\mathbf{2},\mathbf{1})]^*$ to minimize resources
- Already attempted in homogeneous systems & other fields

Strategy to solve two-time equations



$$\mathcal{G}^<(t_1, T+\Delta t) = e^{i\varepsilon\Delta t}\mathcal{G}^<(t_1,T) - \varepsilon^{-1}\left(1-e^{i\varepsilon\Delta t}\right)\overline{I_2^<(t_1,T+\Delta t)}$$

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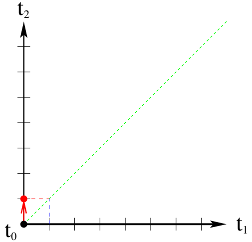
- Each time step involves $2N_t + 1$ operations
- Self-consistency imposed at every time step
- Elimination schemes for time off-diagonal elements?

Strategy to solve two-time equations



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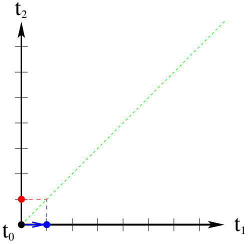

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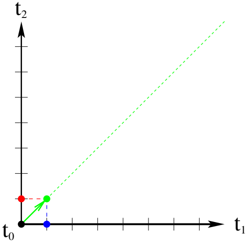

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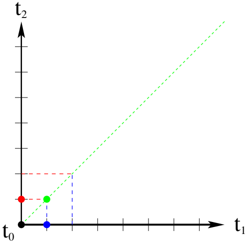

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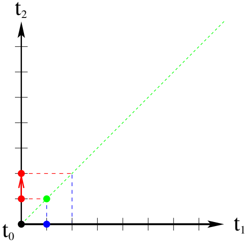

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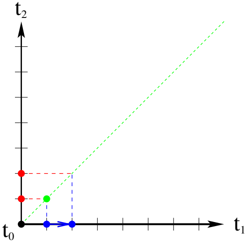

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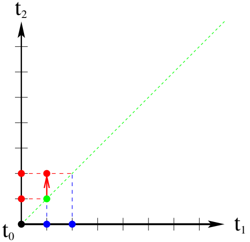

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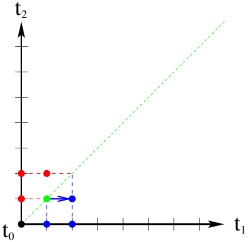

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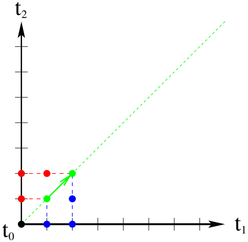

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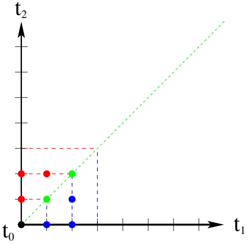

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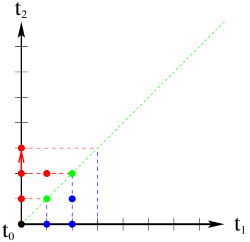

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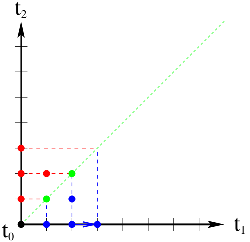

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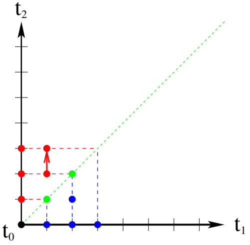

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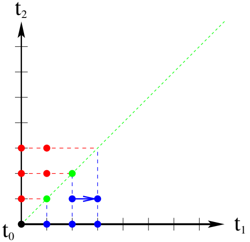

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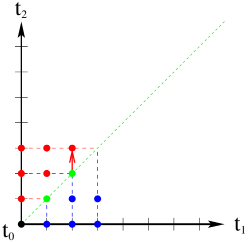

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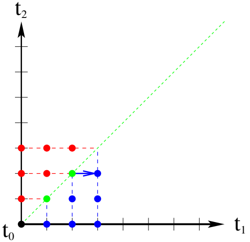

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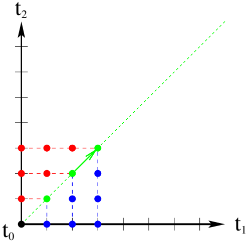

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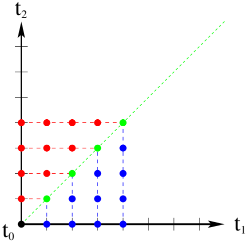

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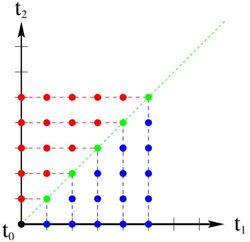

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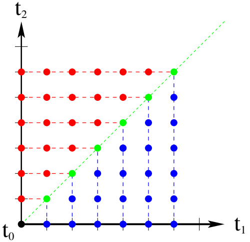

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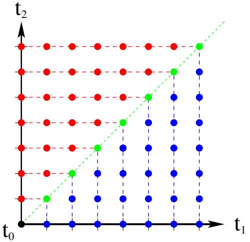

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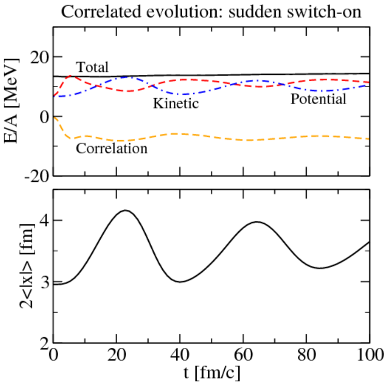
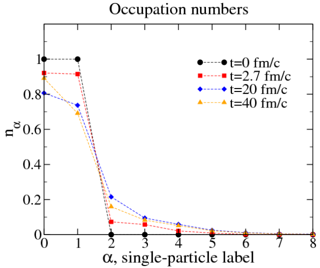
Correlated fermions in a trap

Dynamics in a Harmonic Oscillator trap





Total energy is conserved

Oscillations are damped by dissipative effect of correlations

Initial uncorrelated state has 2 states fully occupied

Thermalization appears over time

Summary

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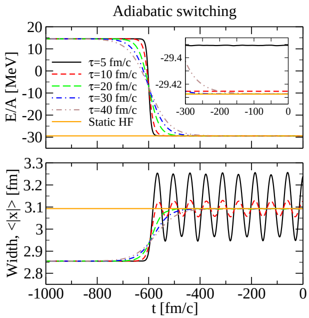

A. Rios *et al.*, Ann. Phys. **326**, 1274 (2011)

- Used adiabatic theorem to solve initial value $\surd$
- Full (N_x^2), damped & cut ($N_a \times N_r$) 1D mean-field evolution $\surd$
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- Full 1D correlated evolution: Born approximation $\sim \surd$
- Lessons learned $\Rightarrow$ Progressive understanding of higher D

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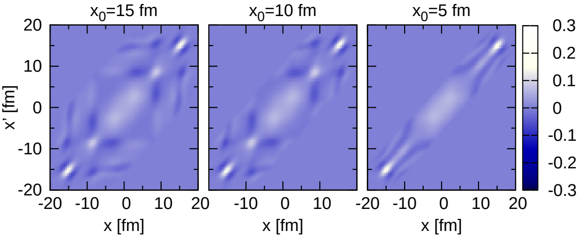
Off-diagonal elements



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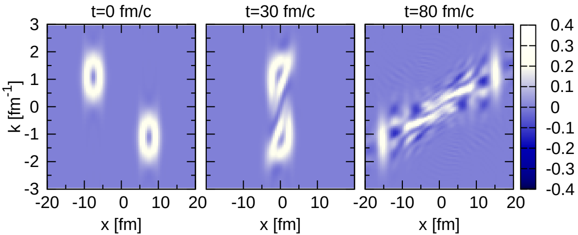

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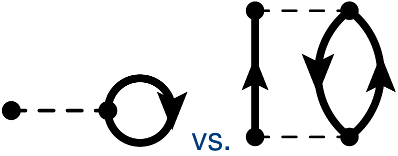

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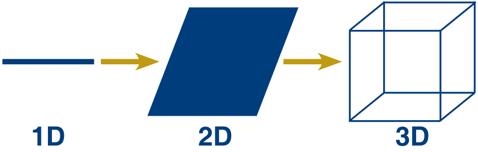

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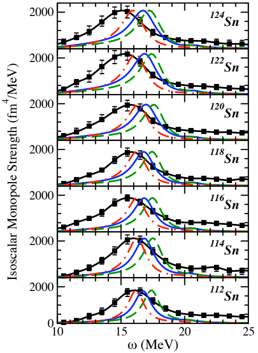
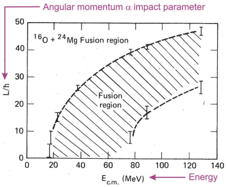
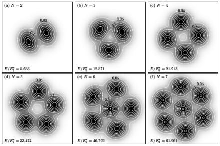
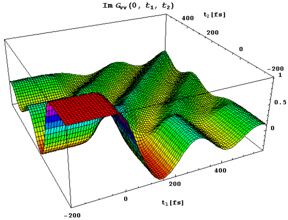
Nuclear Kadanoff-Baym

Potential & challenges





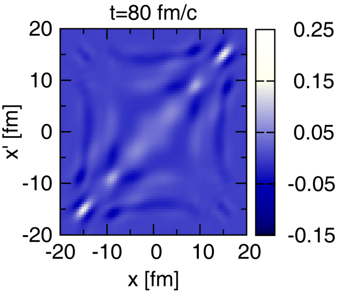


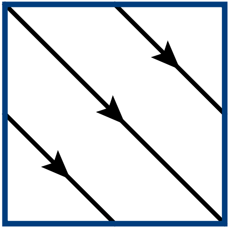


- Potential for applications in nuclear reactions & structure
- Provides a microscopic understanding of dissipation
- Response for nuclei including collision width
- Multidisciplinary research: from quantum dots to cosmology!

Thank you!

Wigner function



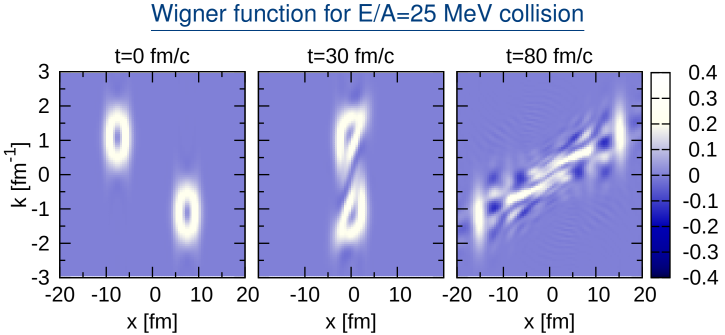


- Fourier transform along relative variable (Wigner transform)

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

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

Wigner function

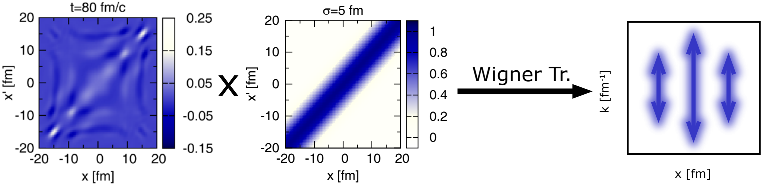


- Fourier transform along relative variable (Wigner transform)

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

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

Smearing out the distribution



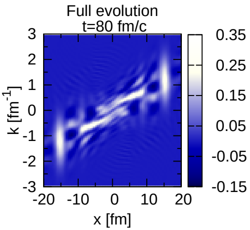
Wigner transform $\mathcal{G}^<$ with gaussian cut off the diagonal...

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

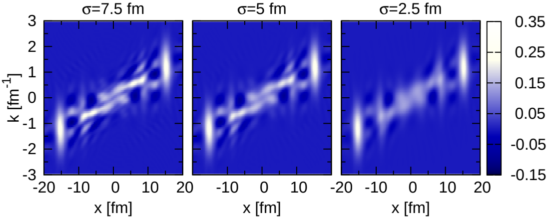
is equivalent to momentum average of $f_W(x,P)$!

Smearing out the distribution

Full evolution Wigner distribution



Gaussian average off the diagonal



Superoperator cut off the diagonal