Time-Dependent Green's Functions approach to nuclear reactions

Understanding the 1D mean-field dynamics

Arnau Rios Huguet, Pawel Danielewicz & Brent Barker

National Superconducting Cyclotron Laboratory
Michigan State University

Time-dependent formalism for nuclear reactions

Our "ambitious" goal:

- Simulate time evolution of nuclear phenomena in 3D
- Use Time-Dependent Green's Functions formalism
  - Good in the static case
  - Fully quantal
  - Correlations in initial state and in dynamics
  - Microscopic conservation laws are preserved

Where we are right now:

- Mean-field simulation of collisions of 1D slabs
- Understanding TDGF formalism before...
  - Including correlations in 1D (NN collisions)
  - Extending to higher dimensions (2D, 3D)

Kadanoff-Baym equations

Eventually:

$$\rho(\mathbf{x}_1 t_1, \mathbf{x}_{1'} t_{1'}) = \mathcal{G}^{<}(\mathbf{1}\mathbf{1}') = i\Big\langle \Phi_0 \Big| \hat{a}^\dagger(\mathbf{x}_{1'} t_{1'}) \hat{a}(\mathbf{x}_1 t_1) \Big| \Phi_0 \Big\rangle$$

$$\mathcal{G}^{>}(\mathbf{1}\mathbf{1}') = i\Big\langle \Phi_0 \Big| \hat{a}(\mathbf{x}_1 t_1) \hat{a}^\dagger(\mathbf{x}_{1'} t_{1'}) \Big| \Phi_0 \Big\rangle$$

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

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

- Evolution equations for non-equilibrium systems (Keldysh)
- Can be derived from general principles
- Include correlation and memory effects
- Complicated numerical solution!

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

Kadanoff-Baym equations

Right now:

$$\rho(\mathbf{x}_1 t_1, \mathbf{x}_{1'} t_{1'}) = \mathcal{G}^<(\mathbf{11'}) = i\Big\langle \Phi_0 \Big| \hat{a}^\dagger(\mathbf{x}_{1'} t_{1'}) \hat{a}(\mathbf{x}_1 t_1) \Big| \Phi_0 \Big\rangle$$

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TDGF in the MF approximation vs. TDHF

- TDGF and TDHF give exactly the same results...
- but are expressed in rather different terms!

Time Dependent Green's Functions	Time Dependent Hartree-Fock
$$i\frac{\partial}{\partial t}\mathcal{G}^<(x,x';t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right\}\mathcal{G}^<(x,x';t)$$ $$-i\frac{\partial}{\partial t}\mathcal{G}^<(x,x';t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x'^2} + U(x')\right\}\mathcal{G}^<(x,x';t)$$	for $\alpha = 1, \dots, N_\alpha$ $$i\frac{\partial}{\partial t}\varphi_\alpha(x,t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right\}\varphi_\alpha(x,t)$$ end
• 2 equations ... $N_x \times N_x$ matrix • Testing ground & new perspective	• 1 equation ... $N_x \times N_\alpha$ matrix • Limited to mean-field!

- First calculation: mean-field time evolution of 1D slabs
- Understand time evolution of uncorrelated density matrices

Collisions of 1D slabs

- Frozen y, z coordinates, dynamics in x
- Simplified Skyrme mean field:

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

- Initial state from adiabatic theorem or static HF
- Ground state of $\mathcal{G}^<$ with $A = 8$ $(N_\alpha = 2)$

Two aspects:

- Phenomenology: dependence on bombarding energy?
- New perspective from Green's functions $\Rightarrow$ off-diagonal elements

Diagonal & off-diagonal matrix elements

- Diagonal elements yield physical properties:

$$n(x) = \mathcal{G}^<(x, x' = x) = \sum_{\alpha=0}^{N_\alpha} n_\alpha |\varphi_\alpha(x)|^2$$

$$K = \sum_k \frac{k^2}{2m} \mathcal{G}^<(k, k' = k)$$

- What happens off the diagonal?

$$\mathcal{G}^<(x, x') = \sum_{\alpha=0}^{N_\alpha} n_\alpha \varphi_\alpha(x) \varphi_\alpha^*(x')$$

  - What is their meaning? $\Rightarrow \mathcal{G}^< \sim$ correlation function
  - Are all $x \neq x'$ necessary for the time-evolution?
  - Eliminate them at higher D's to avoid $N_x^D \times N_x^D \times N_t$ matrices?

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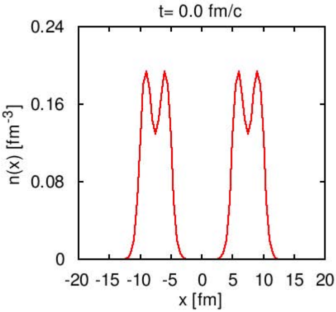
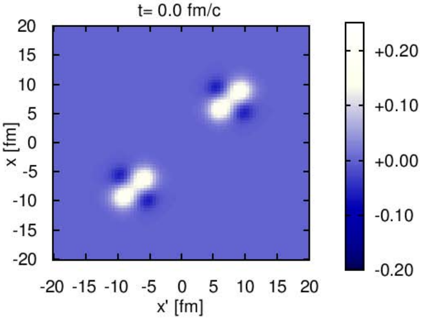
Collisions of 1D slabs: fusion (off-diagonal)

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

$$E_{CM}/A = 0.1 \text{ MeV}$$

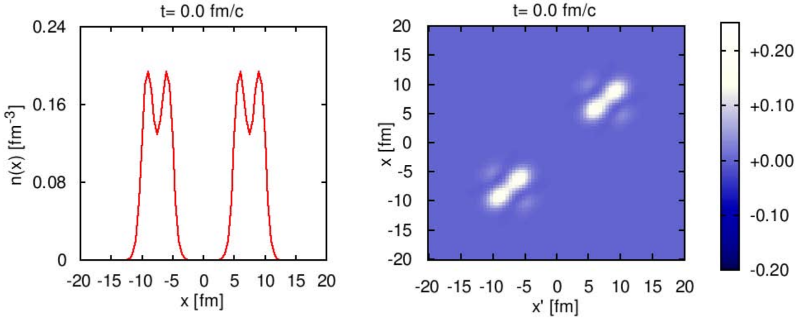




Collisions of 1D slabs: break-up (off-diagonal)

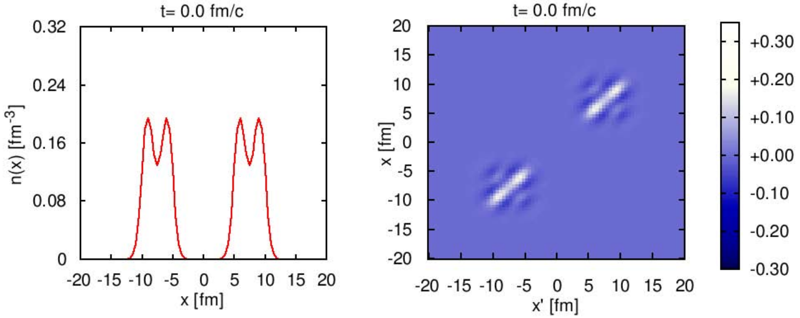
$$\mathcal{G}^{<}(x,x') = \sum_{\alpha} n_\alpha \varphi_\alpha(x) \varphi_\alpha(x')$$

$$E_{CM}/A = 4 \text{ MeV}$$

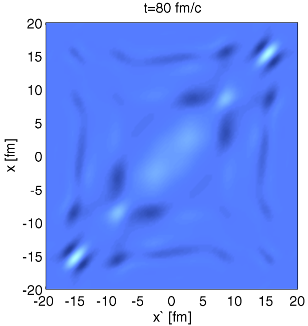


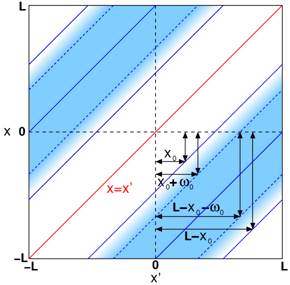
Collisions of 1D slabs: multifrag. (off-diagonal)

$$E_{CM}/A = 25 \text{ MeV}$$



Erasing off-diagonal elements



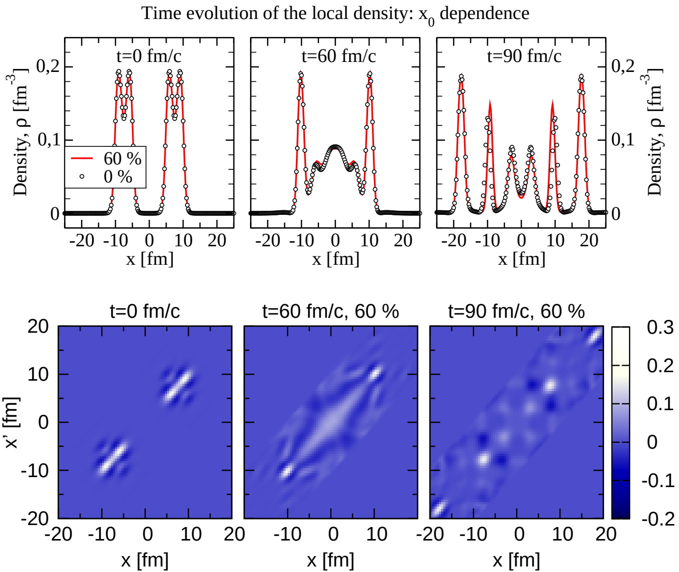


- Use a cut-off imaginary potential off the diagonal $\sim$ superoperator

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

- Properties of the field set to preserve norm, periodicity, etc
- Other choices do not yield good results!

Erasing off-diagonal elements



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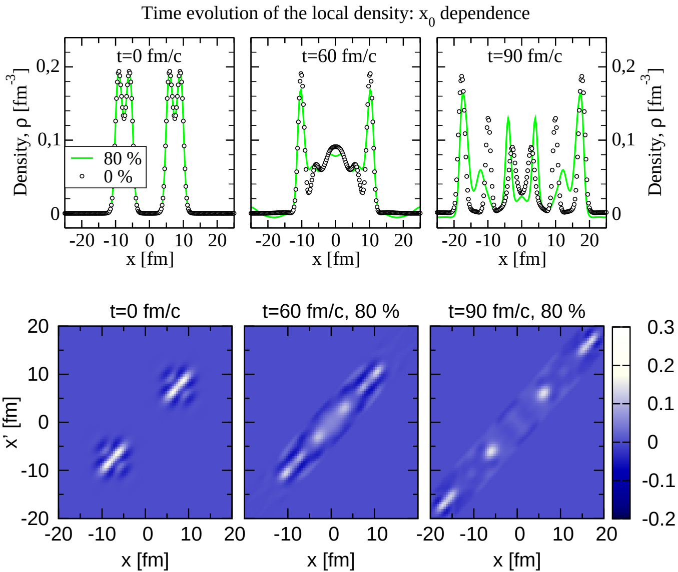

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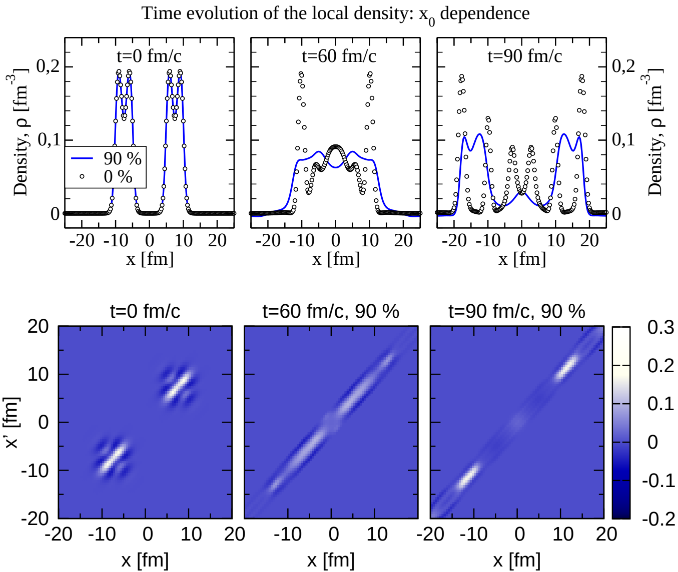

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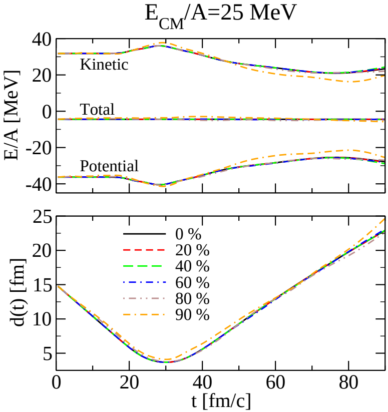


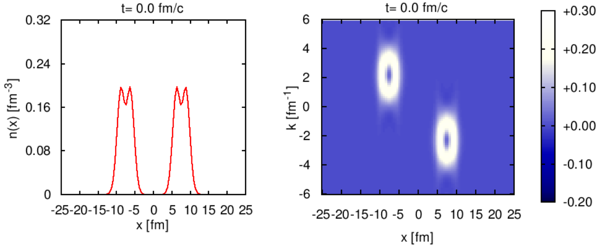
- Up to 60% (safe) off-diagonal elements can be neglected safely?
- Small effect of erasure for observables in high energy reactions!

Connection to transport phenomena

- Wigner transform:

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

- $f(x,P)$ phase space density
- Obeys Boltzmann equation under assumptions
- Momentum average of $f(x,P) \sim$ erasure of off-diagonal elements



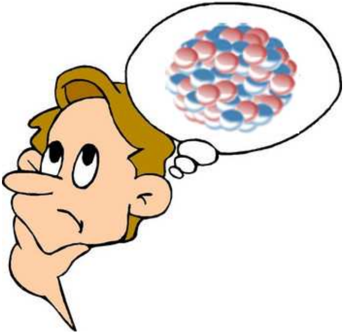
Conclusions

- KB equations offer a consistent framework for TD calculations
- Time evolution of 1D slabs in the mean-field
- New perspective is gained
- 60% off-diagonal elements are unimportant with appropiate cut-off
- Wigner functions are being analyzed

- Qualitative agreement with previous calculations*
- Beyond mean-field calculations are being implemented
- Extension to 2D and 3D $\Rightarrow$ Promising approach to study correlations in time-dependent approaches!

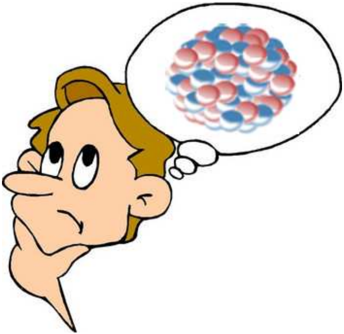
*Bonche, Koonin and Negele, PRC 13, 1226 (1976).

Thank you!



Let me know if you nide a ride back to Kellogg!

Thank you!



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