Correlations within Non-equilibrium Green's Functions method

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- Introduction to Non-Equilibrium Green's functions (NEGF)
- Applications of NEGF
- Infinite nuclear matter
- Finite system

Why NEGF

- Evolution of correlated/uncorrelated quantum many-body systems can be described in a consistent way in NEGF formalism
- TDHF : $$\Phi(x_1 ... x_A; t) = \frac{1}{A!} \sum_{\sigma} \prod_{\alpha=1}^{A} (-1)^{\mathrm{sgn}\sigma} \phi_\alpha(x_{\mathrm{sgn}\sigma}, t)$$

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

- limitations on allowed excitations The validity of TDHF requires a negligible role played by correlations in the dynamics
- NEGF is suitable for central reactions due to averaging over more than one-body effect

The Contour

$$\langle O_H(t)\rangle = \langle U(t_0,t)O_I(t)U(t,t_0)\rangle$$
$$= \left\langle T^a\left[\exp\left(-i\int_{t_0}^{t} d\tau H(\tau)\right)\right] O_I(t)\, T^c\left[\exp\left(-i\int_{t_0}^{t} d\tau H(\tau)\right)\right]\right\rangle$$

where $$U(t_0,t) = T^a\left[\exp\left(i\int_{t_0}^{t} d\tau H(\tau)\right)\right] \qquad t > t_0$$

introducing a contour running along the time and a ***T*** operator ordering along the contour.

P. Danielewicz: Annals of physics 152. 239-304(1984)

Kadanoff-Baym Equations

$$G^{<}(x_1,t_1;x_{1'},t_{1'}) \to G^{<}(1,1') = i\langle \hat{a}^{\dagger}(1)\hat{a}(1')\rangle$$
$$G^{>}(x_1,t_1;x_{1'},t_{1'}) \to G^{>}(1,1') = -i\langle \hat{a}(1)\hat{a}^{\dagger}(1')\rangle$$

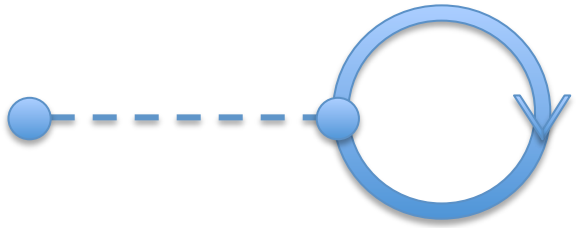
$$\left[i\hbar\frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}\right] G^{\gtrless} = \int d\bar{x}_{\bar{1}}\Sigma_{HF}(1\bar{1})G^{\gtrless}(\bar{1}1') + \int_{t_0}^{t_1} d\bar{1}\left[\Sigma^{>}(1\bar{1}) - \Sigma^{<}(1\bar{1})\right]G^{\gtrless}(\bar{1}1') - \int_{t_0}^{t_{1'}} d\bar{1}\Sigma^{\gtrless}(1\bar{1})\left[G^{>}(\bar{1}1') - G^{<}(\bar{1}1')\right]$$

$$\left[-i\hbar\frac{\partial}{\partial t_1'} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1'^2}\right] G^{\gtrless} = \int d\bar{x}_{\bar{1}}\Sigma_{HF}(1\bar{1})G^{\gtrless}(\bar{1}1') + \int_{t_0}^{t_1} d\bar{1}\left[G^{>}(1\bar{1}) - G^{<}(1\bar{1})\right]\Sigma^{\gtrless}(\bar{1}1') - \int_{t_0}^{t_{1'}} d\bar{1}G^{\gtrless}(1\bar{1})\left[\Sigma^{>}(\bar{1}1') - \Sigma^{<}(\bar{1}1')\right]$$

Kadanoff-Baym Equations

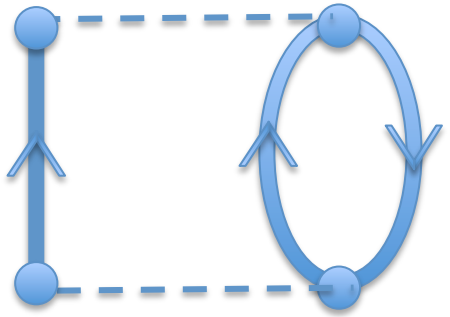
$$\left[i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}\right]G^{\gtrless}=\int dx_{\bar{1}}\Sigma_{HF}(1\bar{1})G^{\gtrless}(\bar{1}1')$$

$$\Sigma_{HF}$$



$$+\int_{t_0}^{t_1}d\bar{1}\left[\Sigma^{>}(1\bar{1})-\Sigma^{<}(1\bar{1})\right]G^{\gtrless}(\bar{1}1')-\int_{t_0}^{t_{1'}}d\bar{1}\Sigma^{\gtrless}(1\bar{1})\left[G^{>}(\bar{1}1')-G^{<}(\bar{1}1')\right]$$

$$\Sigma^{\gtrless}$$



HF approximation

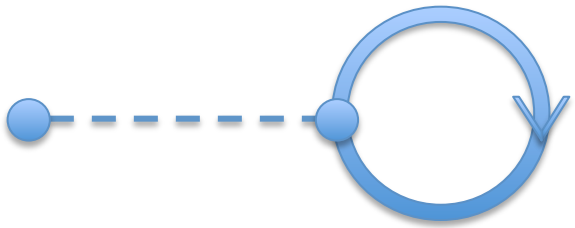
- In HF approximation:

$$\Sigma_{HF}(12) = \delta(t_1 - t_2)\Sigma_{HF}(x_1, x_2)$$

- KB equations reduces to:

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

$$\rho(x, x'; t) = -iG^{<}(x, t; x', t)$$



Adiabatically switching

- Adiabatic switching

$$H(t) = F(t)H_0 + [1 - F(t)]H_1 \qquad F(t) = \begin{cases} 1, & t \to -\infty \\ 0, & t \to t_i \end{cases}$$

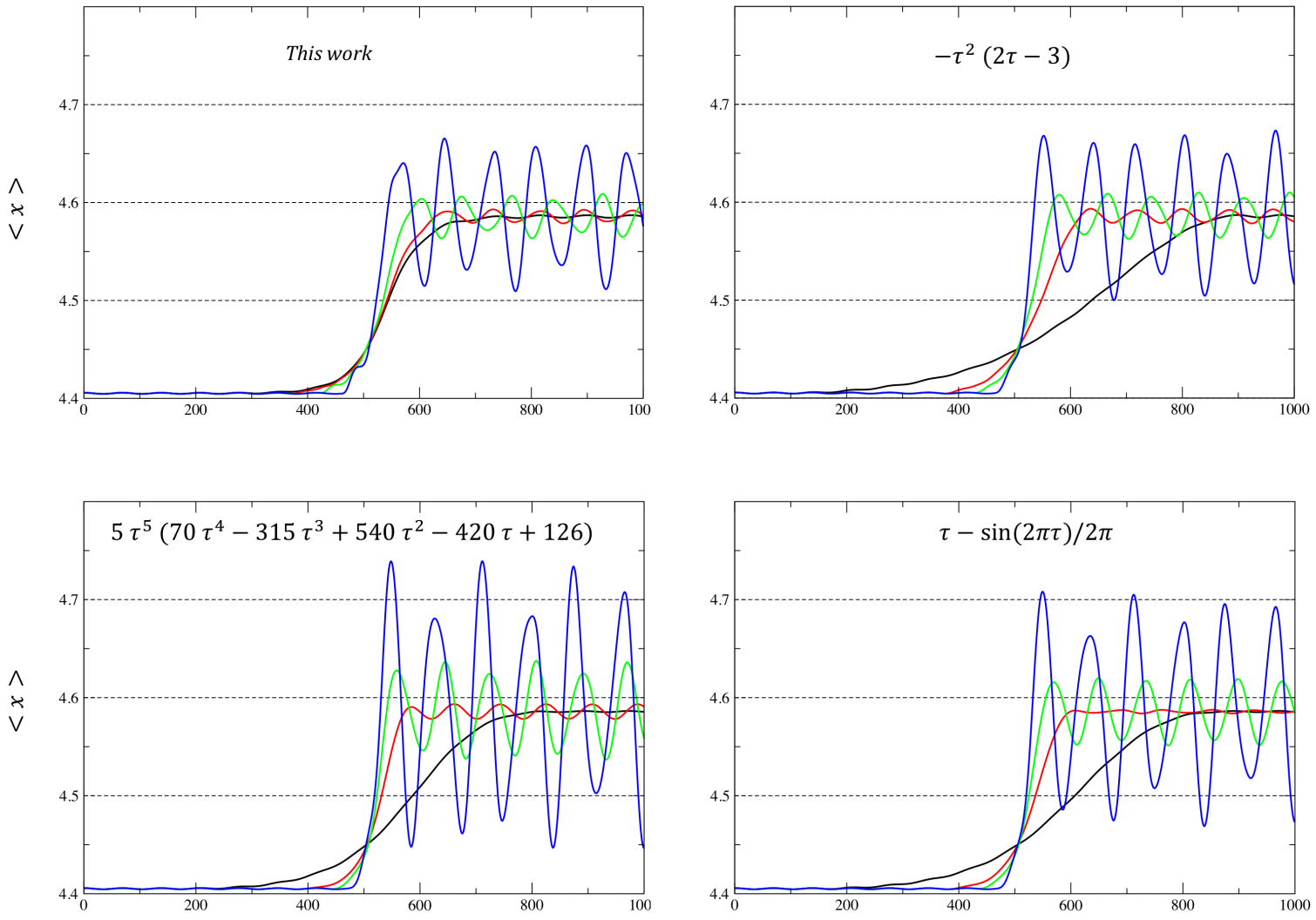
$$f(t) = \frac{1}{1 + e^{t/\tau}} \qquad F(t) = \frac{f(t) - f(t_f)}{f(t_i) - f(t_f)}$$

- Preparing the initial state

$$H_0 = \frac{1}{2}kx^2 \qquad H_1 = U_{mf}$$

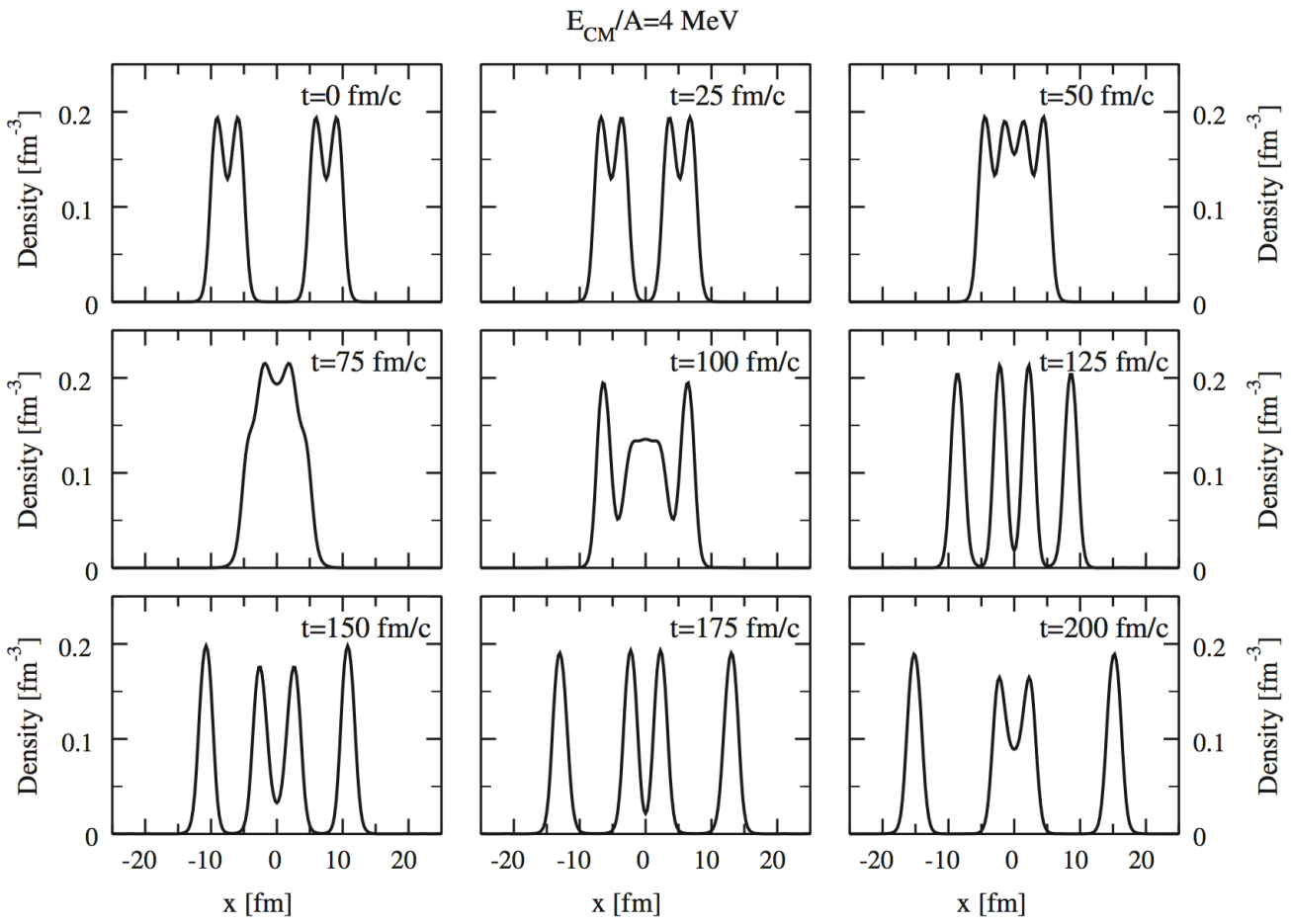
$$U_{mf}(x) = \frac{3}{4}t_0 n(x) + \frac{2+\sigma}{16}t_3 \left[n(x)\right]^{\sigma+1}$$

Switching function



M. Watanaba et all, PRL 65,no. 26, page3301

Collision of two slabs



A. Rios et al :Annals of Physics 326 (2011) 1274

Correlations

- Equation incorporating the interactions:

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

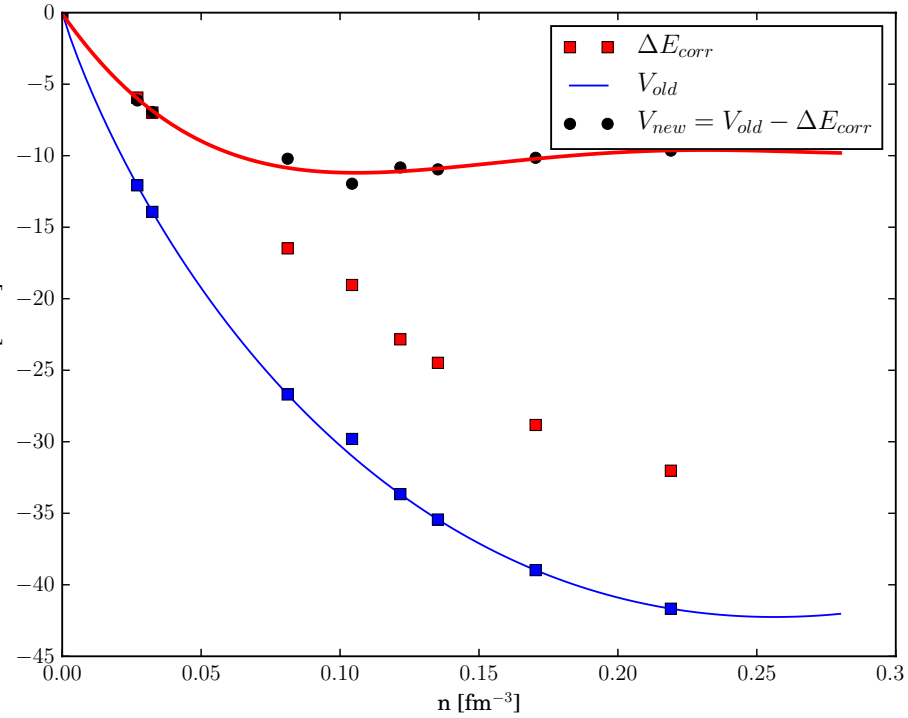
$$\Pi^{\gtrless}(p,t;p',t') = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi} G^{\gtrless}(p_1,t;p_2,t')G^{\gtrless}(p_2-p',t';p_1-p,t)$$

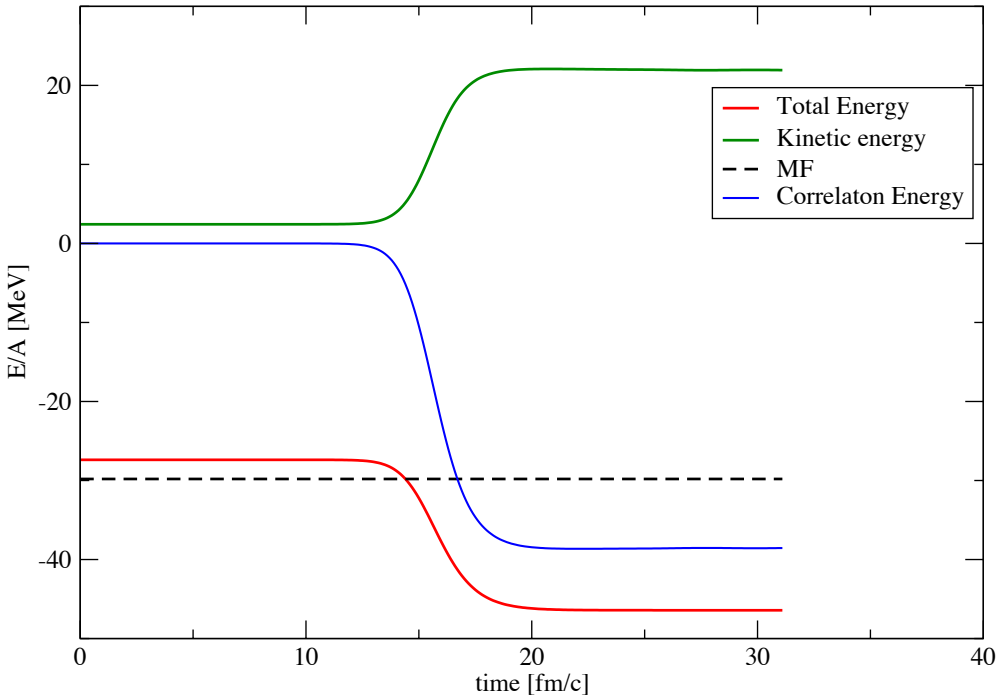
$$V(p) = V_0\sqrt{\pi}(\eta p)^2 e^{-\frac{(\eta p)^2}{4}} \qquad V(x) = V_0\left(1-2\frac{x^2}{\eta^2}\right)e^{-\frac{x^2}{\eta^2}}$$

The parameters are chosen to result reasonable physical quantities such as depletion number

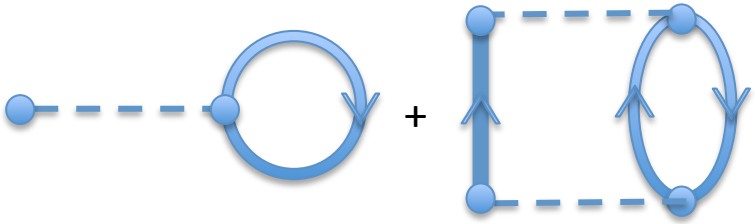
A. Rios et al :Annals of Physics 326 (2011) 1274

infinite nuclear matter

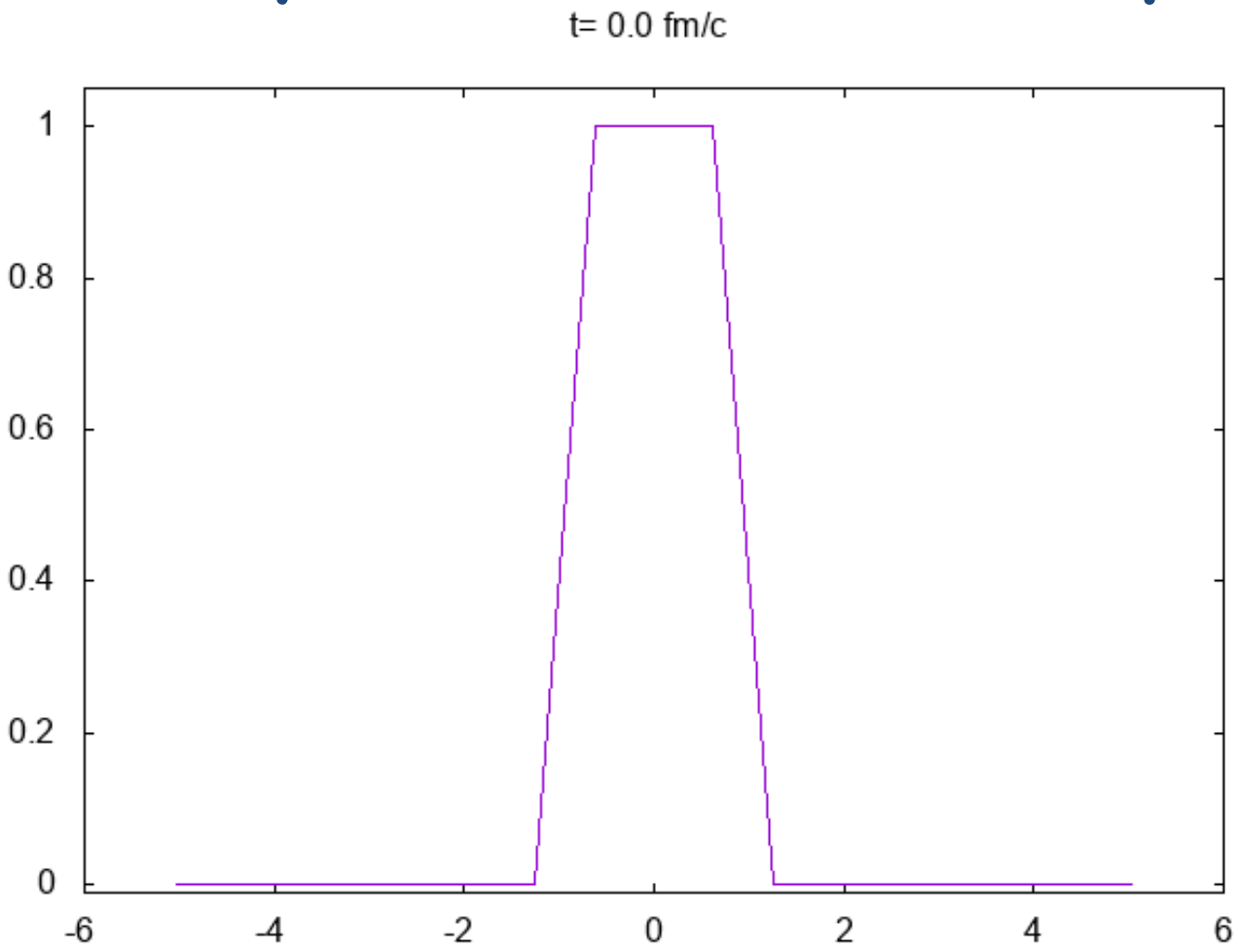




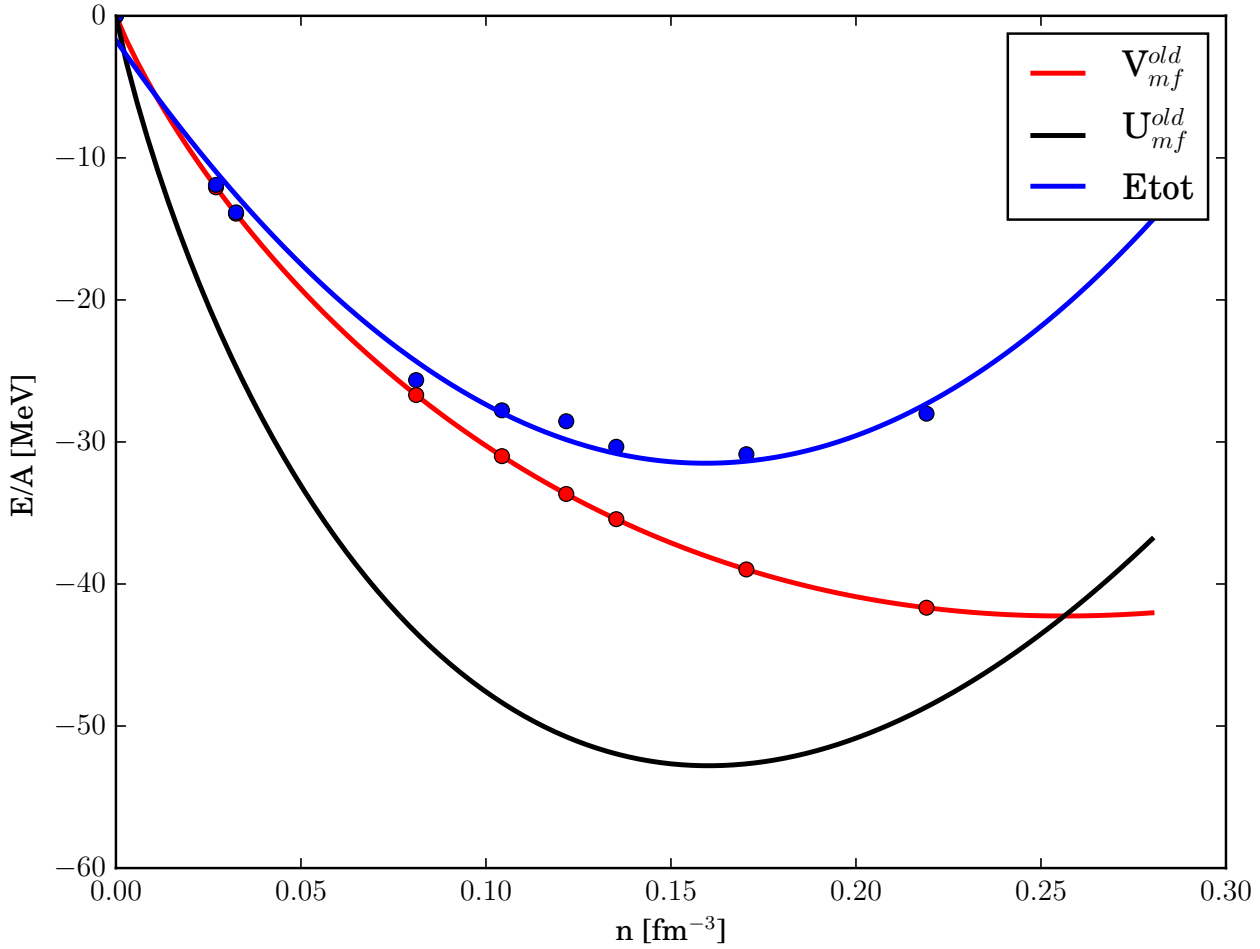
Density in coordinate space



Density in momentum space



EOS in infinite nuclear matter

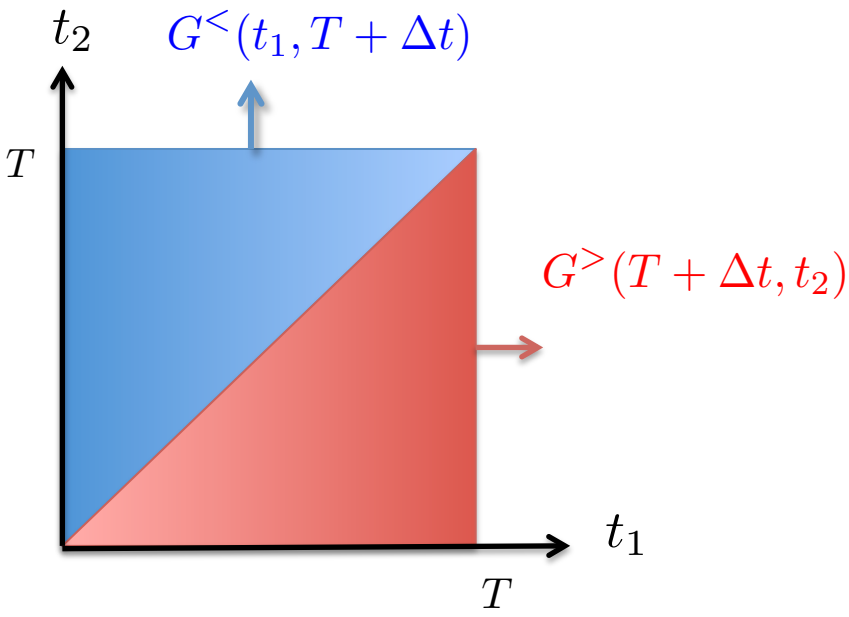


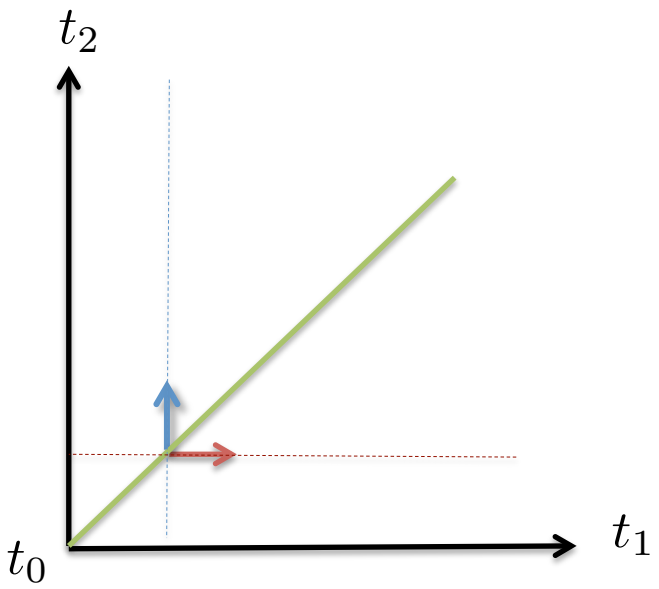
Density in coordinate space

Finite nuclear matter

- Starting from harmonic oscillator Hamiltonian
- Adiabatically switching on mean-field and correlations
- Technicalities:
  - Setting cut-off for energy (dx) and finding the appropriate dt
  - Starting from different initial ω_{HO}
  - Friction term

Solving two-time equations





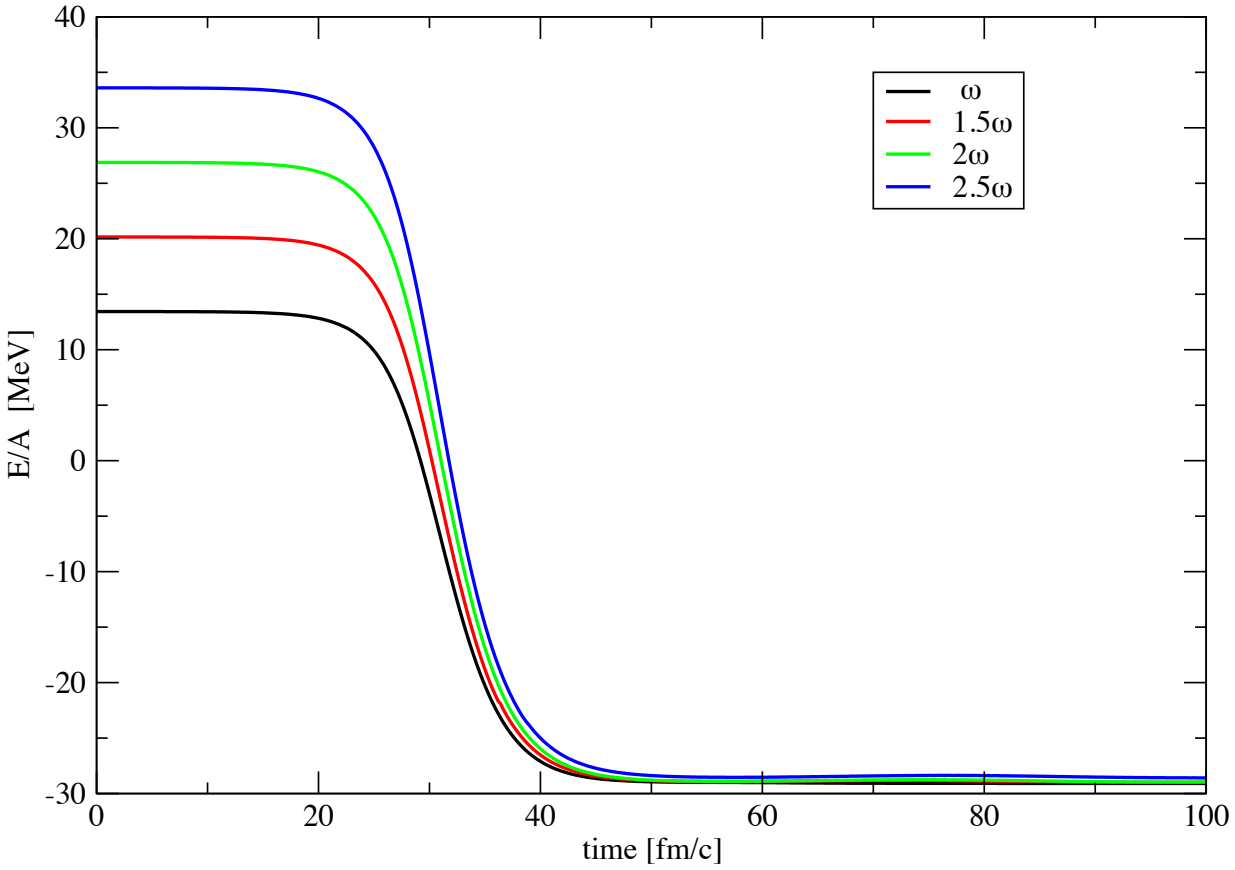
Using symmetries: $G^{\lessgtr}(1,2) = -[G^{\lessgtr}(2,1)]^*$

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

$$G^>(T+\Delta t, t_2) = e^{i\varepsilon\Delta t}G^>(T, t_2) - \left(1 - e^{-i\varepsilon\Delta t}\right)\varepsilon^{-1}I_1^>(T, t_2)$$

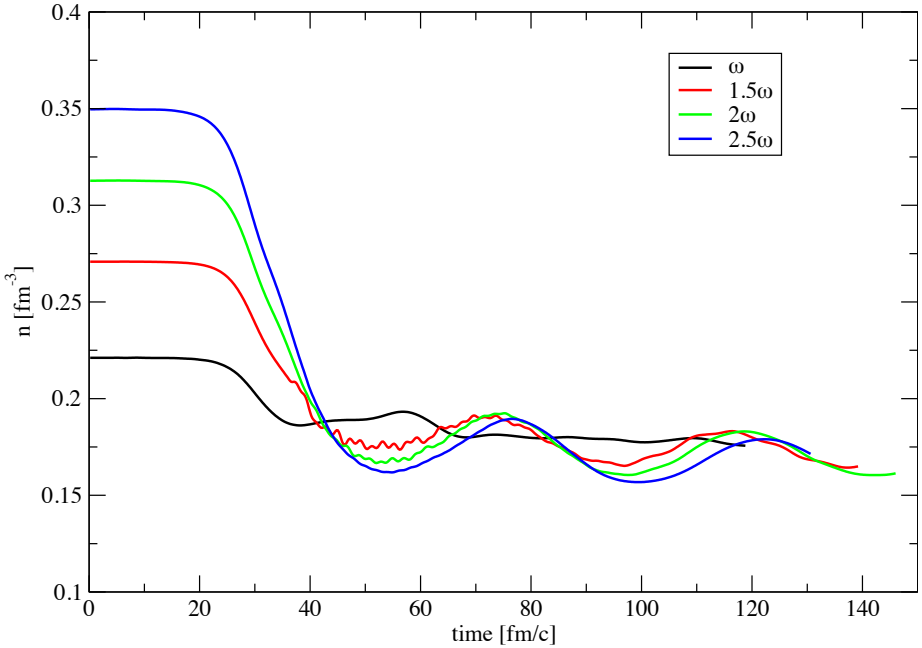
$$G^<(T+\Delta T, T+\Delta T)$$

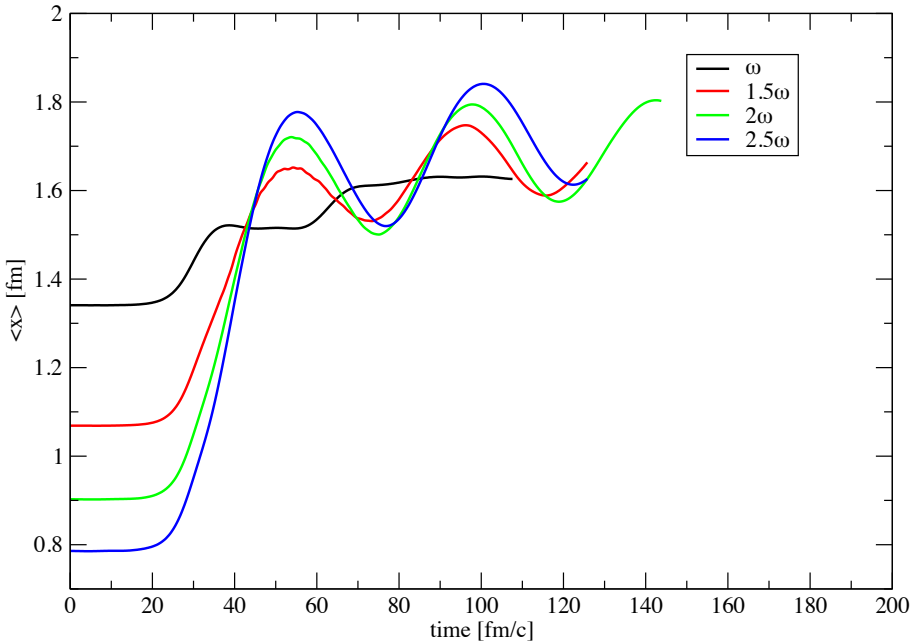
Different starting points



Starting from different frequencies, energy arrives to the same final value

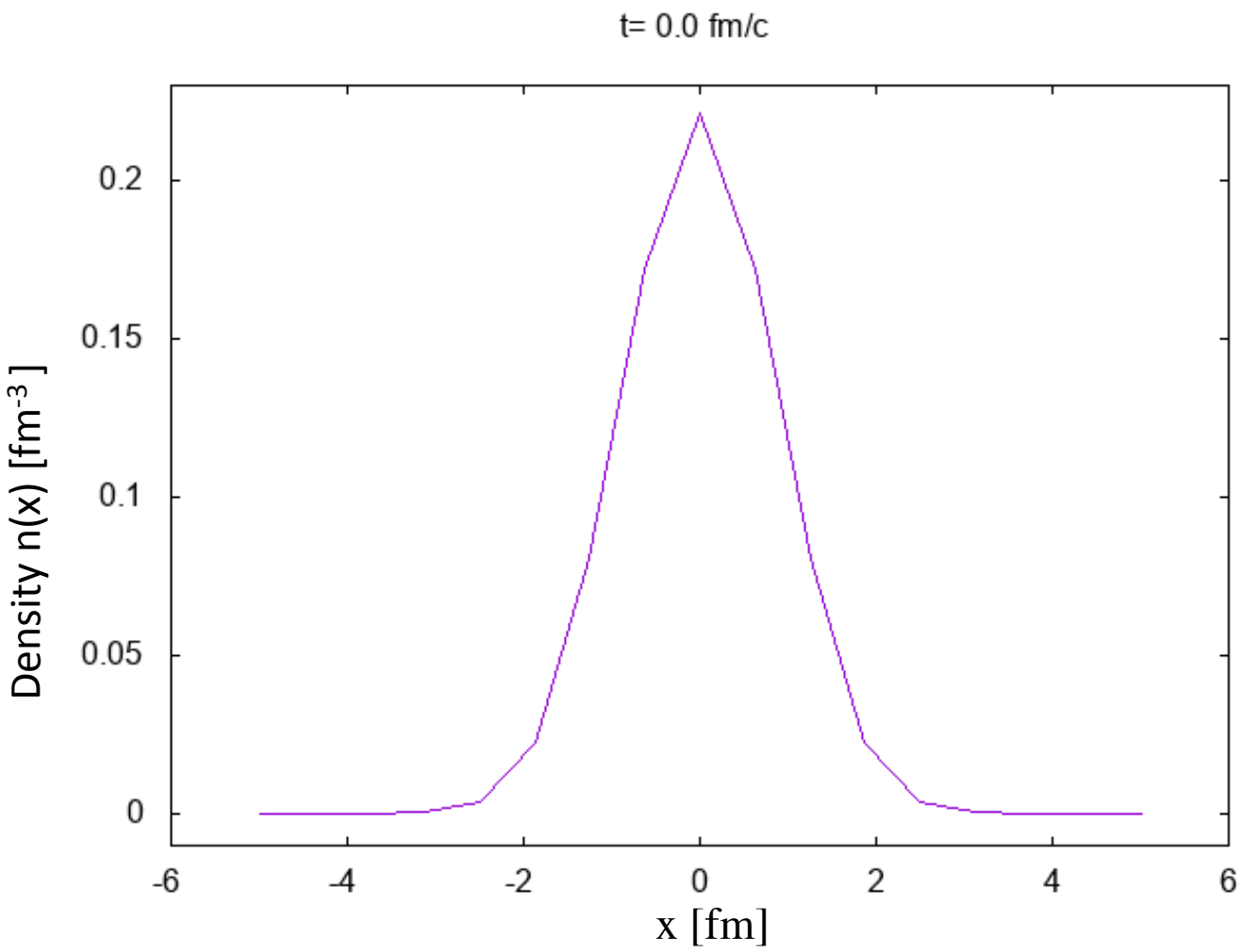
Observables and central density





- Comparing the time evolution of central density (in coordinate space) and the size of the system, for different initial cases,
- They all converge to the same final value

Density



Time evolution of the density in the coordinate space,

Friction term

- A time-dependent external potential

$$U_t \equiv U_t(x)$$

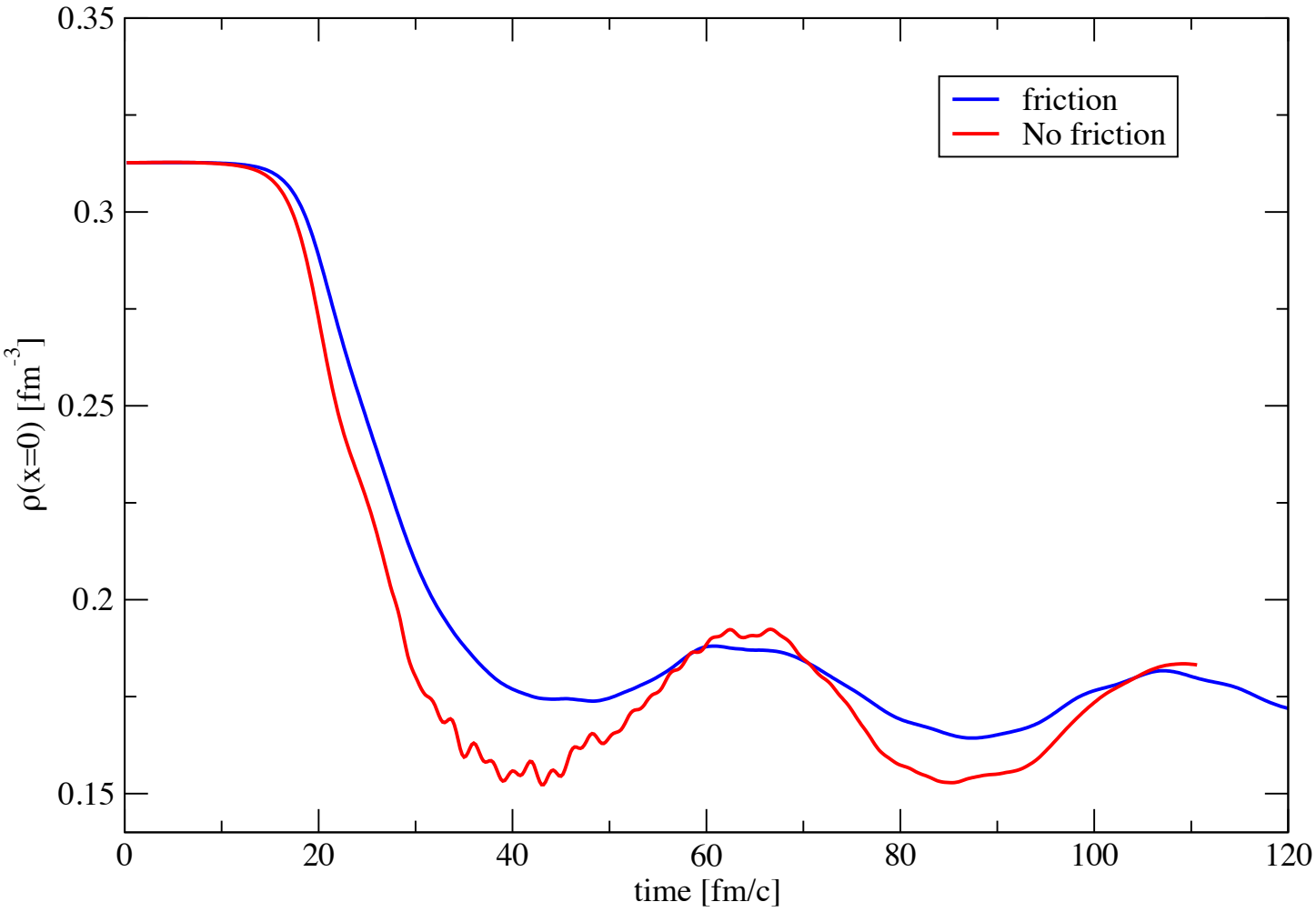
A. Bulgac et. al
https://arxiv.org/abs/1305.6891

- As long as $U_t \propto \dot{\rho}$,

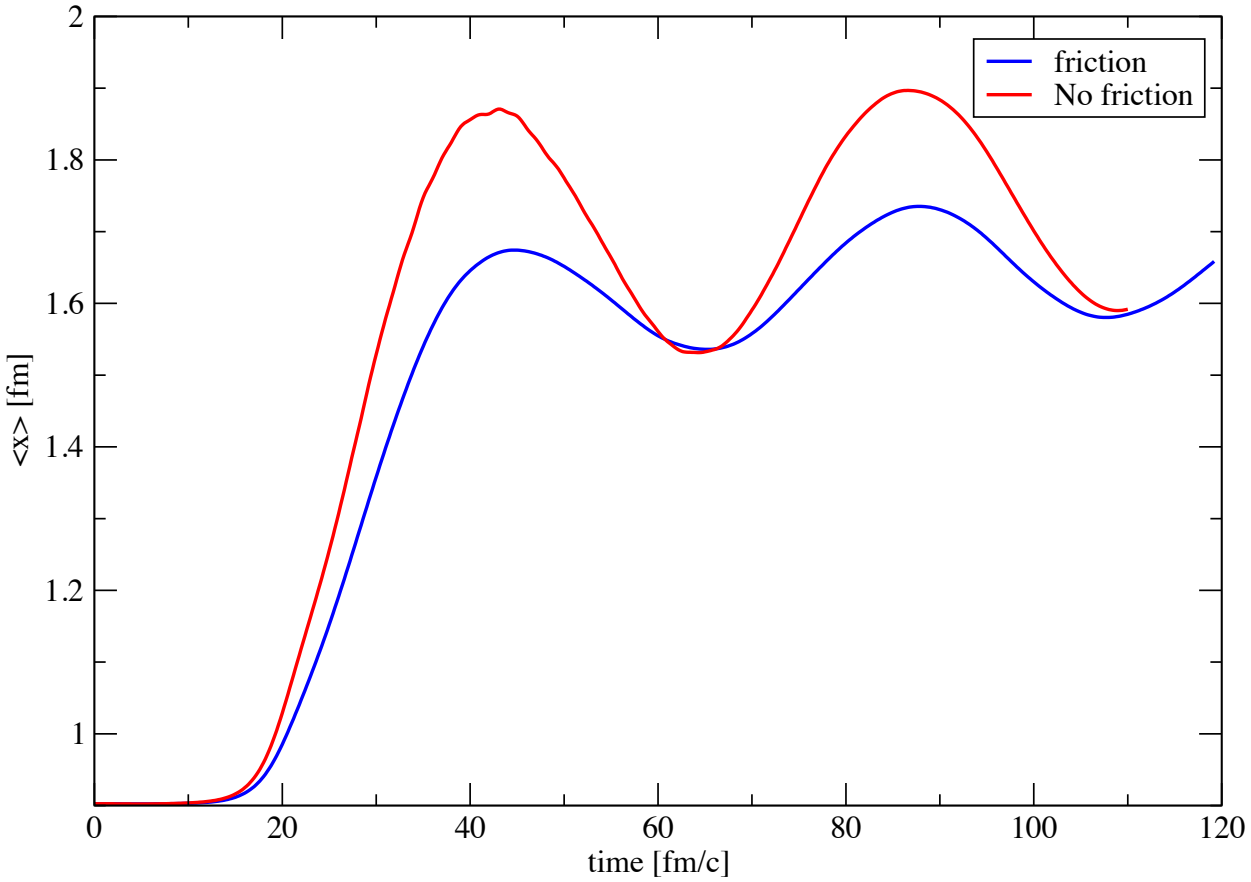
the local quantum friction potential $c\dot{\rho}$ cools the system

- The friction term can be implemented in both momentum and coordinate space

Effect of friction term

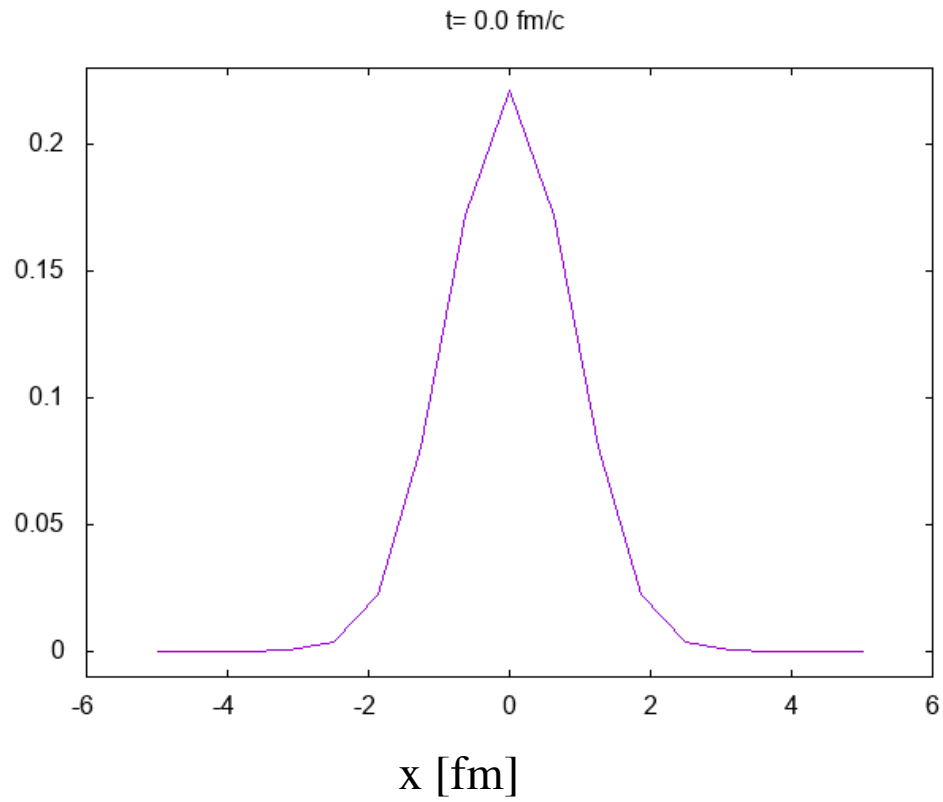


Effect of friction term

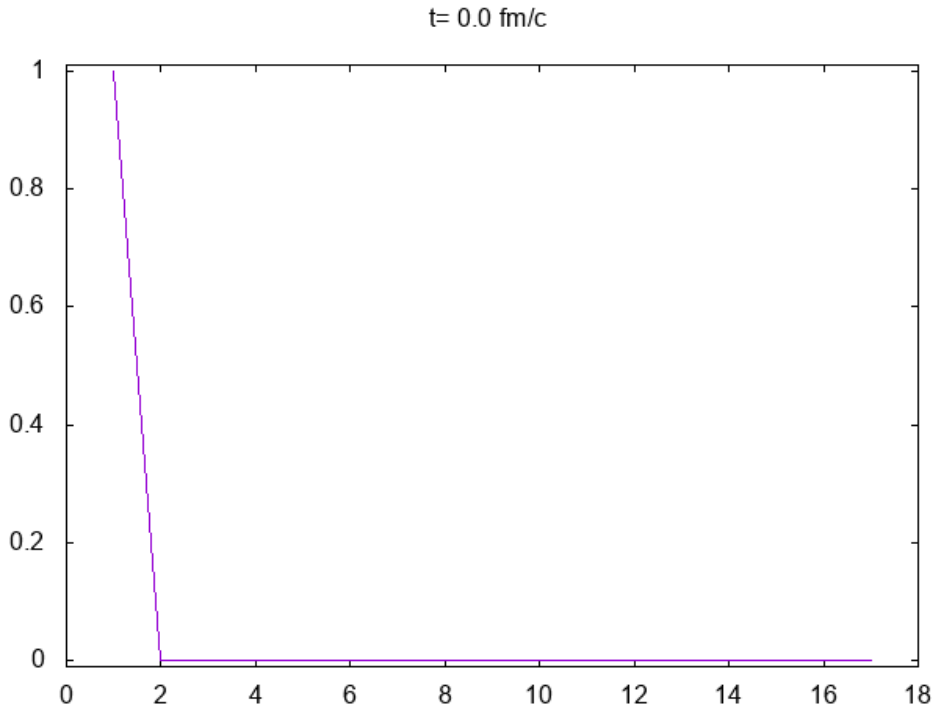


occupation number

Density n(x) [fm^{-3}]



Occupation number

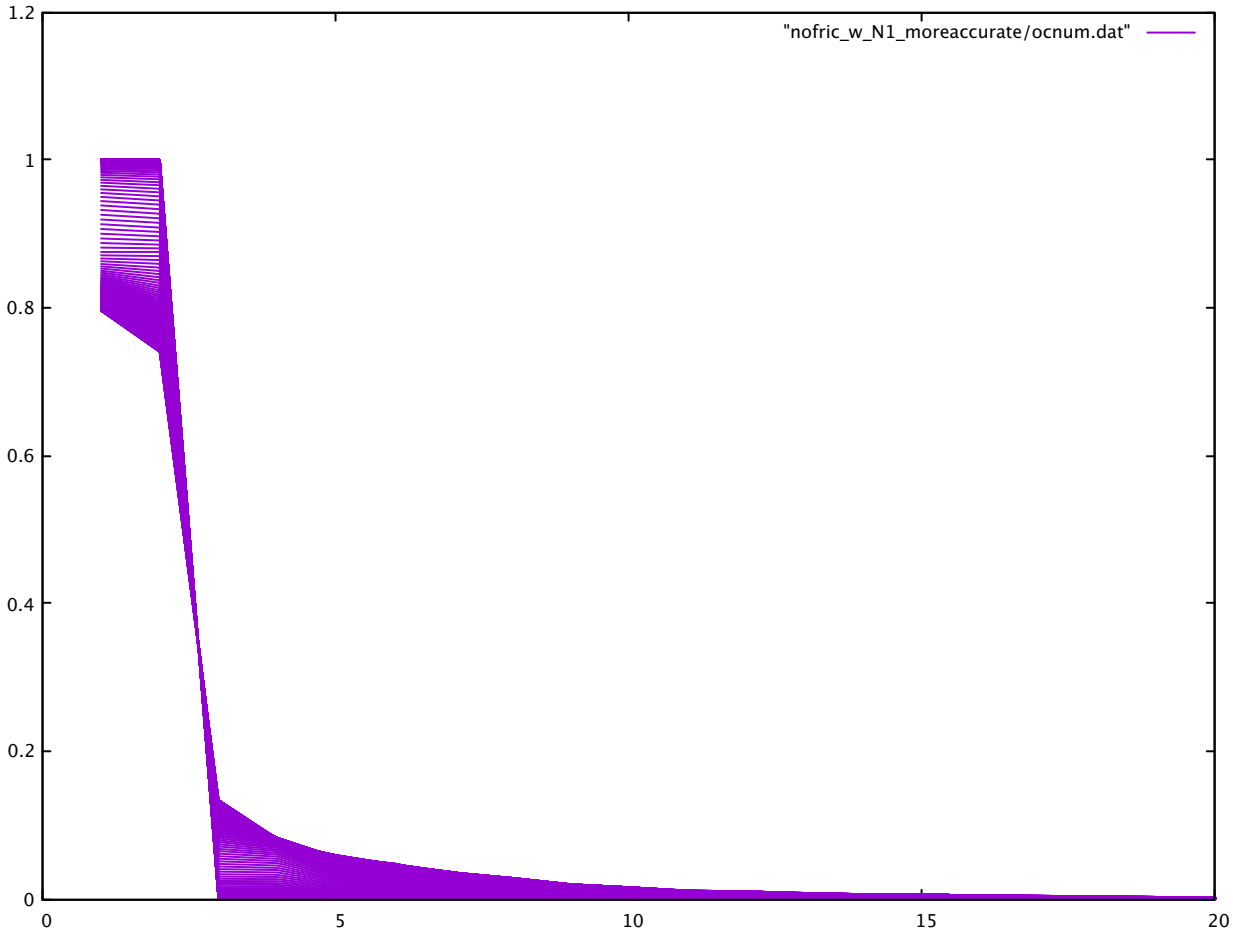


What is next

- Including isospin dependency in the formalism
- Performing the collision of slabs

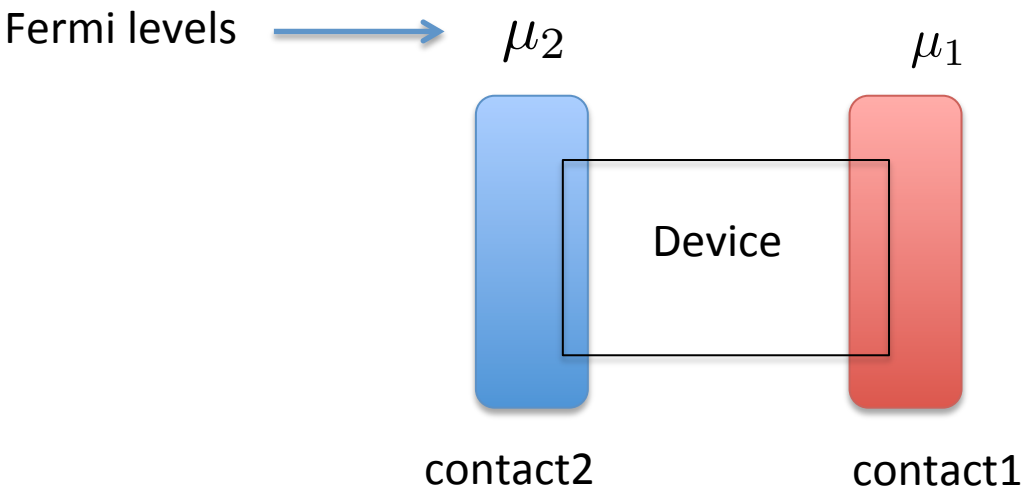
Thanks!

Occupation number



Application: Metal Oxide Semiconductors(MOS)

- The quantitative simulation tools for the new generation of devices will require atomic-level quantum mechanical models.
- The NEGF provides a conceptual basis for this new simulators

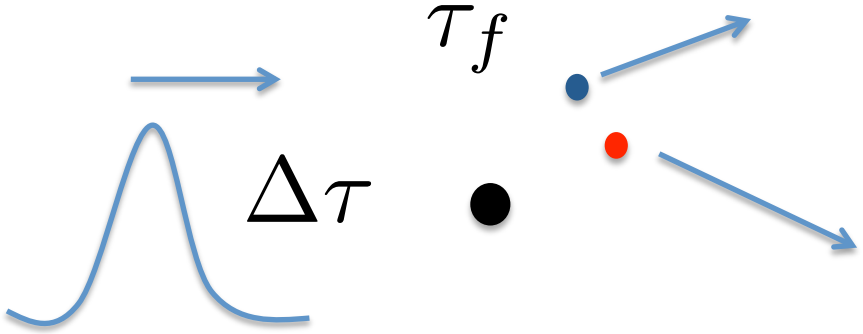


- The device is driven out of equilibrium by two contacts with different Fermi levels
- NGF can be used to determine the density matrix

Supriyo Datta : Superlattices and Microstructures, Vol. 28, No. 4, 2000

Scale

$$\Delta\tau = \frac{\hbar}{\epsilon}$$



$$\tau_f = \frac{\hbar}{\Gamma}$$

$$\Gamma = \hbar n \sigma v \sim 50 MeV$$

The energy, ϵ, is of the same order