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:

  \[ \Phi(x_1 \ldots x_A; t) = \frac{1}{A!} \sum_{\sigma} \prod_{\alpha=1}^{A} (-1)^{\text{sgn}\sigma} \phi_\alpha(x_{\text{sgn}\sigma}, t) \]

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

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

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

introducing a contour running along the time and a \( T \) operator ordering along the contour.
Kadanoff-Baym Equations

\[ G^<(x_1, t_1; x_1', t_1') \rightarrow G^<(1, 1') = i\langle \hat{a}^\dagger(1)\hat{a}(1') \rangle \]

\[ G^>(x_1, t_1; x_1', t_1') \rightarrow G^>(1, 1') = -i\langle \hat{a}(1)\hat{a}^\dagger(1') \rangle \]

\[
\left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} \right] G^\lessgtr = \int dx_1 \Sigma_{HF}(\bar{1}\bar{1}) G^\lessgtr(\bar{1}\bar{1}') \\
+ \int_{t_0}^{t_1} d\bar{1} \left[ \Sigma^>(\bar{1}\bar{1}) - \Sigma^<(\bar{1}\bar{1}) \right] G^\lessgtr(\bar{1}\bar{1}') - \int_{t_0}^{t_{1'}} d\bar{1} \Sigma^\lessgtr(\bar{1}\bar{1}) \left[ G^>(\bar{1}\bar{1}') - G^<(\bar{1}\bar{1}') \right]
\]

\[
\left[ -i\hbar \frac{\partial}{\partial t_1'} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1'^2} \right] G^\lessgtr = \int dx_1 \Sigma_{HF}(\bar{1}\bar{1}) G^\lessgtr(\bar{1}\bar{1}') \\
+ \int_{t_0}^{t_1} d\bar{1} \left[ G^>(\bar{1}\bar{1}) - G^<(\bar{1}\bar{1}) \right] \Sigma^\lessgtr(\bar{1}\bar{1}') - \int_{t_0}^{t_{1'}} d\bar{1} G^\lessgtr(\bar{1}\bar{1}) \left[ \Sigma^>(\bar{1}\bar{1}') - \Sigma^<(\bar{1}\bar{1}') \right]
\]
Kadanoff-Baym Equations

\[
\left[i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2}\right] G^\geq = \int dx_1 \Sigma_{HF}(1\bar{1}) G^\geq(\bar{1}1')
\]

\[
\Sigma_{HF}
\]

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

\[
\Sigma^\geq
\]

\[
\Sigma^\geq
\]
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

\[ H(t) = F(t)H_0 + [1 - F(t)]H_1 \]

\[ F(t) = \begin{cases} 
1, & t \to -\infty \\
0, & t \to t_i 
\end{cases} \]

\[ f(t) = \frac{1}{1 + e^{t/\tau}} \]

\[ F(t) = \frac{f(t) - f(t_f)}{f(t_i) - f(t_f)} \]

- Preparing the initial state

\[ H_0 = \frac{1}{2}kx^2 \]

\[ H_1 = U_{mf} \]

\[ U_{mf}(x) = \frac{3}{4}t_0n(x) + \frac{2 + \sigma}{16}t_3 [n(x)]^{\sigma+1} \]
Switching function

\[ \tau^2 (2\tau - 3) \]

\[ 5\tau^5 (70\tau^4 - 315\tau^3 + 540\tau^2 - 420\tau + 126) \]

\[ \tau - \sin(2\pi\tau)/2\pi \]

\[ \text{time [fm/c]} \]

M. Watanaba et al., PRL 65, no. 26, page 3301
Collision of two slabs

Correlations

- Equation incorporating the interactions:

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

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

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

The parameters are chosen to result reasonable physical quantities such as depletion number.
infinite nuclear matter

Density in coordinate space

\[
\frac{E}{A} \quad \Delta E_{\text{corr}} = \Delta E_{\text{corr}}
\]
Density in momentum space

$t = 0.0 \text{ fm/c}$
EOS in infinite nuclear matter

\begin{figure}
\centering
\includegraphics[width=\textwidth]{plot.png}
\caption{Density in coordinate space}
\end{figure}
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 \(\omega_{HO}\)
  – Friction term
Solving two-time equations

Using symmetries:

\[ G^\leq(1, 2) = -[G^\leq(2, 1)]^* \]

\[ G^\leq(t_1, T + \Delta t) = G^\leq(t_1, T)e^{i\varepsilon\Delta t} - I_2^\leq(t_1, T)e^{-1}(1 - e^{i\varepsilon\Delta t}) \]

\[ G^\geq(T + \Delta t, t_2) = e^{i\varepsilon\Delta t}G^\geq(T, t_2) - (1 - e^{-i\varepsilon\Delta t})e^{-1}I_1^\geq(T, t_2) \]

\[ G^\leq(T + \Delta T, T + \Delta T) \]
Different starting points

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

![Graph showing the effect of friction term on density](image-url)
Effect of friction term

![Graph showing the effect of friction term over time with two curves: one with friction and one without. The x-axis represents time in fm/c, and the y-axis represents the variable \( \langle x \rangle \) in fm. The graph illustrates the behavior of the system with and without friction.]
Density $n(x)$ [fm$^{-3}$]

$t = 0.0$ fm/c

Occupation number

$t = 0.0$ fm/c

$x$ [fm]
What is next

• Including isospin dependency in the formalism

• Performing the collision of slabs
Thanks!
Occupation number

"nofric_w_N1_moreaccurate/ocnum.dat"
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
$\Delta \tau = \frac{\hbar}{\epsilon}$

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

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

The energy, $\epsilon$, is of the same order