Nuclear matter properties from self-consistent Green’s function methods

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Outline

- Introduction
  - *what* is nuclear matter
    - definitions, limits of validity, EOS
  - *why* we study it
    - applications and constraints
  - *how* we study it
    - phenomenological vs. ab-initio approaches

- Self-consistent Green’s functions at zero & finite temperature

- The need for three-body forces

- Results I: equation of state
  - Results II: in-medium single-particle properties

- Conclusions and current plans
Introduction: *what* is nuclear matter
Nuclear matter

- strongly interacting nucleons (symmetric/pure neutron matter)
- spin-unpolarized
- homogeneous system
- thermodynamic limit

\[ N, V \to \infty \]
\[ \rho = \frac{N}{V} \]

Weizsäcker semi-empirical mass formula

\[ E(N_p, N_n) = E_B N + E_{\text{surf}} N^{2/3} + E_{\text{Coul}} N_p^2 N^{-1/3} + E_{\text{Pauli}} (N_n - N_p)^2 / N \]

energy per particle in symmetric nuclear matter at saturation density \( \rho_0 \)
Limits of validity

- low density → clusters
- high density → hyperons, etc...

\[ T = T_{c}^{LG} \] liquid-gas phase transition
\[ T = T_{c}^{A} \] superfluidity

Challenges

- nuclear matter as a thermodynamic ensemble
  - equation of state
- nuclear matter as a system of interacting nucleons
  - modified single-particle properties
Introduction: *why* we study nuclear matter
Applications and constraints

- low-density neutron matter
  - universal properties of Fermi systems

- nuclear matter near saturation density
  - low-energy nuclear reactions
  - benchmark development of EDF (e.g. extensions to neutron-rich systems)

- high-density/high-temperature nuclear matter
  - astrophysical environment (SN, (proto-)neutron stars, ...)

- high-density/high-temperature nuclear matter
  - heavy-ion collisions
Cooling of neutron stars

- direct Urca cooling
  \[ n \rightarrow p + e^- + \bar{\nu}_e, \quad p \rightarrow n + e^+ + \nu_e \]

- modified Urca cooling
  \[ n + (n, p) \rightarrow p + (n, p) + e^- + \bar{\nu}_e \]
  \[ p + (n, p) \rightarrow n + (n, p) + e^+ + \nu_e \]
  much less efficient ( \(< 10^{-4} \))

- neutrino emissivities depend on the in-medium nucleon properties,
  in particular of the superfluid phase
Global constraints from flow observables

- not excluded a phase transition above $4\rho_0$

- extrapolation to neutron matter model for the symmetry energy

[ Danielewicz et al., Science 298 (2002) ]
Introduction: *how* we study nuclear matter
Ab-initio approaches

- model for the nuclear Hamiltonian

\[ H(\Lambda) = T + V_{\text{NN}}(\Lambda) + V_{\text{3N}}(\Lambda) + V_{\text{4N}}(\Lambda) + \cdots \]

fits two-body observables (NN phase shifts, deuteron)

- traditional/hard-core potentials (large cutoff)
  - self-consistent Green’s functions
  - Brueckner-Hartree-Fock
  - variational approaches
  - AFDMC

- EFT interactions (intermediate cutoff)

- renormalized/soft potentials (small cutoff)
  - perturbation theory
Phenomenological approaches

- effective interactions (Skyrme, Gogny, ...)
  - energy density functionals
    - fit selected nuclei and nuclear matter properties

- phenomenological effective Lagrangian
  - relativistic mean field
    - fit nuclear matter properties

lack predictive power
Self-consistent Green’s functions at zero and finite temperature
Finite temperature Green’s functions

- single-particle propagator on the time-contour
  \[ i G_{\alpha\beta}(r, t; r', t') = \mathcal{J} \psi_{\alpha}(r, t) \psi_{\beta}^\dagger(r', t') \]

carry statistical mechanics information of the system

\[ \langle \hat{O} \rangle = \text{tr} \left[ \hat{\rho} \hat{O} \right] = \frac{\text{tr} \left[ e^{-\beta(H-\mu N)} \hat{O} \right]}{\text{tr} \left[ e^{-\beta(H-\mu N)} \right]} \]

consistency between macroscopic and microscopic observables

other ab-initio approaches:

- Bloch-De Dominicis (⇒ BBG) → "frozen correlations" approximation
- variational → work in progress
Equations of motion

- equations of motion for the single-particle propagator

\[
\left( i \frac{\partial}{\partial t_1} + \frac{\nabla_{1'}^2}{2m} \right) G(1, 1') = \delta(1, 1') - i \int d \mathbf{r}_2 \, V(\mathbf{r}_1 - \mathbf{r}_2) \, G_2(1, \mathbf{r}_2, t_1; 1', \mathbf{r}_2, t_1^+) 
\]

\[ \rightarrow \quad \text{.... N-1 coupled equations} \]

decouple the hierarchy

- self-energy

\[
\int_C d^3 \mathbf{r} \, \Sigma(1, 3) \, G(3, 1') = -i \int d \mathbf{r}_2 \, V(\mathbf{r}_1 - \mathbf{r}_2) \, G_2(1, \mathbf{r}_2, t_1; 1', \mathbf{r}_2, t_1^+) 
\]

- Dyson equation

\[
G(1, 1')^{-1} = G_0(1, 1')^{-1} - \Sigma(1, 1') 
\]
In-medium T-matrix

- T-matrix approximation for the two-particle propagator

\[
\begin{align*}
\frac{G_2}{N} &= \\
\frac{H_{\text{tot}}}{\mathcal{V}} &= \\
\frac{H_{\text{kin}}}{\mathcal{V}} + \frac{H_{\text{pot}}}{\mathcal{V}}
\end{align*}
\]

- Energy per particle

\[
\frac{E}{N} = \frac{1}{\rho} \left[ \frac{\langle H_{\text{tot}} \rangle}{\mathcal{V}} \right] = \frac{1}{\rho} \left[ \frac{\langle H_{\text{kin}} \rangle}{\mathcal{V}} + \frac{\langle H_{\text{pot}} \rangle}{\mathcal{V}} \right]
\]

- Grand-canonical potential

\[
\Omega = -\text{tr}\{\ln[G^{-1}]\} - \text{tr}\{\Sigma G\} + \Phi \quad \rightarrow \quad \Omega[G, \Sigma, \Phi] = -P \mathcal{V}
\]
There exists a class of approximations which automatically fulfills thermodynamic constraints [Baym & Kadanoff '61, '62]

\[ \Sigma(1, 1') = \frac{\delta \Phi[G, V]}{\delta G(1, 1')} \]

Hartree-Fock, second order, T-matrix belong to this class
Spectral representation

- matrix representation \( i \mathbf{G}(1, 1') = i \begin{pmatrix} G^r(1, 1') & G^< (1, 1') \\ G^>(1, 1') & G^a (1, 1') \end{pmatrix} \)

\( = \begin{pmatrix} \langle T \psi(1) \psi^\dagger (1') \rangle & - \langle \psi^\dagger (1') \psi(1) \rangle \\ \langle \psi(1) \psi^\dagger (1') \rangle & \langle T^a \psi(1) \psi^\dagger (1') \rangle \end{pmatrix} \)

- equilibrium & homogeneous system: spectral GFs

\( i G^> (\mathbf{p}, \omega) = [1 - f(\omega)] \mathbf{A}(\mathbf{p}, \omega) \)
\(-i G^< (\mathbf{p}, \omega) = f(\omega) \mathbf{A}(\mathbf{p}, \omega) \)

\[ \int \frac{d\omega}{2\pi} \mathbf{A}(\mathbf{p}, \omega) = 1 \]

- free particles \( \mathbf{A}_0 (\mathbf{p}, \omega) = 2\pi \delta(\omega - p^2/2m) \)

- momentum distribution \( n(\mathbf{p}) = \int \frac{d\omega}{2\pi} \mathbf{A}(\mathbf{p}, \omega) f(\omega) \)
Self-consistent procedure

1. Start with an ansatz for $A(p, \omega)$
2. Compute the T-matrix
   $$\langle k | T^R(P, \Omega) | k' \rangle = V(k, k') + \int \frac{dp}{(2\pi)^3} \frac{dq}{(2\pi)^3} V(k, p) \langle p | G^{mc R}_2(P, \Omega) | q \rangle \langle q | T^R(P, \Omega) | k' \rangle$$
3. Compute the self-energy
   $$\text{Im} \Sigma^R(p, \omega) = \int \frac{dk}{(2\pi)^3} \frac{d\omega'}{2\pi} \left[ \left\langle \frac{p-k}{2} | \text{Im} T^R(p+k, \omega+\omega') | \frac{p-k}{2} \right\rangle \right] - \left\langle \frac{p-k}{2} | \text{Im} T^R(p+k, \omega+\omega') | \frac{k-p}{2} \right\rangle \right] [b(\omega + \omega') + f(\omega')] A(k, \omega')$$
   $$\text{Re} \Sigma^R(p, \omega) = \Sigma_{HF}(p, \omega) + \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} \Sigma^R(p, \omega')}{\omega' - \omega}$$
4. Compute the spectral function
   $$A(p, \omega) = \frac{-2 \text{Im} \Sigma^R(p, \omega)}{[\omega - p^2/2m - \text{Re} \Sigma^R(p, \omega)]^2 + [\text{Im} \Sigma^R(p, \omega)]^2}$$

→ Repeat until convergence is achieved
Technical aspects

- numerical solution of coupled integro-differential equations
  - iterative scheme
- use Fast Fourier Transform (FFT) and convolution theorem
  \[ \int d\omega' F_1(\omega' - \omega) F_2(\omega') = \left[ F_1^T(t) F_2^T(t) \right]^T \]
- discretization on a fixed-spacing grid
- cut-off dependence under control
- each point \((T, \rho, \delta, V) \sim 100\) hours
The need for three-body forces

- empirical values for saturation

\[ \rho_{\text{sat}} \equiv \rho_0 = 0.16 \pm 0.01 \text{ fm}^{-3} \]
\[ E_{\text{sat}}/N \equiv B = 16 \pm 1 \text{ MeV} \]
Three-body forces
Three-body forces

- Realistic microscopic calculations cannot avoid the use of NNN forces
  - Binding energies, saturation properties and radii
  - Shell evolution
  - Three-nucleon scattering

- Currently: microscopic NNN interactions only in light systems and INM
  - Normal-ordered (average) part of NNN possibly sufficient

- Coupled-cluster in $^4$He [Hagen et al. 2007]
- SCGF in INM [Somà, Božek 2008]
- Perturbation theory in INM [Hebeler, Schwenk 2009]
Urbana three-body forces

\[ V_{ijk}^{\text{Urbana}} = V_{ijk}^{2\pi} + V_{ijk}^R \]

\[ \Delta\text{-excitation} \]

\[ \leftrightarrow 2\pi \text{ exchange} \]

\[ \text{and others:} \]
Derivation of the effective potential

- need to derive an effective two-body potential

\[ V_{3}^{\text{eff}}(q, q') = \sum_{\sigma \tau} \int \frac{dk}{(2\pi)^3} n(k) V_{3}^{FT}(k, q, q') \]

to be inserted in the T-matrix

\[ V \rightarrow V' = V + V_{3}^{\text{eff}} \]

Fourier transform

spin-isospin average

projection into partial waves

\[ \langle q| V_{j}^{S=0}(P)|q' \rangle = \frac{1}{4\pi^2} \int d\Omega_{qq'} P_{j}(\Omega_{qq'}) \times \left\{ V_{s}^{R} + V_{s}^{2\pi} - 3V_{\sigma \tau}^{2\pi} \right\} \text{ for } J \text{ even} \]

\[ V_{s}^{R} + V_{s}^{2\pi} + 9V_{\sigma \tau}^{2\pi} \text{ for } J \text{ odd} \]
Results I: equation of state
Energy per particle in symmetric matter

CD-Bonn

\[
\begin{align*}
E/N &= -16.3 \text{ MeV} \\
\rho &= 0.171 \text{ fm}^{-3}
\end{align*}
\]

Nijmegen

\[
\begin{align*}
E/N &= -16.4 \text{ MeV} \\
\rho &= 0.164 \text{ fm}^{-3}
\end{align*}
\]

[Somà and Božek, Phys. Rev. C 78 (2008)]
**Energy in neutron matter & symmetry energy**

![Graph](image)

- **parabolic approximation**

\[
\frac{E}{N}(\rho, \delta) = \frac{E}{N}(\rho, \delta = 0) + \delta^2 E_{sym}(\rho) + \mathcal{O}(\delta^4)
\]

\[\delta \equiv \frac{\rho_n - \rho_p}{\rho_{tot}}\]

### Experimental constraints on the EoS

- **incompressibility**: $$K_0 = 9 \left( \rho^2 \frac{\partial^2 E/N}{\partial \rho^2} \right)_{\rho=\rho_0, \delta=0}$$
- **symmetry energy**: $$S_0 = \frac{1}{2} \left( \frac{\partial^2 E/N}{\partial \delta^2} \right)_{\rho=\rho_0, \delta=0} = E_{\text{sym}}(\rho_0)$$
- **effective mass**: $$\frac{\partial \omega_p}{\partial p^2} = \frac{1}{2m^*} \quad \omega_p = \frac{p^2}{2m} + \text{Re} \, \Sigma(p, \omega_p)$$

<table>
<thead>
<tr>
<th></th>
<th>$\rho_0$ [fm$^{-3}$]</th>
<th>$E_0$ [MeV]</th>
<th>$K_0$ [MeV]</th>
<th>$S_0$ [MeV]</th>
<th>$m^*/m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>0.16 ± 0.01</td>
<td>−16 ± 1</td>
<td>210 ± 30</td>
<td>32 ± 6</td>
<td>≈0.8</td>
</tr>
<tr>
<td>CD-Bonn</td>
<td>0.287</td>
<td>−19.9</td>
<td>70</td>
<td>32.2</td>
<td>0.90</td>
</tr>
<tr>
<td>CD-Bonn + TBF</td>
<td>0.171</td>
<td>−16.3</td>
<td>148</td>
<td>39.7</td>
<td>0.87</td>
</tr>
<tr>
<td>Nijmegen</td>
<td>0.235</td>
<td>−18.4</td>
<td>76</td>
<td>30.5</td>
<td>0.87</td>
</tr>
<tr>
<td>Nijmegen + TBF</td>
<td>0.164</td>
<td>−16.4</td>
<td>158</td>
<td>37.1</td>
<td>0.90</td>
</tr>
</tbody>
</table>
Pressure and entropy

- direct (diagrammatic) calculation of $P$
  \[
  \Phi = \int_0^1 \frac{d\lambda}{\lambda} H_{pot}(\lambda V, G_{\lambda=1})
  \]

- entropy from
  \[
  \frac{S}{N} = \frac{1}{T} \left( \frac{E}{N} - \mu + \frac{P}{\rho} \right)
  \]

\[
\Omega[G, \Sigma, \Phi] = -P \mathcal{V}
\]

Spinodal region
\[
\left. \frac{\partial P}{\partial \rho} \right|_T < 0 \quad \left. \frac{\partial \mu}{\partial \rho} \right|_T < 0
\]

Coexistence region
\[
\mu(\rho_g) = \mu(\rho_l) \\
P(\rho_g) = P(\rho_l)
\]
Spinodal region

![Spinodal region graph](image)

<table>
<thead>
<tr>
<th>potential</th>
<th>$T_c$ (MeV)</th>
<th>$\rho_c$ (fm$^{-3}$)</th>
<th>$P_c$ (MeV fm$^{-3}$)</th>
<th>$\frac{P_c}{\rho_c T_c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD-Bonn</td>
<td>18</td>
<td>0.107</td>
<td>0.43</td>
<td>0.22</td>
</tr>
<tr>
<td>CD-Bonn + TBF</td>
<td>12.5</td>
<td>0.096</td>
<td>0.14</td>
<td>0.12</td>
</tr>
<tr>
<td>Nijmegen</td>
<td>20.5</td>
<td>0.094</td>
<td>0.50</td>
<td>0.26</td>
</tr>
<tr>
<td>Nijmegen + TBF</td>
<td>11.5</td>
<td>0.088</td>
<td>0.15</td>
<td>0.14</td>
</tr>
</tbody>
</table>

[Somà and Božek, Phys. Rev. C 80 (2009)]
Critical temperature in nuclear matter

- Bloch-De Dominicis → 9 - 20 MeV [Das et al.; Baldo et al.]
- Dirac-Brueckner-Hartree-Fock → 10 - 13 MeV [Ter Haar et al.; Huber et al.]
- Green’s functions (NN only) → 16 - 19 MeV [Rios et al.; VS, Božek]
- Green’s functions (NN+NNN) → ~12 MeV [VS, Božek]

“Limiting temperature” in finite nuclei

- Coulomb and surface effects

  the nucleus undergoes a mechanical instability before reaching $T_c$

  $\delta P = P_c + P_s (T)$

Results II: *single-particle properties*
Single-particle properties

- spectral representation
  
  $-i\, G^<(p, \omega) = f(\omega) \, A(p, \omega)$
  
  $i\, G^>(p, \omega) = [1 - f(\omega)] \, A(p, \omega)$

  recall that the free spectral function is
  
  $A_0(p, \omega) = 2\pi \, \delta(\omega - p^2/2m)$

  \textit{quasiparticle approximation}
  
  $A_{qp}(p, \omega) = 2\pi \, \delta(\omega - p^2/2m - \text{Re} \, \Sigma(p, \omega))$

- effective mass

\[ \left. \frac{\partial \omega_p}{\partial p^2} \right|_{p=p_F} = \frac{1}{2m^*} \]

where

\[ \omega_p = \frac{p^2}{2m} + \text{Re} \, \Sigma(p, \omega_p) \]
Spectral function

\[ A(p=0, \omega) \text{ [MeV}^{-1}] \]

- \( T = 0 \)
- \( 0.4 \rho_0 \)
- \( \rho_0 \)
- \( 2 \rho_0 \)

- \( T = 10 \text{ MeV} \)
- \( 0.4 \rho_0 \)
- \( \rho_0 \)
- \( 2 \rho_0 \)
Effective mass

\[ m^* / m \]

\[ p \text{ [MeV]} \]

\[ T = 0 \]

\[ T = 10 \text{ MeV} \]

\[ 0.4 \rho_0 \]

\[ \rho_0 \]

\[ 2 \rho_0 \]

\[ \text{CD-Bonn} \]

\[ \text{CD-Bonn + TBF} \]
Spectral function - neutron matter

\[ A(p=0, \omega) \text{ [MeV}^{-1}] \]

\( T=0 \)

\( 0.4 \rho_0 \)

\( \rho_0 \)

\( 2 \rho_0 \)

\( T=10 \text{ MeV} \)

\( 0.4 \rho_0 \) - CD-Bonn

\( \rho_0 \) - CD-Bonn + TBF

\( 2 \rho_0 \) - CD-Bonn + TBF

\( \omega \) [MeV]
Effective mass - neutron matter

\[ \frac{m^*}{m} \]

\[ p \text{ [MeV]} \]

\[ T = 0 \]

\[ \rho_0 \]

\[ 0.4 \rho_0 \]

\[ 2 \rho_0 \]

\[ T = 10 \text{ MeV} \]

\[ \text{CD-Bonn} \]

\[ \text{CD-Bonn + TBF} \]
Conclusions

- first spectral calculations of the nuclear matter EOS with TBF
- correct saturation properties
- entropy not affected by nucleon correlations
- study of the liquid-gas phase transition $T_c \approx 12$ MeV
- single-particle properties $\rightarrow$ TBF effects above saturation density
- spectral function $\rightarrow$ opposite effect in symmetric and in pure neutron matter

Extensions of the technique:
- asymmetric nuclear matter
- explicit inclusion of superfluidity
- application to nuclei
Gorkov approach to pairing

- Saclay-Surrey collaboration (V.S., C. Barbieri, T. Duguet)

- Gorkov-Green’s function formalism at 2\textsuperscript{nd} order
  - many-body long-range correlations (quenching of spectroscopic factors, ...)
  - pairing beyond HFB
  - ab-initio no-core calculations in large spaces
  - link between g.s. energy and normal/anomalous densities (EDF)
Integrated quantities.

QUASIPARTICLE AND QUASIHOLE STATES OF NUCLEI

that indeed the N-matrix, which involves an integral sum over each hole pole of

by the addition of a nucleon, occupied states are accessed by

with electron scattering measurements on

tion rather than occupation numbers, because the latter are

by analyzing the spectroscopic factors and strength distribu-

fragmentation pattern still leads to large occupation numbers.

Eq. (1)

corresponding to orbits in the 1

as tr o n s i n g l e - p a r t i c l e character event thought they are further

2

with the 1

Spectral function

LO interaction tends to overestimate the

2

f

−

3

ε

−

3

−

5/2

strengths for one-neutron transfer on

Analogous fragmentation patterns extend to the shells

A

k

A

0

A

A

/2

A

A

/2

A

A

/2

A

A

/2

+ FRPA

1st order (HFB)

63Ni

55Ni

65Ni

57Ni

P_{1/2}

P_{3/2}

f_{5/2}

f_{7/2}

Dyson 2nd order (+ FRPA)

55Ni

57Ni

Dyson 1st order (HF)

63Ni

65Ni

Gorkov 1st order (HFB)

Gorkov 2nd order

in progress

Gorkov 2nd order + FRPA

next