Self-consistent Green’s functions with three-body forces

Arianna Carbone
Collaborators: Artur Polls, Arnau Rios, Carlo Barbieri & Andrea Cipollone

5th of May, 2014 - Three-Body Forces: from Matter to Nuclei - ECT*
Objective

The SCGF method with 3B forces in infinite and finite nuclear systems:

**Symmetric nuclear matter**
See Arnau Rios’ talk on Wednesday

**Finite nuclei**
See Carlo Barbieri’s talk later today, and Andrea Cipollone’s talk on Friday
Self-consistent Green’s functions


★ The Green’s function as a tool to solve the many-body problem:

\[
G_{\alpha\beta}(\omega) = \sum_m \frac{\langle \Psi_0^N | a_\alpha | \Psi_m^{N+1} \rangle \langle \Psi_m^{N+1} | a_\beta^\dagger | \Psi_0^N \rangle}{\omega - (E_m^{N+1} - E_0^N) + i\eta} + \sum_n \frac{\langle \Psi_0^N | a_\beta^\dagger | \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle}{\omega - (E_0 - E_n^{N-1}) + i\eta}
\]

★ Self-consistent:

- Green’s function
- Vertex function
- Self-energy

★ Nonrelativistic Hamiltonian:

\[
\hat{H} = \sum_\alpha \varepsilon_\alpha^0 a_\alpha^\dagger a_\alpha - \sum_{\alpha\beta} U_{\alpha\beta} a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\gamma\beta\delta} V_{\alpha\gamma,\beta\delta} a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta + \frac{1}{36} \sum_{\alpha\gamma\epsilon,\beta\delta\eta} W_{\alpha\gamma\epsilon,\beta\delta\eta} a_\alpha^\dagger a_\gamma^\dagger a_\epsilon^\dagger a_\eta a_\delta a_\beta
\]

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**Self-consistent Green’s functions**


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\]

energy with an added particle

energy with a removed particle

★ Self-consistent:

**Nonrelativistic Hamiltonian:**

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\hat{H} = \sum_\alpha \varepsilon_\alpha^0 a_{\alpha}^\dagger a_\alpha - \sum_{\alpha\beta} U_{\alpha\beta} a_{\alpha}^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\gamma, \beta\delta} V_{\alpha\gamma, \beta\delta} a_{\alpha}^\dagger a_{\gamma}^\dagger a_\delta a_\beta + \frac{1}{36} \sum_{\alpha\gamma, \beta\delta, \epsilon\eta} W_{\alpha\gamma\epsilon, \beta\delta\eta} a_{\alpha}^\dagger a_{\gamma}^\dagger a_{\epsilon}^\dagger a_\eta a_\delta a_\beta
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Self-consistent Green’s functions


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Energy with a removed particle

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★ Nonrelativistic Hamiltonian:

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Self-consistent Green’s functions


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\]

\[
\hat{H}_0 = \bullet \bullet \bullet \times \bullet - - - - \bullet
\]

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Self-consistent Green’s functions

SCGF... how does it work?

★ Start:
  SP propagator

★ Construct:
  Vertex function

★ Obtain:
  Self-energy

★ Calculate:
  SP propagator

★ Procedure is repeated until self-consistency is achieved
Self-consistent Green’s functions

SCGF... how does it work?

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Steps to our objective

How to include 3-body forces in the SCGF method:

1. **Extend** the SCGF theory consistently
2. **Build** a density dependent 2-body force (for infinite matter)
3. **Define** new sum rules to calculate the total energy
Steps to our objective

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Effective interactions

Carbone, Cipollone, Barbieri, Rios, Polls, PRC 88, 054326 (2013)

Define **effective interactions** to include correctly 3B terms:

\[
\begin{align*}
2B & \quad \rightarrow \quad 2B + 3B \\
\text{Interaction:} & \quad \rightarrow \\
\text{Example: 2nd order diagrams} & \\
\end{align*}
\]

Number of diagrams decreases!
Effective interactions: 1\textsuperscript{st}, 2\textsuperscript{nd}, 3\textsuperscript{rd} order

Carbone, Cipollone, Barbieri, Rios, Polls, PRC 88, 054326 (2013)

1\textsuperscript{st}  

2\textsuperscript{nd}  

3\textsuperscript{rd}  

Self-energy expansion
The 4-pt vertex function

Obtain the interacting vertex function including 3body forces:

It’s an equation including the 4-pt, 6-pt and 8-pt interacting vertex functions!
The self-energy

Carbone, Cipollone, Barbieri, Rios, Polls, PRC 88, 054326 (2013)

Calculate self-energy paying attention to the effective terms:

Self-energy: \[ 2B \]

\[ \Sigma^* = \frac{1}{4} \Gamma_{4\text{-pt}} + \Gamma_{6\text{-pt}} \]

\[ \gamma^* = \cdots \cdots \cdots + \Gamma_{4\text{-pt}} + \frac{1}{4} \Gamma_{6\text{-pt}} \]

\[ \Gamma_{4\text{-pt}} + \Gamma_{6\text{-pt}} \]

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The self-energy

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Calculate self-energy paying attention to the effective terms:

Self-energy:

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2B + 3B

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Steps to our objective

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In the present work we use:

- **2NF: N3LO** (Entem & Machleidt, PRC 68, 041001, 2003)

- **3NF: N2LO** (Epelbaum et al., PRC 66, 064001, 2002), in a density dependent form (Carbone, Rios, Polls, in preparation)

3NFs at N2LO in the chiral expansion

* **3NF at N2LO:**
  - two-pion exchange
  - one-pion exchange
  - contact

* **2NF density-dependent** at N2LO (following Holt et al. PRC 81, 024002, 2010):

  - $c_1, c_3, c_4$ fit to NN and $\pi N$ data (Entem & Machleidt PRC 68, 041001, 2003)
  - $c_D, c_E$ fit to $^3\text{H}$ and $^4\text{He}$ binding energies (Nogga et al., PRC 73, 064002, 2006)
Density-dependent 2B forces

\[ V(k,k) \text{ [fm]} \]

\begin{align*}
\rho_0 &= \text{N3LO+N2LOdd} (p) \\
\rho_0 &= \text{N3LO} + \text{N2LOdd} (p)
\end{align*}

\[ c_1 = -0.81 \text{ GeV}^{-1} \quad c_3 = -3.2 \text{ GeV}^{-1} \quad c_4 = 5.4 \text{ GeV}^{-1} \]


\[ c_D = -1.11 \quad c_E = -0.66 \]

Nogga et al., PRC 73, 064002 (2006)

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Density-dependent 2B forces

The average:

- small effect
- enhanced absolute values

Holt et al. PRC 81, 024002, 2010
Density-dependent 2B forces

The regulator function:

\[
f(k, k', p_3) = \exp \left[ -\left( \frac{k}{\Lambda_{3NF}} \right)^4 - \left( \frac{k'}{\Lambda_{3NF}} \right)^4 \right] \exp \left[ -\frac{2}{3} \frac{p_3^2}{\Lambda_{3NF}^4} \left( \frac{p_3^2}{3} + (k^2 + k'^2) \right) \right]
\]

\(\Lambda_{3NF} = 500\) MeV

- small effect
- enhanced absolute values

Extrapolation for off-diagonal matrix elements: \(k^2 \rightarrow \frac{(k^2 + k'^2)}{2}\)
Steps to our objective

How to include 3-body forces in the SCGF method:

1. **Extend** the SCGF theory consistently

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3. **Define** new sum rules to calculate the total energy
Koltun sum rule

* Total energy of the system:

\[ E^N = \langle \Psi^N | \hat{H} | \Psi^N \rangle = \langle \Psi^N | \hat{T} | \Psi^N \rangle + \langle \Psi^N | \hat{V} | \Psi^N \rangle \]

* **Koltun sum rule**: first developed by Galitskii & Migdal (1958), later applied to finite system by Koltun ('70s)

\[ \sum_{\alpha} \int_{-\infty}^{E^N-E^{N-1}} d\omega \, \omega \frac{1}{\pi} \text{Im} G_{\alpha\alpha}(\omega) = \langle \Psi^N | \hat{T} | \Psi^N \rangle + 2\langle \Psi^N | \hat{V} | \Psi^N \rangle \]

\[
\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{2} \left\{ \frac{p^2}{2m} + \omega \right\} A(p, \omega) f(\omega)
\]
Koltun sum rule

★ Total energy of the system:

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E^N = \langle \Psi^N | \hat{H} | \Psi^N \rangle = \langle \Psi^N | \hat{T} | \Psi^N \rangle + \langle \Psi^N | \hat{V} | \Psi^N \rangle
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**Koltun sum rule**

* Total energy of the system:

\[
E_N = \langle \Psi_N | \hat{H} | \Psi_N \rangle = \langle \Psi_N | \hat{T} | \Psi_N \rangle + \langle \Psi_N | \hat{V} | \Psi_N \rangle
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\]

The spectral function
Koltun sum rule with 3B forces

* Total energy of the system with three-body forces:

\[ E^N = \langle \Psi^N | \hat{H} | \Psi^N \rangle = \langle \Psi^N | \hat{T} | \Psi^N \rangle + \langle \Psi^N | \hat{V} | \Psi^N \rangle + \langle \Psi^N | \hat{W} | \Psi^N \rangle \]

* Koltun sumrule modified:

\[ \sum_{\alpha} \int_{-\infty}^{E^N - E^{N-1}} \frac{1}{\pi} \text{Im} \ G_{\alpha\alpha}(\omega) = \langle \Psi^N | \hat{T} | \Psi^N \rangle + 2\langle \Psi^N | \hat{V} | \Psi^N \rangle + 3\langle \Psi^N | \hat{W} | \Psi^N \rangle \]

\[
\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{2} \left\{ \frac{p^2}{2m} + \omega \right\} A(p, \omega) f(\omega) - \frac{1}{2} \langle \Psi^N | \hat{W} | \Psi^N \rangle
\]

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Koltun sum rule with 3B forces

- Total energy of the system with three-body forces:

\[ E^N = \langle \Psi^N | \hat{H} | \Psi^N \rangle = \langle \Psi^N | \hat{T} | \Psi^N \rangle + \langle \Psi^N | \hat{V} | \Psi^N \rangle + \langle \Psi^N | \hat{W} | \Psi^N \rangle \]

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\[ \frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \left[ \frac{p^2}{2m} + \omega \right] A(p, \omega) f(\omega) - \frac{1}{2} \langle \Psi^N | \hat{W} | \Psi^N \rangle \]
Koltun sum rule with 3B forces

Written in other words, we are calculating:

\[
\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{2} \left\{ \frac{p^2}{2m} + \omega \right\} A(p, \omega) f(\omega) - \frac{1}{2} \langle \Psi^N | \hat{W} | \Psi^N \rangle
\]

Hartree-Fock approximation

\[
\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{2} \left\{ \frac{p^2}{2m} + \omega + \frac{1}{3} \sum_{HF}^3 \right\} A(p, \omega) f(\omega)
\]
Koltun sum rule with 3B forces

Written in other words, we are calculating:

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\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{2} \left\{ \frac{p^2}{2m} + \omega \right\} A(p, \omega) f(\omega) - \frac{1}{2} \langle \Psi^N | \hat{W} | \Psi^N \rangle
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\]
Symmetric nuclear matter

Pure neutron matter
Summary

* Extended the SCGF method defining effective interactions

* Consistently included three-body forces in the self-energy

* Constructed a density-dependent force

* Defined a new sum rule for the energy

\[
\frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \left[ \frac{p^2}{2m} + \omega \right] A(p, \omega) f(\omega) - \frac{1}{2} \langle \Psi^N | \hat{W} | \Psi^N \rangle
\]

* Analyzed the microscopic properties

* Investigated the total energy
Needs…

* Calculate **off-diagonal matrix elements** for density-dependent potential

* Test the **chiral nuclear force convergence**
Thank you for your attention!
Backup
Step 1. Extend the SCGF approach

- **Start:**
  - $\Sigma^* = T$
  - $\Sigma^* = T$

- **Construct:**
  - $T = \ldots + T$
  - $T = \ldots + T$

- **Obtain:**
  - $\Sigma^* = T$
  - $\Sigma^* = T$

- **Calculate:**
  - $\Sigma^* = T + \Sigma^*$
  - $\Sigma^* = T + \Sigma^*$

- Procedure is repeated until **self-consistency** is achieved.
Step 1. Extend the SCGF approach

Procedure is repeated until **self-consistency** is achieved

<table>
<thead>
<tr>
<th>Start</th>
<th>Construct</th>
<th>Obtain</th>
<th>Calculate</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="NN force" /></td>
<td><img src="image2" alt="2B" /></td>
<td><img src="image3" alt="NN + 3N force" /></td>
<td><img src="image4" alt="2B + 3B" /></td>
</tr>
</tbody>
</table>

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Steps to our objective... Recap!

How to include 3-body forces:

✓ **Extend** the SCGF theory consistently

✓ **Build** a density dependent 2-body force

✓ **Define** new sum rules to calculate the total energy

➡ **Microscopic properties:** momentum distribution, self-energy

➡ **Macroscopic properties:** total energy of SNM and PNM, the symmetry energy

**Notice:** all results are presented at \( T=5 \) MeV to avoid pairing instability
Conclusions

★ **Microscopic properties:**

★ **overall:** small 3-body force effect, except for single-particle potential; small modifications due to averaging procedures

★ **momentum distribution:** depletion is density dependent; presence of high-momentum components

★ **single particle potential:** visible repulsive effect

★ **Macroscopic properties:**

★ **overall:** striking 3-body force effect; small modifications due to averaging procedures

★ **SNM:** good saturation density; saturation energy underbound; SRG improves over energy value

★ **PNM:** repulsion at all densities; neutron matter is perturbative for the chiral force

★ **SYM:** 2B+3B value can be improved with different LECs
The need for three-body forces

- **Infinite nuclear matter:**
  - nuclear matter is overbound with only two-body forces
  - Saturation point of nuclear matter not reproduced

- **Finite nuclei:**
  - light nuclei are underbound
  - many-body forces are necessary to draw the neutron drip line
Previous work

Somà & Bozek, PRC 78, 054003 (2008)
Step 3. Define a new sum rule

* Written in other words, we are calculating:

\[ \sum_\alpha \int_{-\infty}^{E^N - E^{N-1}} d\omega \omega \frac{1}{\pi} \text{Im} \ G_{\alpha\alpha}(\omega) = \langle \Psi^N | \hat{T} | \Psi^N \rangle + 2 \langle \Psi^N | \hat{V} | \Psi^N \rangle + 3 \langle \Psi^N | \hat{W} | \Psi^N \rangle \]

* Koltun sumrule modified:

\[ \frac{E}{A} = \frac{\nu}{\rho} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \left( \frac{p^2}{2m} + \omega \right) A(p, \omega) f(\omega) + \frac{1}{3} \langle \Psi^N | \hat{V} | \Psi^N \rangle \]

\[ G^{4\text{-pt}} = ----- - + \Gamma^4 \]

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Outlooks

- Complete 1B effective potential
- Add terms to sum rule correction
- Test different modified sum rule
- Calculate off-diagonal matrix elements for density-dependent potential
- Test the chiral nuclear force convergence
- Investigate high temperature behavior $T \sim 10-20$ MeV
Thank you for your attention!