Gorkov-Green's function approach to open-shell systems

Based on:

- Somà, Duguet, Barbieri, PRC 84 064317 (2011)
- Somà, Barbieri, Duguet, PRC 87 011303(R) (2013)
- Barbieri, Cipollone, Somà, Duguet, Navrátil, arXiv:1211.3315
- Somà, Barbieri, Duguet, arXiv:1304.xxxx
- Somà, Cipollone, Barbieri, Duguet, Navrátil, *in preparation*

INT Workshop

*Advances in many-body theory: from nuclei to molecules*

Seattle, 4 April 2013
Towards a first-principle description of nuclei

- **Light nuclei**
  - NCSM, GFMC, ...
  - Configuration interaction limited to small valence/model spaces

- **Medium-mass nuclei**
  - Mircroscopic SM, ...
  - Usual expansion schemes fail to account for pairing correlations

- **Medium-mass nuclei**
  - GF, CC, IM-SRG, ...
  - Limited to doubly-closed-shell ± 1 and ± 2 nuclei
Error estimates in *ab initio* calculations

★ Long-term goal: predictive nuclear structure calculations

→ With quantified theoretical errors
→ Consistent description of structure and reaction

Estimation of theoretical errors in *ab initio* methods

<table>
<thead>
<tr>
<th></th>
<th>Gorkov GF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Hamiltonian</td>
<td>×</td>
</tr>
<tr>
<td>2) Many-body expansion</td>
<td>×</td>
</tr>
<tr>
<td>3) Model space truncation</td>
<td>✓</td>
</tr>
<tr>
<td>4) Numerical algorithms</td>
<td>✓</td>
</tr>
</tbody>
</table>
Paths to open-shell systems

Two ways to address (near)-degenerate systems

(a) Multi-reference approaches
   ➞ e.g. IMSRG + CI, MR-CC, microscopic VS-SM

(b) Single-reference approaches
   ➞ explicit account of pairing mandatory

Self-consistent Gorkov-Green’s functions:

- Bogoliubov algebra + Green’s function theory
- Address explicitly the non-perturbative physics of Cooper pairs
  ➞ Formulate the expansion scheme around a Bogoliubov vacuum
  ➞ Breaking of particle-number conservation (eventually restored)
Gorkov’s framework

★ Auxiliary many-body state

⇒ Mixes various particle numbers \( |\Psi_0\rangle \equiv \sum_A c_A |\psi_A^0\rangle \)

⇒ Introduce a “grand-canonical” potential \( \Omega = H - \mu A \)

⇒ |\Psi_0\rangle minimizes \( \Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle \) under the constraint \( A = \langle \Psi_0 | A | \Psi_0 \rangle \)

⇒ Observables of the N system \( \Omega_0 = \sum_{A'} |c_{A'}|^2 \Omega_{0}^{A'} \approx E_0^A - \mu A \)

★ Set of 4 Green’s functions

\[
\begin{align*}
&i G_{ab}^{11}(t,t') \equiv \langle \Psi_0 | T \{ a_a(t) a_b^\dagger(t') \} | \Psi_0 \rangle \equiv \begin{array}{c}
\text{a} \\
\text{b}
\end{array} \\
&i G_{ab}^{12}(t,t') \equiv \langle \Psi_0 | T \{ a_a(t) a_b(t') \} | \Psi_0 \rangle \equiv \begin{array}{c}
\text{a} \\
\bar{\text{b}}
\end{array} \\
&i G_{ab}^{21}(t,t') \equiv \langle \Psi_0 | T \{ a_a^\dagger(t) a_b^\dagger(t') \} | \Psi_0 \rangle \equiv \begin{array}{c}
\bar{\text{a}} \\
\text{b}
\end{array} \\
&i G_{ab}^{22}(t,t') \equiv \langle \Psi_0 | T \{ a_a^\dagger(t) a_b(t') \} | \Psi_0 \rangle \equiv \begin{array}{c}
\bar{\text{a}} \\
\bar{\text{b}}
\end{array}
\end{align*}
\]

[Gorkov 1958]
Spectrum and spectroscopic factors

**Separation energy spectrum**

\[
G^{11}_{ab}(\omega) = \sum_{k} \left\{ \frac{U^{k}_{a} U^{k*}_{b}}{\omega - \omega_{k} + i\eta} + \frac{\tilde{V}^{k*}_{a} \tilde{V}^{k}_{b}}{\omega + \omega_{k} - i\eta} \right\}
\]

Lehmann representation

where

\[
\begin{align*}
U^{k*}_{a} &\equiv \langle \Psi_{k} | a^{\dagger}_{a} | \Psi_{0} \rangle \\
V^{k*}_{a} &\equiv \langle \Psi_{k} | a_{a} | \Psi_{0} \rangle
\end{align*}
\]

and

\[
\begin{align*}
E^{+}_{k}(A) &\equiv E^{A+1}_{k} - E^{A}_{0} \equiv \mu + \omega_{k} \\
E^{-}_{k}(A) &\equiv E^{A}_{0} - E^{A-1}_{k} \equiv \mu - \omega_{k}
\end{align*}
\]

**Spectroscopic factors**

\[
\begin{align*}
SF^{+}_{k} &\equiv \sum_{a \in \mathcal{H}_{1}} |\langle \psi_{k} | a^{\dagger}_{a} | \psi_{0} \rangle|^{2} = \sum_{a \in \mathcal{H}_{1}} |U^{k}_{a}|^{2} \\
SF^{-}_{k} &\equiv \sum_{a \in \mathcal{H}_{1}} |\langle \psi_{k} | a_{a} | \psi_{0} \rangle|^{2} = \sum_{a \in \mathcal{H}_{1}} |V^{k}_{a}|^{2}
\end{align*}
\]
Self-energy expansion

**Gorkov equations**  ➔  energy *dependent* eigenvalue problem

\[
\sum_b \left( \begin{array}{c}
t_{ab} - \mu_{ab} + \Sigma_{1b}^{11}(\omega) \\
\Sigma_{21}^{11}(\omega)
\end{array} \right) \left( \begin{array}{c}
- t_{ab} + \mu_{ab} + \Sigma_{2b}^{12}(\omega)
\end{array} \right) \mid_{\omega_k} \left( \begin{array}{c}
U_b^k \\
V_b^k
\end{array} \right) = \omega_k \left( \begin{array}{c}
U_a^k \\
V_a^k
\end{array} \right)
\]

**1st order**  ➔  energy-*independent* self-energy

\[
\Sigma_{1b}^{11} = \begin{array}{cc}
\bullet & \circ \\
\downarrow & \\
\omega'
\end{array}
\]

**2nd order**  ➔  energy-*dependent* self-energy

\[
\Sigma_{1b}^{11}(2)(\omega) = \uparrow \omega' \downarrow \omega'' + \uparrow \omega' \downarrow \omega'' \\
\Sigma_{1b}^{12}(2)(\omega) = \downarrow \omega' \uparrow \omega'' + \downarrow \omega' \uparrow \omega''
\]
**Scaling of Gorkov’s problem**

★ Transformed into an energy *independent* eigenvalue problem

\[
\begin{pmatrix}
T - \mu + \Lambda & \tilde{h} & C & -D^\dagger \\
\tilde{h}^\dagger & -T + \mu - \Lambda & -D^\dagger & C \\
C^\dagger & -D & E & 0 \\
-D & C^\dagger & 0 & -E
\end{pmatrix}
\begin{pmatrix}
U^k \\
V^k \\
W_k \\
Z_k
\end{pmatrix}
= \omega_k
\begin{pmatrix}
U^k \\
V^k \\
W_k \\
Z_k
\end{pmatrix}
\]

★ Numerical scaling

\[
m_{p,1} \approx \left( \frac{N_b}{3} \right) \propto \frac{N_b^3}{6}
\]

\[2N_b \begin{cases}
h & \tilde{h} & C & -D^\dagger \\
\tilde{h}^\dagger & -h & -D^\dagger & C \\
C^\dagger & -D & E & 0 \\
-D & C^\dagger & 0 & -E
\end{cases}
\]

\[N_{tot,1} = 2N_b + M_{p,1} \approx N_b^3 \]

\[N_{tot,n} = 2N_b + M_{p,n} \approx N_b^{3n} \]

\[N_b \rightarrow \text{dimension of the s.p. basis} \]

\[n \rightarrow \text{number of iterations} \]
Tame the dimension growth

★ How do we select the poles?
We do not...

Krylov projection of Gorkov matrix

\[
\begin{pmatrix}
T - \mu + \Lambda & \tilde{h} & C & -D^\dagger \\
\tilde{h}^\dagger & -T + \mu - \Lambda & -D & C \\
C^\dagger & -D & E & 0 \\
-D & C^\dagger & 0 & -E
\end{pmatrix}
\begin{pmatrix}
U_k \\
V_k \\
\mathcal{W}_k \\
\mathcal{Z}_k
\end{pmatrix} = \omega_k
\begin{pmatrix}
U_k \\
V_k \\
\mathcal{W}_k \\
\mathcal{Z}_k
\end{pmatrix}
\]

⇒ Conserves moments of spectral functions

⇒ Equivalent to exact diagonalization for $N_1 \to \text{dim}(E)$
Testing Krylov projection

★ Energy and spectral independent of the projection

★ Same behavior for all model spaces

favorable scaling

Density of states

Spectral strength

40Ti

N_{\text{max}} = 13

N = 10

N = 50

N = 100

E [MeV]

N_L

40Ti

(\nu s1/2)

\nu s1/2

N_{\text{max}} = 13

DOS

\omega [MeV]

\omega [MeV]
Self-consistency and scaling

🌟 Fully (dashed) vs. partially (solid) SC

Scaling does not depend on $A$

Partial self-consistency grasps most of the correlations

MBPT(2) inadequate
Towards medium/heavy open-shell

$^{74}\text{Ni}$

- **NN interaction:**
  - chiral $N^3LO$ SRG-evolved to 2.0 fm$^{-1}$
  - [Entem and Machleidt 2003]
  - Very good convergence
  - From $N=13$ to $N=11 \rightarrow 200$ keV

$E(N=13) = -1269.6$ MeV
$E(N=\infty) = -1269.7(2)$ MeV

(Extrapolation to infinite model space from [Furnstahl, Hagen, Papenbrok 2012] and [Coon et al. 2012])
Calcium isotopic chain

- NN only

→ Systematic along isotopic/isotonic becomes available
→ Overbinding (increasing with A): need for three-body forces
Three-body forces

🌟 Inclusion of 3NF as effective 2NF

▶️ Average over the 3rd nucleon in each nucleus

![Diagram of HFB limit](https://via.placeholder.com/150)

▶️ Additional term in the Galitskii-Koltun sum rule [Cipollone et al. 2013]

\[ E_0^A = \frac{1}{4\pi i} \int_{C^\uparrow} d\omega \text{Tr}_{\mathcal{H}_1} [G^{11}(\omega) [T + (\mu + \omega) \mathbf{1}]] - \frac{1}{2} \langle \Psi_0 | W | \Psi_0 \rangle \]

🌟 3N interaction: chiral N^2LO (400 MeV) SRG-evolved to 2.0 fm^{-1} [Navrátil 2007]

▶️ Fit to three- and four-body systems only

▶️ Modified cutoff to reduce induced 4N contributions [Roth et al. 2012]
Calcium isotopic chain

First \textit{ab initio} calculation of the whole Ca chain with NN + 3N forces

- 3NF bring energies close to experiment
- Induced 3NF and full 3NF investigated
Calcium isotopic chain

→ Original 3NF correct the energy curvature
→ Good agreement with IM-SRG (quantitative when 3\(^{rd}\) order included)

\[ E \, [\text{MeV}] \]

- exp.
- GGF Indc3NF
- GGF Full3NF
- IMSRG-Indc
- IMSRG-Full

[Hergert et al. 2013]
Exploit the odd-even formalism: application to K

- Trend and agreement similar to calcium

- Future: consistent description of medium-mass driplines
Two-neutron separation energies

🌟 Neutron-rich extremes of the nuclear chart

⇒ Good agreement with measured $S_{2n}$

⇒ Towards a quantitative \textit{ab initio} description of the medium-mass region
Pairing gaps

★ Three-point mass differences

\[
\Delta_n^{(3)}(A) = \frac{(-1)^A}{2} \left[ E_0^{A+1} - 2E_0^A + E_0^{A-1} \right]
\]
Pairing gaps

★ Inversion of odd-even staggering

- Second order and 3NF necessary to invert the staggering
**Pairing gaps**

*Comparison with other microscopic SM and EDFs*

![Graph](image1.png)

- **General agreement with other methods**
- **Initial 3NF increase the gaps with respect to NN + induced 3NF**

---

**Figure 2.** (Color online) Three-point mass differences $\Delta^{(3)}_n$ from $^{40}$Ca to $^{60}$Ca calculated to third-order ladders in MBPT with empirical SPEs, panel (a), compared with the EDF results of Ref. [15], panel (b). Results with and without the leading chiral 3N forces are shown following the legend of Fig. 1, and in comparison with experiment [24, 67].

**Figure 3.** (Color online) Three-point mass differences $\Delta^{(3)}_n$ in the calcium isotopes calculated to third order in MBPT with and without the leading chiral 3N forces, and in comparison with experiment [24, 67]. The legend is as in Fig. 1. Panel (a) shows the results of the third-order ladder contributions. Panel (b) and (c) include MBPT diagrams to third order in the pf-shell and the extended pfg$^{9/2}$ valence space, respectively. The results in the pf-shell are with empirical SPEs. For the pfg$^{9/2}$ space, we show pairing gaps for both the MBPT and empirical SPEs.

Pairing gaps calculated at this level are clearly deficient with respect to experiment. In addition to being below the experimental pairing strength, the odd-even staggering of $\Delta^{(3)}_n$ is inverted compared to experiment ($\Delta^{(3)}_n$ is stronger for odd masses than for even ones). This inverted staggering is a sign that the mean-field part at this level is too attractive, resulting in a lack of saturation and an incorrect symmetry energy, similar to the calculations discussed in Ref. [37]. The correct odd-even staggering of $\Delta^{(3)}_n$ seen in the EDF results of Ref. [15] (see the right panel of Fig. 2) is already built into the Skyrme functional used in Ref. [15].

Taking into account 3N force contributions at the ladders level, we find in Fig. 1 that the repulsive effect of chiral 3N forces leads to a systematic suppression of $\Delta^{(3)}_n$. Ranging from $0.2 - 0.5$ MeV, this is similar to the decrease in pairing strength observed in the EDF study of Ref. [15], as can be seen in Fig. 2. Note that the incorrect odd-even staggering of $\Delta^{(3)}_n$ persists in the NN+3N case, but the repulsive 3N forces make it less pronounced.

**Holt, Menéndez, Schwenk 2013**

**Lesinski, Hebeler, Duguet, Schwenk 2012**
**Benchmarks and chiral EFT interactions**

- *Ab initio* calculations as a test for chiral EFT interactions

- Different approaches agree in O and Ca chains

  - Current chiral NN+3N forces overbind medium/heavy-mass nuclei

---

![Graph](image)

- E\(_{\text{g.s.}}\) [MeV] vs. atomic mass number (A)

  - 2N+3N(full)
  - 2N+3N(ind)
  - Exp

---

[Note]: Cipollone, Barbieri, Navrátil, 2013

[Note]: Hergert et al., 2013
Spectral strength distribution

Dyson 1\textsuperscript{st} order (HF)

\begin{align*}
\text{Dyson 1\textsuperscript{st} order (HF)} & \quad \text{Gorkov 1\textsuperscript{st} order (HFB)} \\
& \quad \text{Dyson 2\textsuperscript{nd} order} \\
& \quad \text{Gorkov 2\textsuperscript{nd} order}
\end{align*}

Fragmentation

Static pairing

Dynamical fluctuations

\begin{align*}
\text{Dyson 1\textsuperscript{st} order (HF)} & \quad \text{Gorkov 1\textsuperscript{st} order (HFB)} \\
& \quad \text{Dyson 2\textsuperscript{nd} order} \\
& \quad \text{Gorkov 2\textsuperscript{nd} order}
\end{align*}
Shell structure evolution

One-neutron separation energies

\begin{align*}
\text{NN} & \\
\text{NN + 3NF} & \\
\end{align*}

\begin{align*}
E_k^\pm & [\text{MeV}] \\
40 & \quad 42 & \quad 44 & \quad 46 & \quad 48 & \quad 50 \\
5/2^- & \\
1/2^- & \\
3/2^- & \\
7/2^- & \\
3/2^+ & \\
\end{align*}
Shell structure evolution

ESPE collect fragmentation of “single-particle” strengths from both $N \pm 1$

$$\varepsilon_a^{cent} \equiv h_a^{cent} \delta_a = t_{aa} + \sum_{cd} \tilde{V}_{acad}^{NN} \rho_{dc}^{[1]} + \sum_{cde} \tilde{V}_{acdaef}^{NNN} \rho_{efcd}^{[2]} \equiv \sum_k S_{k}^{+a} E_{k}^{+} + \sum_k S_{k}^{-a} E_{k}^{-}$$

[Baranger 1970, Duguet and Hagen 2011]
Towards medium/heavy nuclei

- Static and dynamic pairing correlations
- Second order compresses spectrum
- Many-body correlations screened out from ESPEs

\[
E_{\pm}^k \quad SF_{k}^\pm
\]

\[
\epsilon_a \quad \text{cent}
\]

\[
\begin{align*}
7/2^+ & \quad 3/2^+ \\
1/2^+ & \quad 5/2^+ \\
9/2^+ &
\end{align*}
\]

\[
\begin{align*}
74^{Ni} & \\
73^{Ni} \quad 75^{Ni}
\end{align*}
\]
Conclusions and outlook

- **Gorkov-Green’s functions:**
  - Manageable route to (near) degenerate systems
  - *Ab initio* description of medium-mass chains
  - 2NF + 3NF: towards predictive calculations
  - Energies: quantitative agreement
  - Spectra: study of shell structure evolution

- **Improvement of the self-energy expansion**
- **Proper coupling to the continuum**
- **Formulation of particle-number restored Gorkov theory**
- **Towards consistent description of structure and reactions**
Acknowledgements

Collaborators:

Carlo Barbieri (University of Surrey, UK)
Andrea Cipollone (University of Surrey, UK)
Thomas Duguet (CEA Saclay, France)
Petr Navrátil (TRIUMF, Canada)

Funding:

German Research Foundation

Computing resources:

Centre de Calcul Recherche et Technologie