Superfluidity in nuclei from ab-initio many-body methods

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Outline

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Question of present interest

Fully microscopic description of pairing in nuclei

- Long term challenge
- Quantitative account rely on delicate interplay
- Relevant to structure and reaction properties of (exotic) nuclei

Non-perturbative many-body physics

- Necessary to account quantitatively for
  1. Particle motion ⇔ shell structure and fragmentation
  2. Pair attraction ⇔ direct and induced processes
- Ab-initio methods for mid-mass open-shell nuclei
  1. Self-consistent Gorkov Green's Function theory = in place [V. Somà, C. Barbieri, T. Duguet]
  2. Bogoliubov Coupled-Cluster theory = on the way [A. Signoracci, T. Duguet, G. Hagen]

Realistic Hamiltonian

- Nuclear NN and NNN (at least) as well as Coulomb interactions
  1. From Chiral Effective Field Theory (χ-EFT)
  2. Scaled down through, e.g., Similarity Renormalization Group (SRG) method

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1. Question of present interest
2. Self-consistent Gorkov Green's Function calculations
   - Elements of formalism
   - Inclusion of NNN forces
   - First results
3. Conclusions

Ab-initio theory for mid-mass open-shell nuclei

Gorkov self-consistent Green's function method

1. Extends Dyson SCGF to open-shell nuclei
2. Extends reach from $\sim 10^1$ to $\sim 10^2$ nuclei
3. Treatment of superfluidity built in

[V. Somà, T. Duguet, C. Barbieri, PRC 84 (2011) 064317]

Green's functions [L. P. Gorkov, JETP 7 (1958) 505]

$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle$$

$$i\,G^{12}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle$$

$$i\,G^{21}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle$$

$$i\,G^{22}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle$$

whose poles provide $\omega_k \equiv \Omega_k - \Omega_0$

Gorkov's equation of motion

$$G_{ab}(\omega) = G^{(0)}_{ab}(\omega) + \sum_{cd} G^{(0)}_{ac}(\omega)\Sigma_{cd}(\omega)G_{db}(\omega)$$

$T = 0$ grand potential

$$\Omega \equiv H_{\text{int}} - \mu A$$

Eigenstates

$$\Omega|\Psi_k\rangle = \Omega_k|\Psi_k\rangle$$

Irreducible self-energy

$$\Sigma_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & \Sigma^{22}_{ab}(\omega) \end{pmatrix}$$

Observables

$$E^A_0 = \sum_{ab}\int \frac{d\omega}{4\pi i} G^{11}_{ab}(\omega)[T_{ba} + \omega\delta_{ab}]$$

$$r^2 = \sum_{ab}\int \frac{d\omega}{2\pi i} G^{11}_{ab}(\omega)\, r^2_{ba}$$

$$E^\pm_k \equiv \pm[E^{A\pm1}_k - E^A_0] = \mu \pm \omega_k$$

$$\Delta^{(3)}(A) = (-1)^A[E^+_0 - E^-_0]/2$$

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Kadanoff-Baym Φ-derivable scheme

- ✔ Thermodynamically consistent
- ✔ Symmetry conserving
- ✘ Ward-Takahashi identities

Luttinger-Ward potential $\Omega_0[G] \equiv \langle \Psi_0 | \Omega | \Psi_0 \rangle$

$$\Omega_0[G] \equiv \mathrm{Tr}\left\{G^{(0)-1}\, G - 1\right\} - \mathrm{Tr}\left\{\ln G\right\} + \Phi[G]$$

Two-particle irreducible Φ-functional

$$\Phi[G] \equiv \sum_{n=1}^{\infty} \Phi^{(n)}[G]$$

Variational principle

$$\frac{\delta \Omega_0[G]}{\delta G(\omega)} = 0 \Longrightarrow \begin{cases} G(\omega) = G^{(0)}(\omega) + G^{(0)}(\omega)\,\Sigma(\omega)\,G(\omega) \\ \Sigma_{ab}^{gg'}(\omega) \equiv -\delta\Phi[G] / \delta G_{ba}^{g'g}(\omega) \end{cases}$$

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Kadanoff-Baym Φ-derivable scheme

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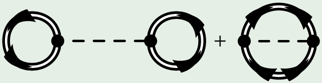
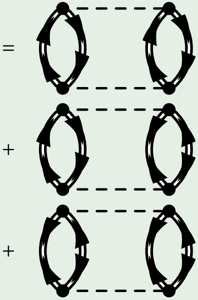
Self-consistent second-order

$\Phi^{(1)}[G] =$



$\Phi^{(2)}[G] =$



Eigenvalue problem

Lehmann representation

$$G^{11}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \mathcal{U}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \bar{\mathcal{V}}^k_b}{\omega + \omega_k - i\eta} \right\} \quad , \quad G^{12}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \mathcal{V}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \bar{\mathcal{U}}^k_b}{\omega + \omega_k - i\eta} \right\}$$

$$G^{21}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{V}^k_a \mathcal{U}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{U}}^{k*}_a \bar{\mathcal{V}}^k_b}{\omega + \omega_k - i\eta} \right\} \quad , \quad G^{22}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{V}^k_a \mathcal{V}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{U}}^{k*}_a \bar{\mathcal{U}}^k_b}{\omega + \omega_k - i\eta} \right\}$$

Gorkov's equation as an energy-dependent eigenvalue problem

$$\sum_b \left(\begin{array}{cc} T_{ab} - \mu\delta_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -T_{ab} + \mu\delta_{ab} + \Sigma^{22}_{ab}(\omega) \end{array} \right)\Bigg|_{+\omega_k} \left(\begin{array}{c} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{array} \right) = \omega_k \left(\begin{array}{c} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{array} \right)$$

Practical implementation [V. Somà, C. Barbieri, T. Duguet, in preparation]

1. Transform into energy-*independent* eigenvalue problem of large dimension
2. Tame dimension growth through iterations via Krylov projection technique
3. Check independence of results on number of Lanczos iterations

Outline

Effective two-body interaction (I)

Nuclear Hamiltonian with NN and NNN forces

$$H = \sum_{\alpha\beta} t_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{(2!)^2}\sum_{\alpha\beta\gamma\delta} v_{\alpha\gamma\beta\delta}\, a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta + \frac{1}{(3!)^2}\sum_{\alpha\beta\gamma\delta\epsilon\zeta} w_{\alpha\gamma\epsilon\beta\delta\zeta}\, a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\epsilon a_\zeta a_\delta a_\beta$$

Normal ordering with respect to, e.g., Hartree-Fock Slater determinant $|\Phi\rangle$

$$X = \tilde{x}^{0B} + \sum_{\alpha\beta} \tilde{x}^{1B}_{\alpha\beta} : a^\dagger_\alpha a_\beta : + \frac{1}{(2!)^2}\sum_{\alpha\beta\gamma\delta} \tilde{x}^{2B}_{\alpha\gamma\beta\delta} : a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta : + \frac{1}{(3!)^2}\sum_{\alpha\beta\gamma\delta\epsilon\zeta} \tilde{x}^{3B}_{\alpha\gamma\epsilon\beta\delta\zeta} : a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\epsilon a_\zeta a_\delta a_\beta :$$

$\tilde{t}^{0B} \equiv (1!)^{-1} \sum_{\alpha\beta} t_{\alpha\beta}$	$\tilde{v}^{0B} \equiv (2!)^{-1} \sum_{\alpha\beta\gamma\delta} v_{\alpha\gamma\beta\delta}\, \rho_{\beta\alpha}\, \rho_{\delta\gamma}$	$\tilde{w}^{0B} \equiv (3!)^{-1} \sum_{\alpha\beta\gamma\delta\epsilon\zeta} w_{\alpha\gamma\epsilon\beta\delta\zeta}\, \rho_{\beta\alpha}\, \rho_{\delta\gamma}\, \rho_{\zeta\epsilon}$
$\tilde{t}^{1B}_{\alpha\beta} \equiv (0!)^{-1} t_{\alpha\beta}$	$\tilde{v}^{1B}_{\alpha\beta} \equiv (1!)^{-1} \sum_{\gamma\delta} v_{\alpha\gamma\beta\delta}\, \rho_{\delta\gamma}$	$\tilde{w}^{1B}_{\alpha\beta} \equiv (2!)^{-1} \sum_{\gamma\delta\epsilon\zeta} w_{\alpha\gamma\epsilon\beta\delta\zeta}\, \rho_{\delta\gamma}\, \rho_{\zeta\epsilon}$
$\tilde{t}^{2B}_{\alpha\beta\gamma\delta} \equiv 0$	$\tilde{v}^{2B}_{\alpha\beta\gamma\delta} \equiv (0!)^{-1} v_{\alpha\beta\gamma\delta}$	$\tilde{w}^{2B}_{\alpha\beta\gamma\delta} \equiv (1!)^{-1} \sum_{\epsilon\zeta} w_{\alpha\gamma\epsilon\beta\delta\zeta}\, \rho_{\zeta\epsilon}$
$\tilde{t}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv 0$	$\tilde{v}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv 0$	$\tilde{w}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv (0!)^{-1} w_{\alpha\beta\gamma\delta\epsilon\zeta}$

Effective two-body interaction (I)

Nuclear Hamiltonian with NN and NNN forces

$$H \;=\; \ldots\, a^\dagger_\epsilon a_\zeta a_\delta a_\beta$$

Normal ordering ...

$$X \;=\; \tilde{x}^{0B} + \sum_{\alpha\ldots} \ldots\, a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\epsilon a_\zeta a_\delta a_\beta :$$

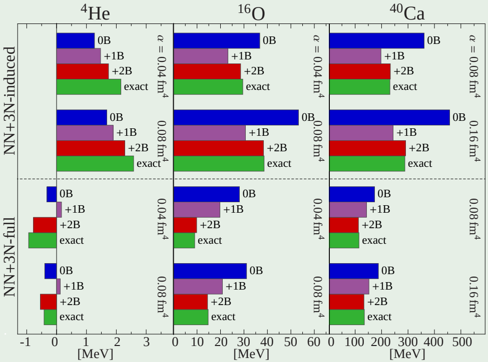
$$\tilde{t}^{0B} \equiv (1!)^{-1} \sum_{\alpha\beta} \ldots\, {}_{\epsilon\beta\delta\zeta}\, \rho_{\beta\alpha}\, \rho_{\delta\gamma}\, \rho_{\zeta\epsilon}$$

$$\tilde{t}^{1B}_{\alpha\beta} \equiv (0!)^{-1} t_{\alpha\beta} \ldots\, {}_{\delta\zeta}\, \rho_{\delta\gamma}\, \rho_{\zeta\epsilon}$$

$$\tilde{t}^{2B}_{\alpha\beta\gamma\delta} \equiv 0 \ldots\, {}_{\delta\zeta}\, \rho_{\zeta\epsilon}$$

$\tilde{t}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv 0$	$\tilde{v}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv 0$	$\tilde{w}^{3B}_{\alpha\beta\gamma\delta\epsilon\zeta} \equiv (0!)^{-1} w_{\alpha\beta\gamma\delta\epsilon\zeta}$

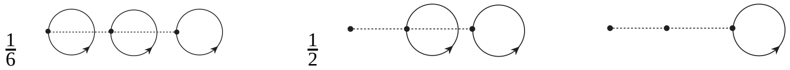
Accuracy of "2B" approx in IT-NCSM calculations



[R. Roth *et al.*, PRL 109 (2012) 052501]

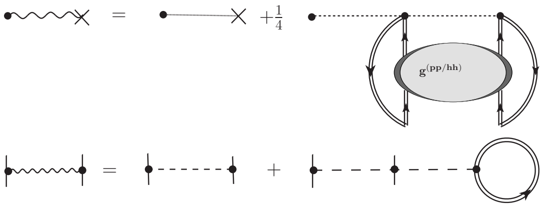
Effective two-body interaction (II)

2B approx based on normal ordering



2B approx beyond normal ordering [A.Carbone, A. Cipollone, C. Barbieri, A. Rios, A. Polls, unpublished]

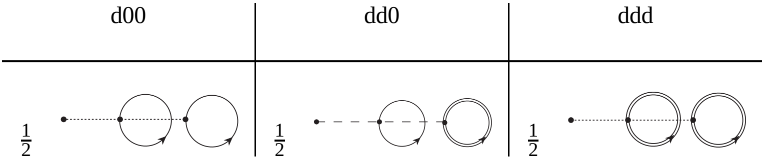
Define effective one- and two-body vertices



Retain one-fermion-line AND *one-interaction-line* irreducible diagrams

Effective two-body interaction (III)

Current implementation of 2B approx beyond normal ordering

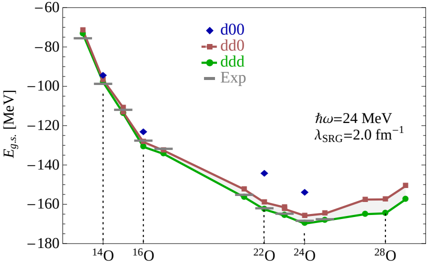


Results

- Beyond normal ordering matters
- Further corrections to be investigated

Open shell - present status

- dd0 in normal state with filling approx
- Procedure withing superfluid state soon

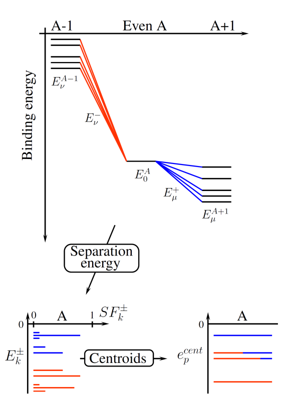


[A. Cipollone, C. Barbieri, P. Navrátil, unpublished]

Outline

Quantities of interest

Separation energies and shell structure



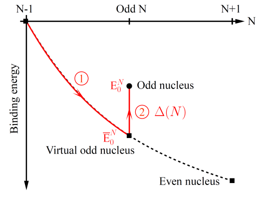
Baranger single-particle energies

$$e_p^{\text{cent}} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_\mu^{+pp} E_\mu^+ + \sum_{\nu \in \mathcal{H}_{A-1}} S_\nu^{-pp} E_\nu^-$$

[M. Baranger, NPA 149 (1970) 225]

Odd-even mass staggering

$$E_0^N \equiv \underbrace{\overline{E}_0^N}_{\text{smooth}} + \underbrace{\Delta(N)}_{\text{odd N only}}$$



Three point mass difference

$$\Delta_n^{(3)}(N) \equiv \frac{(-1)^N}{2}\left[E_0^{N+1} - 2E_0^N + E_0^{N-1}\right]$$
$$= (-1)^N [E_0^+ - E_0^-]/2$$
$$= \underbrace{\frac{(-1)^N}{2}\frac{\partial^2 \overline{E}_0^N}{\partial^2 N}}_{\text{oscillates around 0}} + \underbrace{\Delta(N)}_{\text{dominates}}$$

[T. Duguet *et al.*, PRC 65 (2002) 014311]

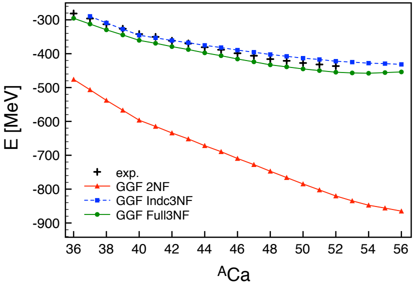
Ground-state energies

Interactions

- NN = χ-N^{3}LO (500 MeV) SRG-evolved to 2.0 fm^{-1} [D. R. Entem, R. Machleidt, PRC 68 (2003) 041001]
- NNN = χ-N^{2}LO (400 MeV) SRG-evolved to 2.0 fm^{-1} [P. Navràtil, FBS 41 (2007) 117]
  1. Fit to three- and four-body systems only
  2. Lowered cutoff to reduce induced 4N contributions [R. Roth *et al.*, PRL 109 (2012) 052501]

Absolute energies

- First such ab initio calculations of Ca
- NN+NN brings energy in the ballpark
- Trend improved by initial NNN
- NNN runs out of steam for $N \gtrsim 34$
- Anticipated agreement with IM-SRG
- Large uncertainty on the interaction side



[V. Somà, A. Cipollone, C. Barbieri, T. Duguet, P. Navrátil, unpublished]

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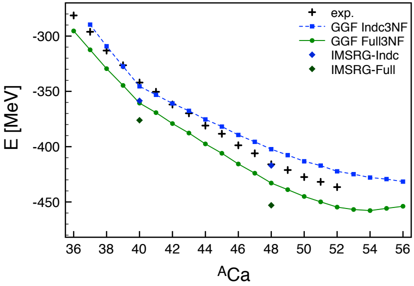

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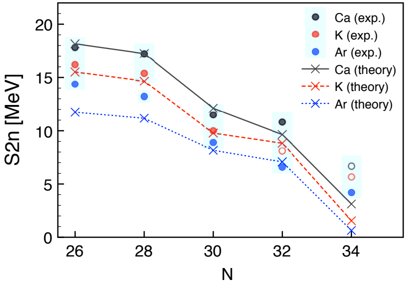
Two-neutron separation energies

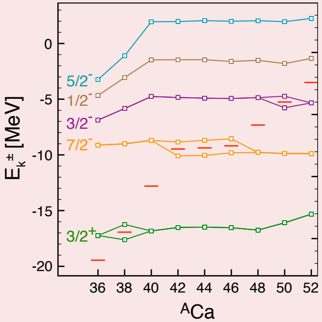
- Very fair reproduction in Ca and K
- Doubly-open shell Ar challenging
- NNN runs out of steam for $N \gtrsim 34$



[V. Somà *et al.*, unpublished]

Spectroscopy of odd-even isotopes and shell structure

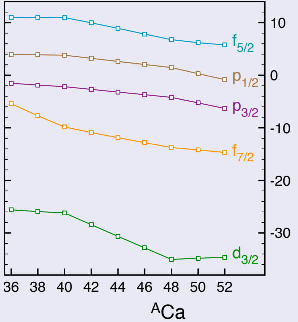
One-neutron separation energies



[V. Somà *et al.*, unpublished]

- Main fragments of given J^Π
- Fragmentation due to pairing visible
- Strongly differ from ESPE
- NNN strongly increase density of states
- Still too spread out

Centroids



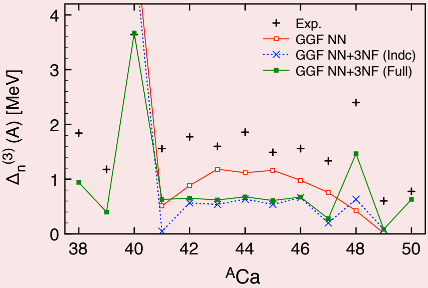
[V. Somà *et al.*, unpublished]

- Recollect fragmented strength
- Defines the shell structure
- Extracted along isotopic/isotonic chains
- Non-observable quantity

T. Duguet, G. Hagen, PRC 85 (2012) 034330]

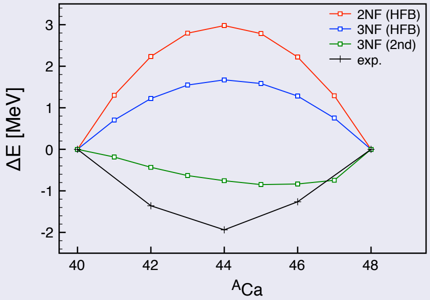
Pairing gaps (I)

Overall scale of $\Delta_n^{(3)}(N)$



- Significantly reduced by induced NNN
- Original NNN
  1. Essential for *magic* gaps
  2. No impact on *pairing* gaps
- Too low pairing gaps
  1. Too low density of states
  2. Too weak pairing vertex

Oscillation of $\Delta_n^{(3)}(N)$



[V. Somà *et al.*, unpublished]

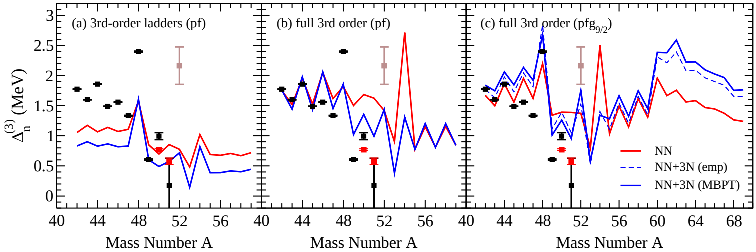
- From curvature of $\bar{E}_0^N$ (symmetry energy)
- NNN improves over NN only
- 2nd-order mandatory for correct sign
- Not quantitatively sufficient

T. Duguet, *50 years of nuclear BCS theory*, p. 229, WS, 2013]

Pairing gaps (II)

Microscopic shell model

- 3^{rd}-order *ladders* qualitatively consistent with our HFB results
  1. Reduction from NNN ($\sim 300 - 500$ keV)
  2. Inverted oscillation compared to experiment
- Remaining 3^{rd}-order contribution provides significant increase of $\Delta_n^{(3)}(N)$
- Need to incorporate (at least) coupling to 3^{rd}-order particle-hole fluctuations



[J. D. Holt, J. Menendez, A. Schwenk, arXiv:1304.0434]

Outline

Summary and perspectives

Ab initio calculation of superfluid properties of nuclei

- Self-consistent Gorkov Green's function (SCGGF) theory
  1. First ab-initio access to pairing gaps in mid-mass nuclei
  2. Contribution of (induced) NNN interaction essential
  3. Soon go to ADC(3) self-energy expansion to reach quantitative description
- Bogoliubov Coupled-Cluster (BCC) theory [A. Signoracci, T. Duguet, G. Hagen, unpublished]
  1. Powerful alternative to Self-consistent Gorkov Green's function theory
  2. Formalism fully developed
  3. Implementation in m-scheme to singles and doubles close to completion
- Symmetry-restored SCGGF and BCC theories [T. Duguet, G. Ripka, unpublished]