Polynomial Similarity Transformation Theory:

From coupled cluster doubles to number projected BCS

Jorge Dukelsky

CONSEJO SUPERIOR
DE INVESTIGACIONES
CIENTÍFICAS

CSIC

INSTITUTO DE ESTRUCTURA
DE LA MATERIA

Future directions for nuclear structure and reaction theories: Ab initio approaches for 2020, March 14-18, 2016,GANIL, Caen, France

Based on:

- **Structure of the number projected BCS wave function.**
  Jorge Dukelsky, Stuart Pittel, Carlos Esebbag.
  Phys. Rev. C **93**, 03413 (2016).

- **Polynomial Similarity Transformation Theory: A smooth interpolation between coupled cluster doubles and projected BCS applied to the reduced BCS Hamiltonian.**
  Matthias Degroote, Thomas M. Henderson, Jinmo Zhao, Jorge Dukelsky, Gustavo E. Scuseria. arXiv:1512.0611.
  Phys. Rev. B (in press).

Ab initio methods for light to medium-mass nuclei

Based on realistic two and three body interactions.

- Green’s function Monte Carlo
- Self-consistent Green’s function
- No-core shell model
- Coupled Cluster
- In-medium similarity renormalization group

Nuclear density functional theory for heavy nuclei

Phenomenological density dependent interactions.

HFB approximations and extensions:

Symmetry restoration (Number, angular momentum, ….)

QRPA, Time-dependent DFT, …..

PoST: an initial attempt to bridge the gap between CCD and NPHFB

The reduced BCS Hamiltonian or the constant pairing model

$$H = \sum_i \varepsilon_i N_i - G \sum_{i,j} P_i^+ P_j, \quad N_i = c_i^+ c_i + c_{\bar{i}}^+ c_{\bar{i}}, \quad P_i^+ = c_i^+ c_{\bar{i}}^+$$

$$\left[N_i, P_j^+ \right] = 2\delta_{i,j} P_j^+, \left[P_i, P_j^+ \right] = \delta_{i,j} \left(1 - N_i \right)$$

The 3 generators close the SU(2) algebra

Richardson solved exactly this Hamiltonian. Phys. Lett. 3 (1963) 277.

The complete set of eigenvectors have the form:

$$\left| \Psi \right\rangle = \prod_{\alpha=1}^{M} \left(\sum_{i=1}^{L} \frac{1}{2\varepsilon_i - E_\alpha} P_i^+ \right) \left| 0 \right\rangle$$

For simplicity we will consider equidistant levels $\boldsymbol{\varepsilon_i = i}$ and systems at half filling $M=L/2$.

Pair Coupled Cluster Doubles (pCCD)

CC theory is based on p-h excitations, singles, doubles, triples, etc. out of a reference |HF>, $T=T_1+T_2+T_3+\dots$ The pairing Hamiltonian conserves seniority. Within the each seniority subspace only even p-h excitations are permitted. Moreover, we will stop at doubles which means that the excitation operator is

$$T=\sum_{p,h} t_{ph} P_p^+ P_h$$

The pCCD wave function and eigenvalue equations are

$$\left|\Psi\right\rangle = e^T \left|HF\right\rangle, \quad H\left|\Psi\right\rangle = Ee^T\left|HF\right\rangle$$

Multiplying by the inverse transformation from the left

$$\overline{H} = e^{-T} H e^T, \quad \overline{H}\left|HF\right\rangle = E\left|HF\right\rangle$$

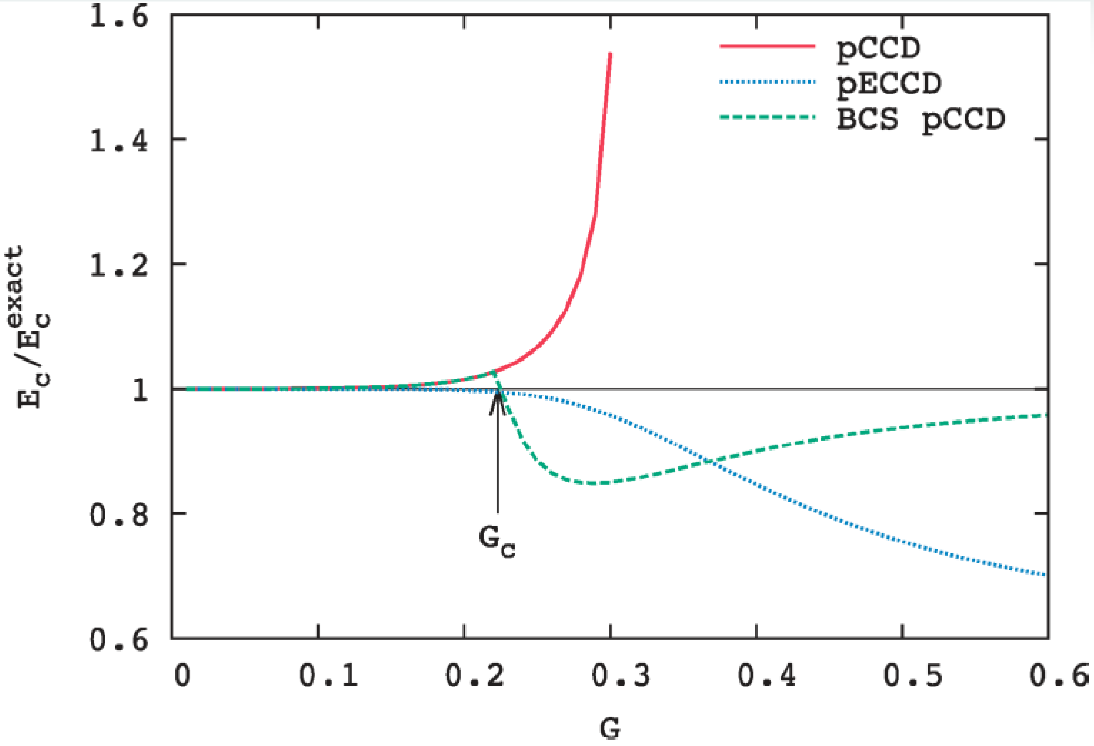
Projecting over the reference state and over 2p-2h states from the left

$$E = \left\langle HF\right|\overline{H}\left|HF\right\rangle, \quad 0 = \left\langle HF\right|P_h^+ P_p \overline{H}\left|HF\right\rangle$$

Energy

Amplitude equations

Similarity transformed Hamiltonian (non-hermitian)



J. Dukelsky, G. G. Dussel, J. G. Hirsch and P. Schuck. Nucl. Phys. A 714 (2003) 63.

T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, and T. Duguet, Phys. Rev. C **89**, 054305 (2014).

T. M. Henderson, I. W. Bulik, and G. Scuseria, J. Chem. Phys. **142**, 214116 (2015).

pCCD fails dramatically around the phase transition. pECCD and BCS oe Bogoliubov pCCD improve but not yet satisfactory.

Number projected BCS pCCD could be an alternative. T. Duguet, A. Signoracci, arXiv:1512.02878

Number Projected BCS (PBCS) Wavefunction

The number projected BCS wavefunction is a pair condensate:

$$\left|PBCS\right\rangle = \left(\Gamma^{+}\right)^{M}\left|0\right\rangle, \quad \Gamma^{+}\left(x\right) = \sum_{i=1}^{L} x_i P_i^{+}$$

We want express PBCS as a correlation operator acting on a HF reference state.

First we separate the correlated pair operator in *p* and *h* parts:

$$\Gamma^{+} = \sum_{p=M+1}^{L} x_p P_p^{+} + \sum_{h=1}^{M} x_h P_h^{+} = \Gamma_p^{+}\left(x\right) + \Gamma_h^{+}\left(x\right)$$

Next we expand the condensate

$$\left|PBCS\right\rangle = \left(\Gamma_p^{+} + \Gamma_h^{+}\right)^{M}\left|0\right\rangle = \sum_{n=0}^{M} \binom{M}{n} \Gamma_p^{+n} \Gamma_h^{+(M-n)}\left|0\right\rangle$$

We now use a trick to replace the vacuum by the HF state

$$\left|HF\right\rangle = \left[\Gamma_h^{+}\left(x\right)\right]^{M}\left|0\right\rangle$$

Acting with the a pair destruction

$$\Gamma_h^n(1/x)\left|HF\right\rangle = \Gamma_h^n(1/x)\,\Gamma_h^{+M}(x)\left|0\right\rangle = \frac{M!\,n!}{(M-n)!}\Gamma_h^{+(M-n)}(x)\left|0\right\rangle$$

The r.h.s is precisely the term appearing the binomial expansion.

Modified Bessel function of the first kind

$$\left|PBCS\right\rangle = \sum_{n=0}^{L}\frac{1}{(n!)^2}\left[\Gamma_p^+(x)\Gamma_h(1/x)\right]^n\left|HF\right\rangle = I_0\left[2\sqrt{\Gamma_p^+(x)\Gamma_h(1/x)}\right]\left|HF\right\rangle$$

Or

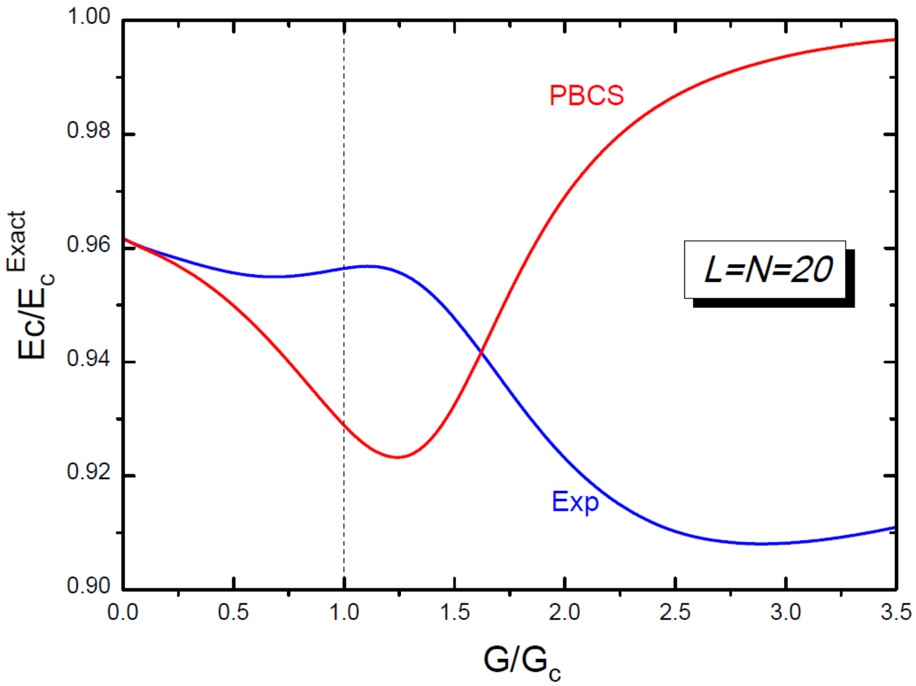
Separable amplitude matrix

$$\left|PBCS\right\rangle = \sum_n \frac{1}{(n!)^2}\left(\sum_{p,h}\frac{x_p}{x_h}P_p^+P_h\right)^n\left|HF\right\rangle$$

Alternatively we will explore the exponential form

$$\left|Exp\right\rangle = \sum_n \frac{1}{(n!)}\left(\sum_{p,h}\frac{x_p}{x_h}P_p^+P_h\right)^n\left|HF\right\rangle$$

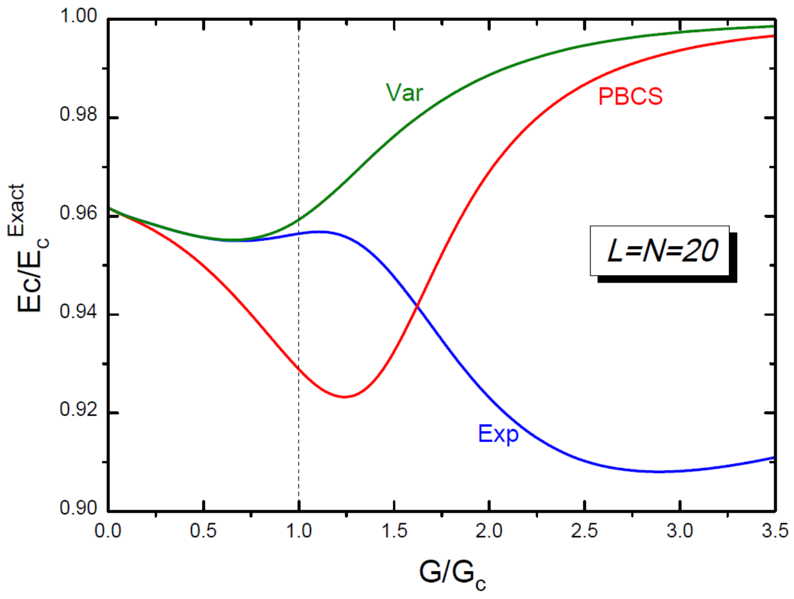
Correlation energies referred to the exact correlations energy for PBCS and Exponential wave function

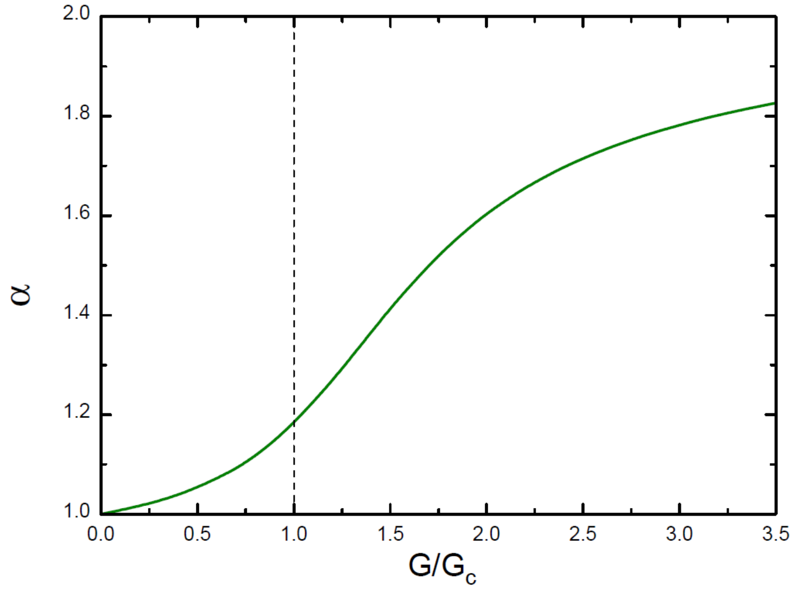


Variational approach (upper bound). Factorized cluster matrix. Factorial exponent $\alpha = 2$ (1) for PBCS (Exponential).

We can still improve using the exponent α as a variational parameter.

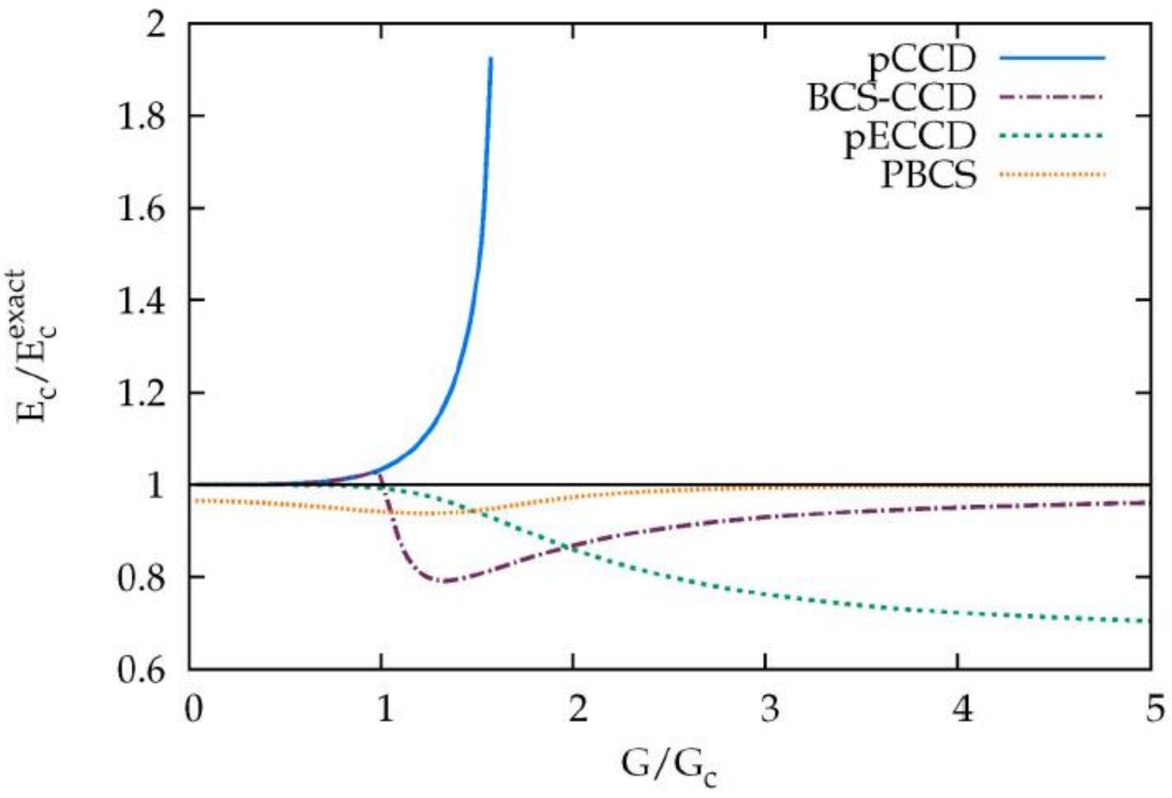
$$\left|Var\right\rangle = N\sum_{l}\frac{1}{(l!)^{\alpha}}\left(\sum_{p,h}\frac{x_p}{x_h}P_p^{+}P_h\right)^{l}\left|HF\right\rangle$$





The bad convergence to g->0 is not related to the coefficients in the expansion.

Comparison between pCCD and PBCS



Would be nice to include results from:

Symmetry broken and restored coupled-cluster theory. II. Global gauge symmetry and particle number. T. Duguet, A. Signoracci. arXiv:1512.02878.

pCCD

- Non-hermitian similarity transformed Hamiltonian. Non-variational theory.
- Complete freedom in cluster amplitudes t_{ph}. Implies correlations between 2p-2h. Quartet correlations.
- Due to the exponential it has nice properties: size consistent, size extensive.
- Accurate for weak pairing correlations.

$$|pCCD\rangle = \sum_i \frac{1}{l!}\left(\sum_{ph} t_{ph} P_p^+ P_h\right)|HF\rangle$$

PBCS

- Variational theory.
- Factorized cluster amplitudes. Implies pair correlations.
- Not size consistent. Includes intensive terms.
- Accurate for superconducting systems

$$|PBCS\rangle = \sum_l \frac{1}{(l!)^2}\left(\sum_{ph} \frac{x_p}{x_h} P_p^+ P_h\right)^l |HF\rangle$$

Polynomial Similarity Transformation Theory (PoST)

- Keep full freedom in the cluster amplitudes t_{ph} (beyond pair correlations)
- Abandoned exponential form and the properties of consistency and extensivity.
- Abandoned Ritz variational property.

Instead of exponential or Bessel, assume a general polynomial of an excitation operator *T,* and the corresponding inverse:

$$F(T) = 1 + T + a_2 T^2 + a_3 T^3 + \cdots, \quad F^{-1}(T) = 1 - T + (1 - a_2) T^2 - (1 - 2a_2 + a_3) T^3 + \cdots$$

The PoST ansatz for the wave function and the similarity transformed Hamiltonian are

$$|\Psi\rangle = F(T)|HF\rangle, \quad \overline{H} = F^{-1}(T) HF(T)$$

Expanding the similarity transformation

Disconnected

$$\overline{H} = H + [H,T] + a_2\left[[H,T],T\right] + (2a_2 - 1)T[H,T] + \mathrm{O}\left(HT^3\right)$$

Whose eigenvalues are the same as the eigenvalues of *H*.

We note that if $a_n = 1/n!$ the term $(2a_2 - 1)$ cancels out and $\overline{H}$ is purely connected (express in terms of nested commutators of *H* and *T*).

In what follow we will restrict PoST to only doubles T_2

Similarly to pCCD the PoST equations are

$$E = \langle HF | \overline{H} | HF \rangle, \quad 0 = \langle HF | P_h^+ P_p \overline{H} | HF \rangle$$

And we can disregard terms of order HT^3.

Moreover, we will parametrized the polynomial coefficients as $a_n = 1/(n!)^\alpha$

Question: How can we determine α ?

No Ritz variational theory. We cannot minimize E with respect to α.

CCD and PoST doubles cancels R_2

$$R_2 = \langle HF | P_h^+ P_p \overline{H} | HF \rangle = 0$$

CCD

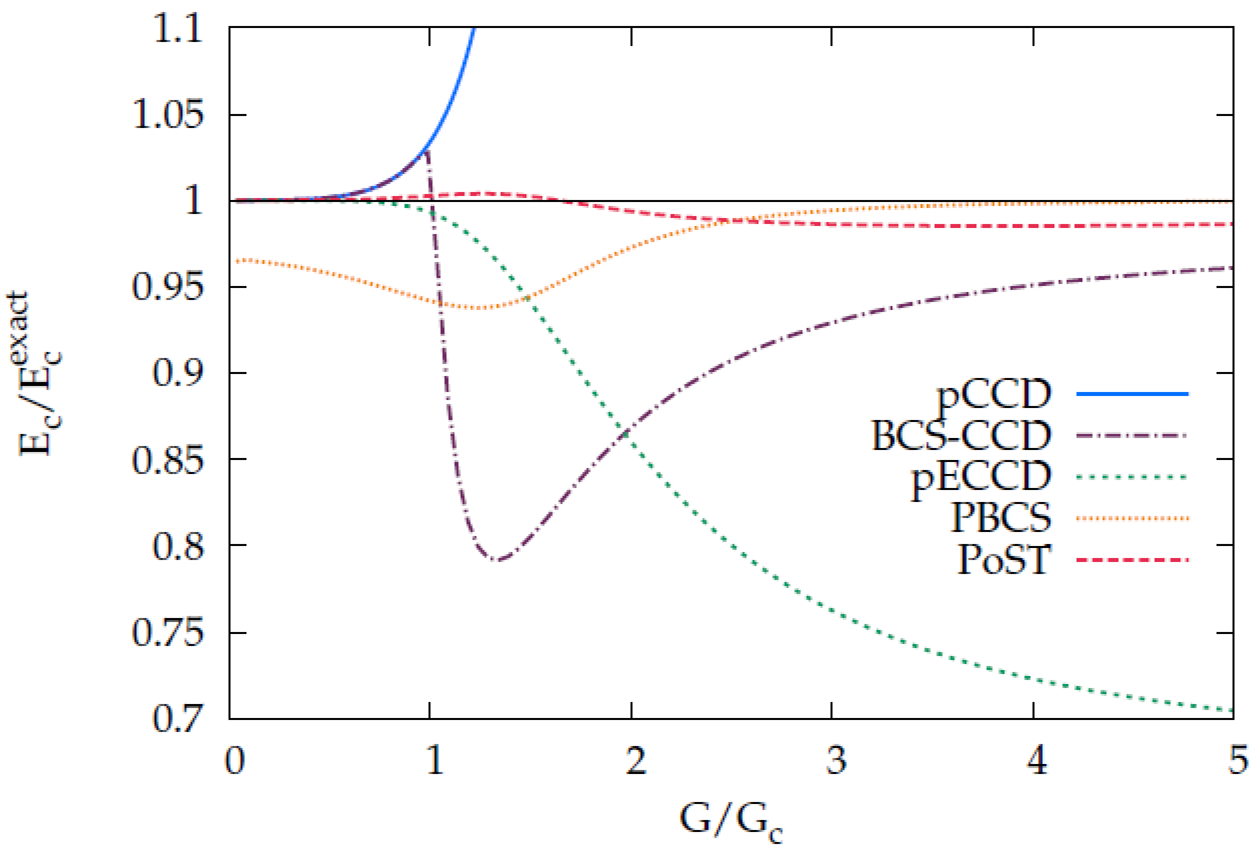
$\overline{H}$	0p-0h	2p-2h	4p-4h
0p-0h	E	■	■
2p-2h	R_2	■	■
4p4h	■	■	■

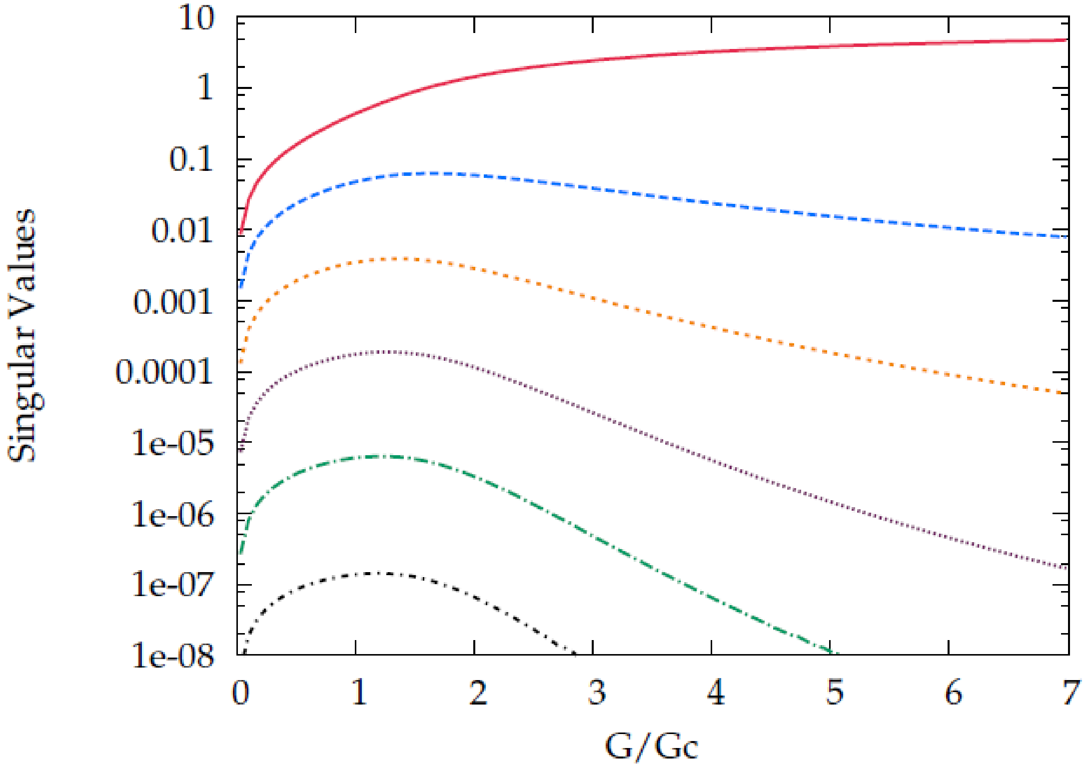
PoST

$\overline{H}$	0p-0h	2p-2h	4p-4h
0p-0h	E	■	■
2p-2h	R_2	■	■
4p4h	R_4	■	■

α Is determine from the minimization of R_4^2

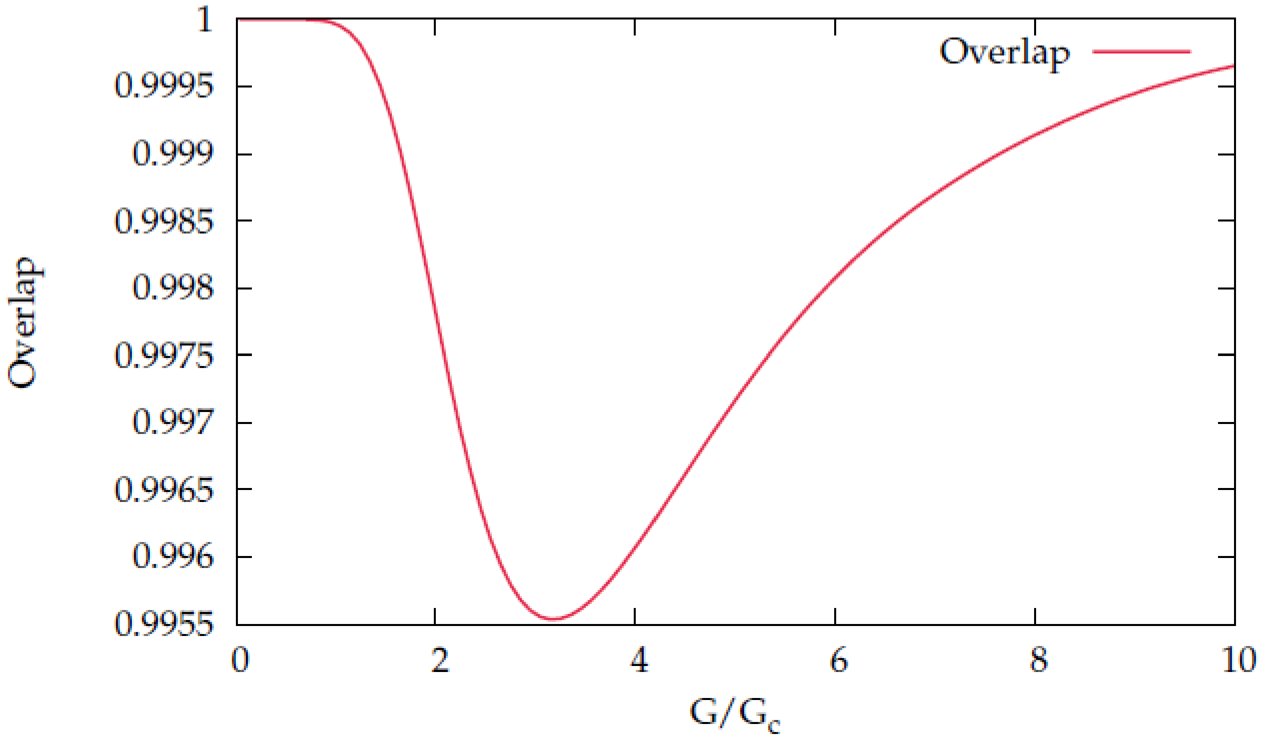
Computational cost N^6, comparable with CCD ($N_h^2\ N_p^4$)


1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
E_c/E_c^{exact}
0
1
2
3
4
5
G/G_c
pCCD
BCS-CCD
pECCD
PBCS
PoST



Singular values of PoST.

For G → ∝ all minus one singular values tend to 0.



Overlap of the PoST wavefunction $|\Psi\rangle = F_\alpha(T)|HF\rangle$ with the exact wavefunction.

PoST with α=2 is exact if PBCS is an exact eigenstate of H

$$|\Psi\rangle = \sum_n \frac{1}{(n!)^\alpha}\left(\sum_{ph} t_{ph} P_p^+ P_h\right)^n |HF\rangle, \quad H|\Psi\rangle = E|\Psi\rangle$$

PBCS is an exact eigenstate in extreme superconducting limit G →∝

The hyperbolic Richardson-Gaudin model has particular point (Moore-Read) at which PBCS is an exact eigenstate.

$$H_{hyp} = \sum_i \varepsilon_i n_i - G\sum_{i,j}\sqrt{\varepsilon_i \varepsilon_j}\, P_i^+ P_j$$

A variant of this Hamiltonian has been proposed in J. D,. S. Lerma H., L. M. Robledo, R. Rodriguez-Guzman, and S. M. A. Rombouts Phys. Rev. C 84, 061301(R) (2011) as an exactly solvable pairing Hamiltonian for heavy nuclei.

The eigenstates are:

$$E = \sum_{\beta=1}^{M} E_\beta, \quad |\Psi\rangle = \prod_{\beta=1}^{M}\left[\sum_{i=1}^{L} \frac{\sqrt{\varepsilon_i}}{\varepsilon_i - E_\beta} P_i^+\right]|0\rangle$$

At the Moore-Read point

$$G_{MR} = \frac{2}{L-M+1}, \quad E_\beta = 0 \quad \forall \beta \Rightarrow E = 0$$

The exact ground state

$$|\Psi_{MR}\rangle = \left[\sum_i \frac{1}{\sqrt{\varepsilon_i}} P_i^+\right]^M |0\rangle$$

From PoST equations we have

$$E = E_{HF} - G\sum_{p,h}\sqrt{\varepsilon_p \varepsilon_h}\, t_{ph}$$

$$R_2 = \left\langle HF \middle| P_h^{+} P_p \left(1-T\right) H \left(1+T+a_2 T^2\right) \middle| HF \right\rangle = 0$$

$$Min\left\{R_4^2\right\}$$

It turns out that we insert the cluster amplitude $t_{ph} = \dfrac{\sqrt{\varepsilon_h}}{\sqrt{\varepsilon_p}}$ as dictated by the exact solution, the three equations are satisfied for

$$G = \frac{2}{L-M+1}, \quad E = 0, \quad R_{2n} = 0 \;\forall n$$

PoST is exact when PBCS is exact

Summary

- PoST seems to interpolate nicely between CCD and PBCS paving the way for using CC type of algorithms for medium to heavy-mass superfluid nuclei.
- The pairing Hamiltonian can be solved exactly for any pairing strength. However, PoSt can deal with non-integrable pairing Hamiltonians, and with more general interactions without seniority conservation.
- Important point to elaborate in the future is the lack of extensivity. A good approximate many-body theory might not fulfil all the constraints but it is required to be as accurate as possible.
- PoST is an approach close CCT. Therefore, many of the tools developed in CCT can be extended to PoST: 1) Incorporate response theory to evaluate observables. 2) Incorporate equation of motion for the description of excited states.
- We are carrying out studies in condensed matter (Hubbard models) and quantum chemistry (molecular structure) where strong correlations are not of the superfluid type. Even so, PoST is improving the results of CCSD.