pphh-TDA (AND BEYOND) FOR PAIRING

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THE PAIRING HAMILTONIAN

⋆ The nuclear many-body pairing hamiltonian reads :

$$H = \sum_{\alpha=1}^{\Omega} (\varepsilon_\alpha - \lambda) N_\alpha - \sum_{\alpha,\beta=1}^{\Omega} G_{\alpha\beta} P_\alpha^\dagger P_\beta$$

where

$$N_\alpha = a_\alpha^\dagger a_\alpha + a_{\bar{\alpha}}^\dagger a_{\bar{\alpha}} \qquad \text{and} \qquad P_\alpha^\dagger = a_\alpha^\dagger a_{\bar{\alpha}}^\dagger$$

⋆ The symmetric (half-filled; $N = \Omega$) picket-fence model ($\varepsilon_\alpha = \alpha\varepsilon$; ε = 1 MeV) with constant pairing G is studied.

⋆ To ensure particle-hole symmetry, one choses the chemical potential λ to be equal to

$$\lambda = \varepsilon(N + \frac{1}{2}) - \frac{G}{2}$$

THE PAIRING HAMILTONIAN

⋆ Refs: J. Hirsch, A. Mariano, J. Dukelski and P. Schuck, Ann. Phys. 296 (2002) 187; N. Dinh Dang, Phys. Rev. C71, 024302 (2005).

$$M_p = N_p, \qquad M_h = 2 - N_h, \qquad Q_p^\dagger = P_p^\dagger, \qquad Q_h = -P_h^\dagger$$

$$D_p = 1 - M_p = 1 - N_p, \qquad D_h = 1 - M_h = -(1 - N_h)$$

⋆ Single-particle energies:

$$\varepsilon_p = \varepsilon(N + p), \qquad \varepsilon_h = \varepsilon(N - h + 1), \qquad p, h = 1, ..., N.$$

⋆ The hamiltonian can be written in the form:

$$\begin{aligned} H &= -\varepsilon N^2 + \sum_{p=h=1}^{N} \left[\varepsilon(p - \frac{1}{2}) + \frac{G}{2}\right](M_p + M_h) \\ &- G\sum_{pp'} Q_p^\dagger Q_{p'} - G\sum_{hh'} Q_h^\dagger Q_{h'} + G\sum_{ph}(Q_p^\dagger Q_h^\dagger + Q_p Q_h) \end{aligned}$$

SCRPA CALCULATIONS

⋆ Ref.: J. Hirsch, A. Mariano, J. Dukelski and P. Schuck, Ann. Phys. 296 (2002) 187.

⋆ The two-particle addition operator is defined as:

$$A^{\dagger}_{\tau} = \sum_{p} X^{\tau}_{p} \bar{Q}^{\dagger}_{p} - \sum_{h} Y^{\tau}_{h} \bar{Q}_{h}$$

where

$$\bar{Q}^{\dagger}_{p} = \frac{Q^{\dagger}_{p}}{\sqrt{\langle D_p \rangle}}, \qquad \bar{Q}^{\dagger}_{h} = \frac{Q^{\dagger}_{h}}{\sqrt{\langle D_h \rangle}}$$

⋆ This leads to the SCRPA equations in matrix form:

$$\begin{pmatrix} A & B \\ -B & C \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar \Omega_{\tau} \begin{pmatrix} X \\ Y \end{pmatrix}$$

EXPLICIT FORM FOR SCRPA

⋆ Ref.: J. Hirsch, A. Mariano, J. Dukelski and P. Schuck, Ann. Phys. 296 (2002) 187.

$$
\begin{aligned}
A_{pp'}^{SCRPA} &= 2\Big\{\Big[\varepsilon\Big(p-\tfrac{1}{2}\Big)+\tfrac{G}{2}\Big] \\
&+ \tfrac{G}{\langle D_p\rangle}\Big[\textstyle\sum_{p''}\langle Q^\dagger_{p''}Q_p\rangle-\sum_{h''}\langle Q_pQ_{h''}\rangle\Big]\Big\}\delta_{pp'} \\
&- G\frac{\langle D_pD_{p'}\rangle}{\sqrt{\langle D_p\rangle\langle D_{p'}\rangle}} \\
B_{ph}^{SCRPA} &= G\frac{\langle D_pD_h\rangle}{\sqrt{\langle D_p\rangle\langle D_h\rangle}} \\
C_{hh'}^{SCRPA} &= -2\Big\{\Big[\varepsilon\Big(h-\tfrac{1}{2}\Big)+\tfrac{G}{2}\Big] \\
&+ \tfrac{G}{\langle D_h\rangle}\Big[\textstyle\sum_{h''}\langle Q^\dagger_hQ_{h''}\rangle-\sum_{p''}\langle Q^\dagger_{p''}Q^\dagger_h\rangle\Big]\Big\}\delta_{hh'} \\
&+ G\frac{\langle D_hD_{h'}\rangle}{\sqrt{\langle D_h\rangle\langle D_{h'}\rangle}}
\end{aligned}
$$

r-RPA AND (pp)-RPA SIMPLIFICATIONS

⋆ The r-RPA equations are obtained if one neglects all the expectation values $\langle Q^\dagger_{p'} Q_p \rangle$, $\langle Q_p Q_h \rangle$ and $\langle Q^\dagger_h Q_{h'} \rangle$, and by the simplification

$$\langle D_i D_j \rangle \simeq \langle D_i \rangle \langle D_j \rangle$$

⋆ The (pp)-RPA equations are obtained if one sets

$$D_p = D_h = 1$$

EXPLICIT FORMS FOR r-RPA AND (pp)-RPA

$$
\begin{aligned}
A_{pp'}^{r-RPA} &= 2\left[\varepsilon\left(p - \tfrac{1}{2}\right) + \tfrac{G}{2}\right]\delta_{pp'} - G\sqrt{\langle D_p\rangle\langle D_{p'}\rangle} \\
B_{ph}^{r-RPA} &= G\sqrt{\langle D_p\rangle\langle D_h\rangle} \\
C_{hh'}^{r-RPA} &= -2\left[\varepsilon\left(h - \tfrac{1}{2}\right) + \tfrac{G}{2}\right]\delta_{hh'} + G\sqrt{\langle D_h\rangle\langle D_{h'}\rangle}
\end{aligned}
$$

$$
\begin{aligned}
A_{pp'}^{(pp)-RPA} &= 2\left[\varepsilon\left(p - \tfrac{1}{2}\right) + \tfrac{G}{2}\right]\delta_{pp'} - G \\
B_{ph}^{(pp)-RPA} &= G \\
C_{hh'}^{(pp)-RPA} &= -2\left[\varepsilon\left(h - \tfrac{1}{2}\right) + \tfrac{G}{2}\right]\delta_{hh'} + G
\end{aligned}
$$

pp-TDA CALCULATIONS

⋆ If in the pp-RPA matrix one sets the off-diagonal blocs to zero (B=0), one obtains the pp-TDA equations.

⋆ The pp-TDA equations can be alternatively derived by postulating

$$|pp - TDA, \tau\rangle = \sum_{m>0} C^{\tau}_{m} a^{\dagger}_{m} a^{\dagger}_{\bar{m}} |HF\rangle$$

and by solving the secular equation

$$\hat{H}|pp - TDA, \tau\rangle = E_{\tau}|pp - TDA, \tau\rangle$$

leading to the matrix form

$$\sum_{m'>0} H_{mm'} C^{\tau}_{m'} = E_{\tau} C^{\tau}_{m}$$

pp-TDA CALCULATIONS

⋆ We notice that the matrix element

$$H_{mm'} = \{ \sum_{i;occ.} [2(\varepsilon_{i;occ.} - \lambda) - G_{ii}] + 2(\varepsilon_m - \lambda) \} \delta_{mm'} - G_{mm'}$$

is equal to $A_{mm'}$ in the pp-RPA equations, up to the constant term

$$\sum_{i;occ.} [2(\varepsilon_{i;occ.} - \lambda) - G_{ii}] = \langle HF | \hat{H} | HF \rangle$$

pphh-TDA CALCULATIONS

⋆ We now postulate

$$|pphh - TDA, \tau\rangle = \mathcal{C}^{\tau}_{00}|HF\rangle + \sum_{mi(>0)} \mathcal{C}^{\tau}_{mi} a^{\dagger}_{m} a^{\dagger}_{\bar{m}} a_{\bar{i}} a_{i} |HF\rangle$$

⋆ This leads to the secular equation

$$\sum_{nj} H_{mi;nj}\, \mathcal{C}^{\tau}_{nj} = E_{\tau}\, \mathcal{C}^{\tau}_{mi}$$

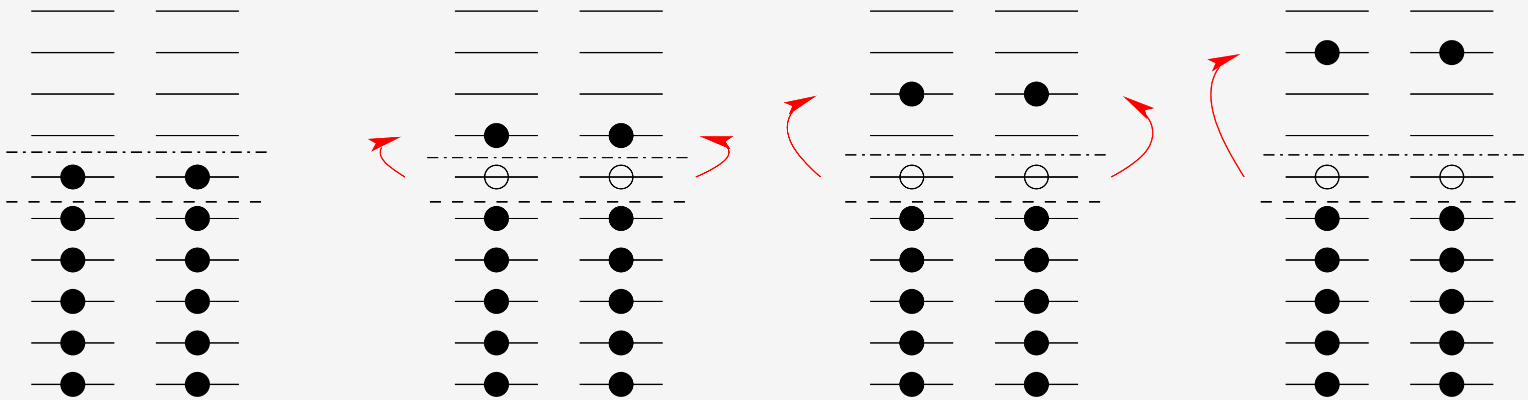
⋆ Where the matrix elements are given by

$$\begin{aligned} H_{mi;nj} &= \{\textstyle\sum_{i'}[2(\varepsilon_{i'} - \lambda) - G_{i'i'}] + 2(\varepsilon_m - \varepsilon_i) + 2G_{ii}\}\delta_{ij}\delta_{mn} \\ &- \delta_{ij} G_{mn} - \delta_{mn} G_{ij} \end{aligned}$$

QUALITATIVE COMPARISON

⋆ In the pphh-TDA formalism, the properties of the (A)-nucleons system are directly described without distinguishing between addition and removal operators.

⋆ For the addition modes, the pp-TDA represent a first approximation to the pphh-TDA calculations, in which one would restrict oneselves to the subclass of 1-pair states originating from the level located immediately below the no-interaction Fermi surface for the (A+2)-nucleons system.



BEYOND pphh-TDA: THE PSY-MB METHOD

⋆ The idea is to enlarge the many-body basis with 2-pairs, 3-pairs etc. configurations, where a certain energy cut-off is used.

⋆ The pphh-TDA is then equivalent to the PSY-MB procedure in which only the ground-state and the 1-pair configurations are taken into account.

⋆ Direct diagonalization of max. 100 000 configurations is performed with the Lanczos procedure.

⋆ Ref.: H.M. and J. Dudek, Phys. Rev. C 56 (1997) 1795

FORMAL MATRIX STRUCTURE

	GS	1-pair	2-pairs	3-pairs	4-pairs	...
GS	X	X	0	0	0	...
1-pair	X	X	X	0	0	...
2-pairs	0	X	X	X	0	...
3-pairs	0	0	X	X	X	...
4-pairs	0	0	0	X	X	...
...	...	...	...	...	...	...

SPACES AND REGIMES STUDIED

⋆ Small space: 24 particles on 48 levels (2 704 156 s=0 states):

⟶ GS

⟶ 144 1-pair states

⟶ 4 356 2-pairs states

⟶ 48 400 3-pairs states

⋆ Large space: 32 particles on 64 levels (601 080 390 s=0 states):

⟶ GS

⟶ 256 1-pair states

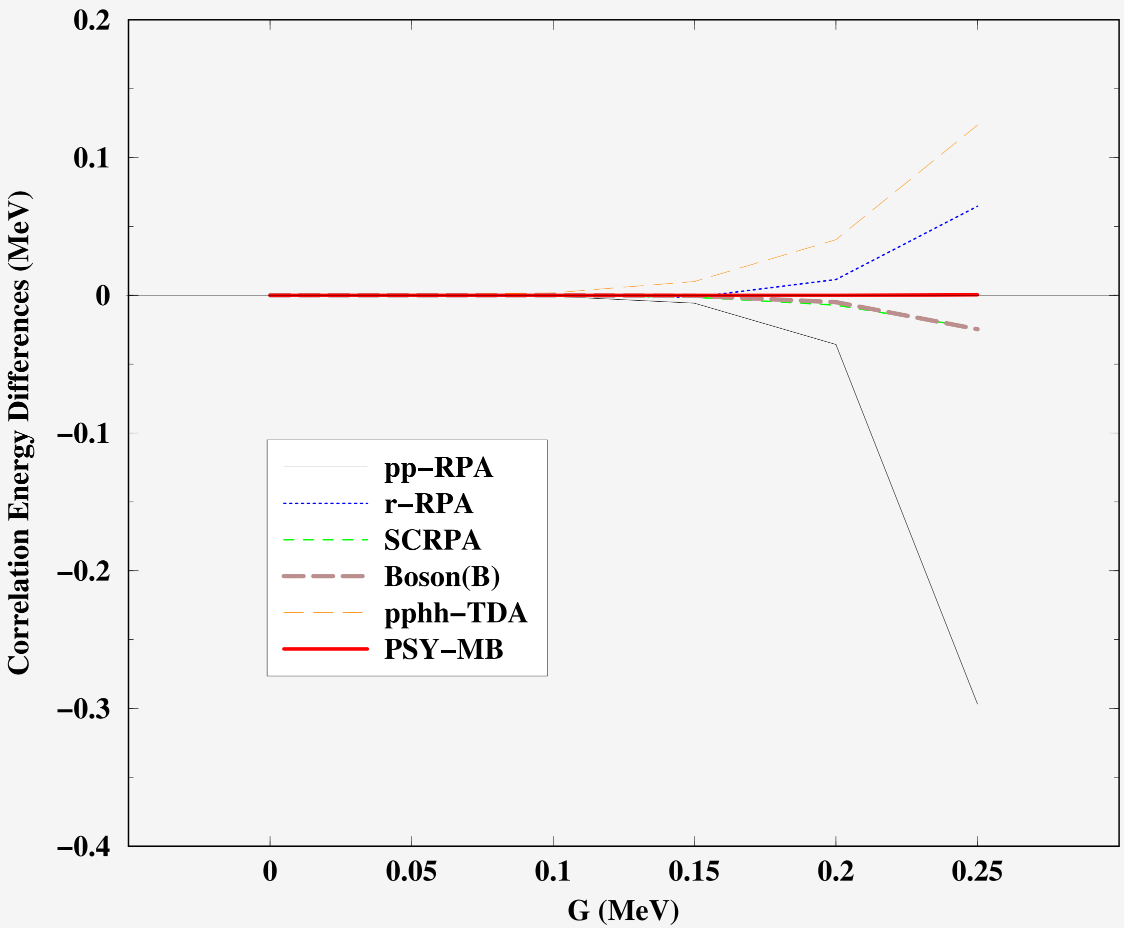
⟶ 14 400 2-pairs states

⟶ 313 600 3-pairs states

⋆ The normal and the superfluid regime is studied.

24/48 - CORR. ENERGY OF THE G.S.

- ⋆ Only small values of the pairing interation strength are considered.
- ⋆ Refs.: J. Hirsch et al., Ann. Phys. 296 (2002) 187, D. Gambacurta et al., Phys. Rev. C73, 014310 (2006).



⟶ Too strong correlations in the RPA ground-state and existence of RPA collapse.

⟶ Too less correlations in the pphh-TDA and r-RPA ground-states.

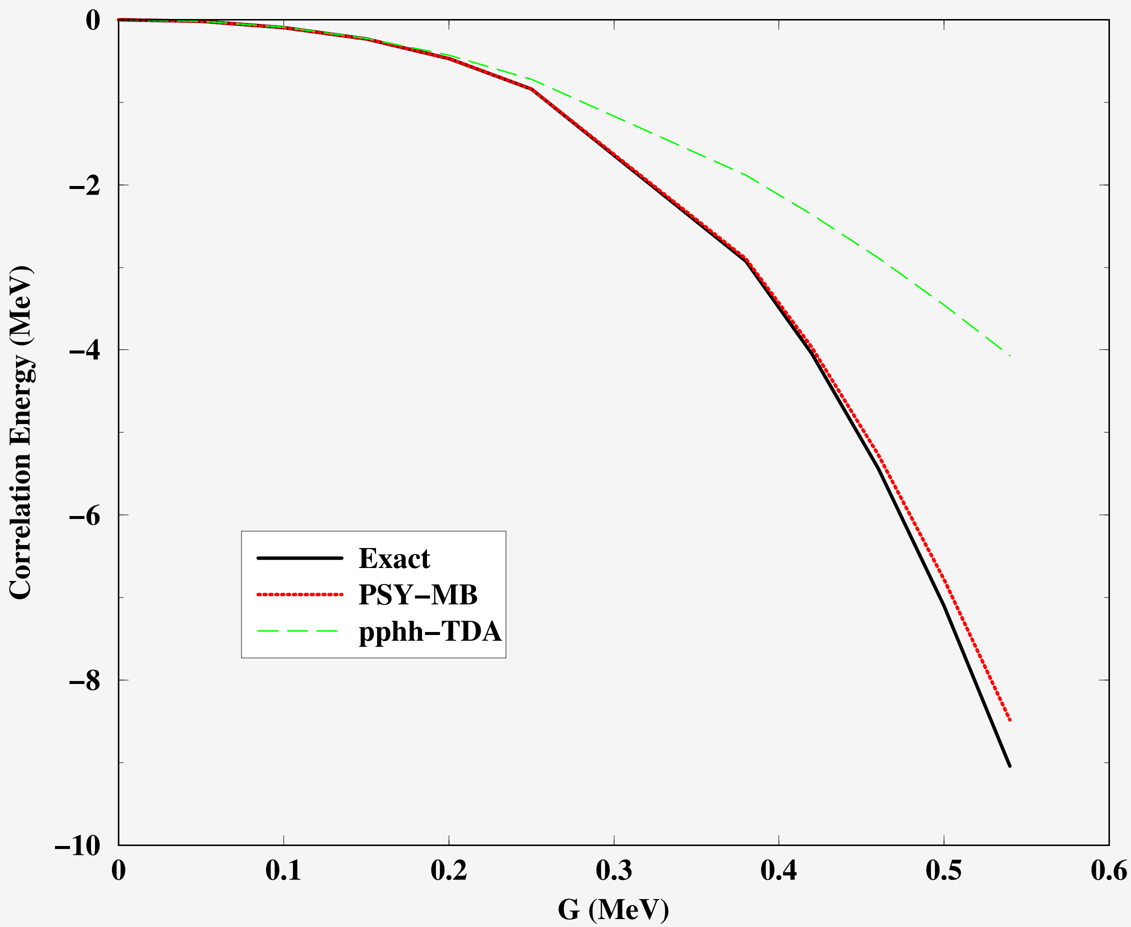
⟶ SCRPA and Boson(B) formalisms give almost identical results.

⟶ PSY-MB gives almost exact results while only 2 % of the s=0 basis states are used.

24/48 - CORR. ENERGY OF THE G.S.

⋆ Correlation energies are plotted.

⋆ Large values of the pairing interation strength are considered.

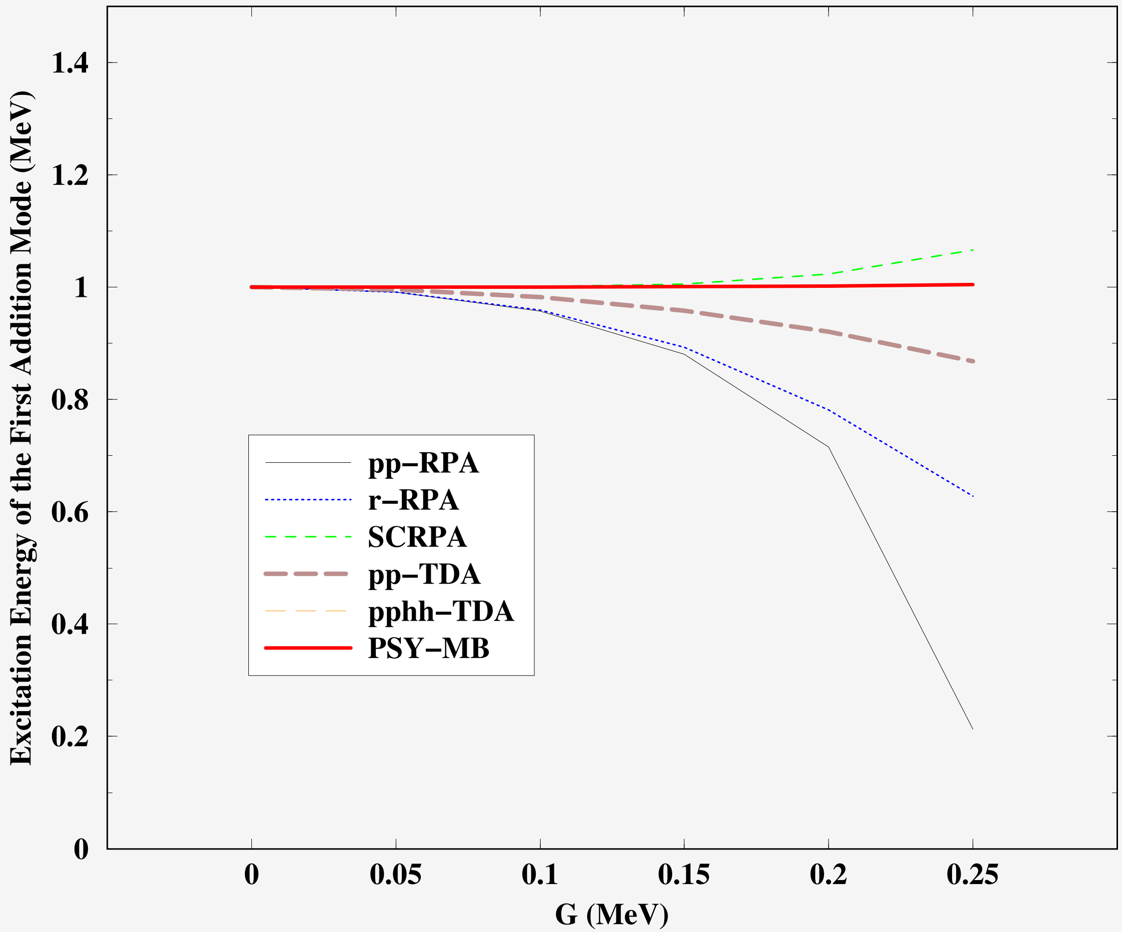


⟶ PSY-MB gives good results also for large values of the pairing strength, where the RPA solution has collapsed. There exists no abrupt phase transition.

⟶ The pphh-TDA method is not powerfull enough in the regime of very strong interactions.

24(26)/48 - EN. OF FIRST ADD. MODE

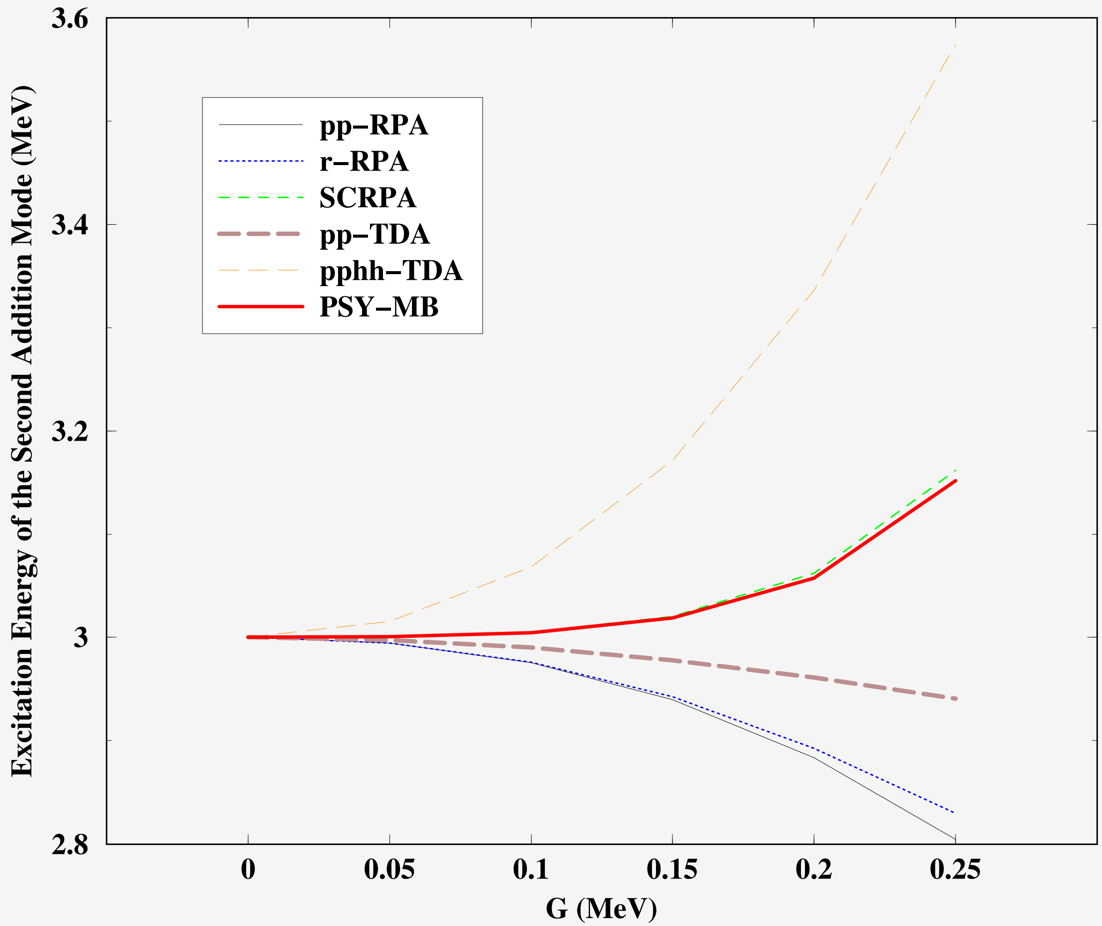
⋆ Excitation energies are given with respect to the ground-state of the 24 particles system.
⋆ Only small values if the pairing interation strength are considered.



⟶ The RPA and r-RPA results show the wrong tendency to <u>decrease</u>, as well as the pp-TDA.
⟶ The correct trend (<u>increase</u>) is given by the SCRPA, pphh-TDA and the PSY-MB methods.
⟶ The results of the pphh-TDA and PSY-MB calculations are almost undistinguishable.
⟶ The simpler pp-TDA calculations are doing better here than the pp-RPA or r-RPA versions.

24(26)/48 - EN. OF SECOND ADD. MODE

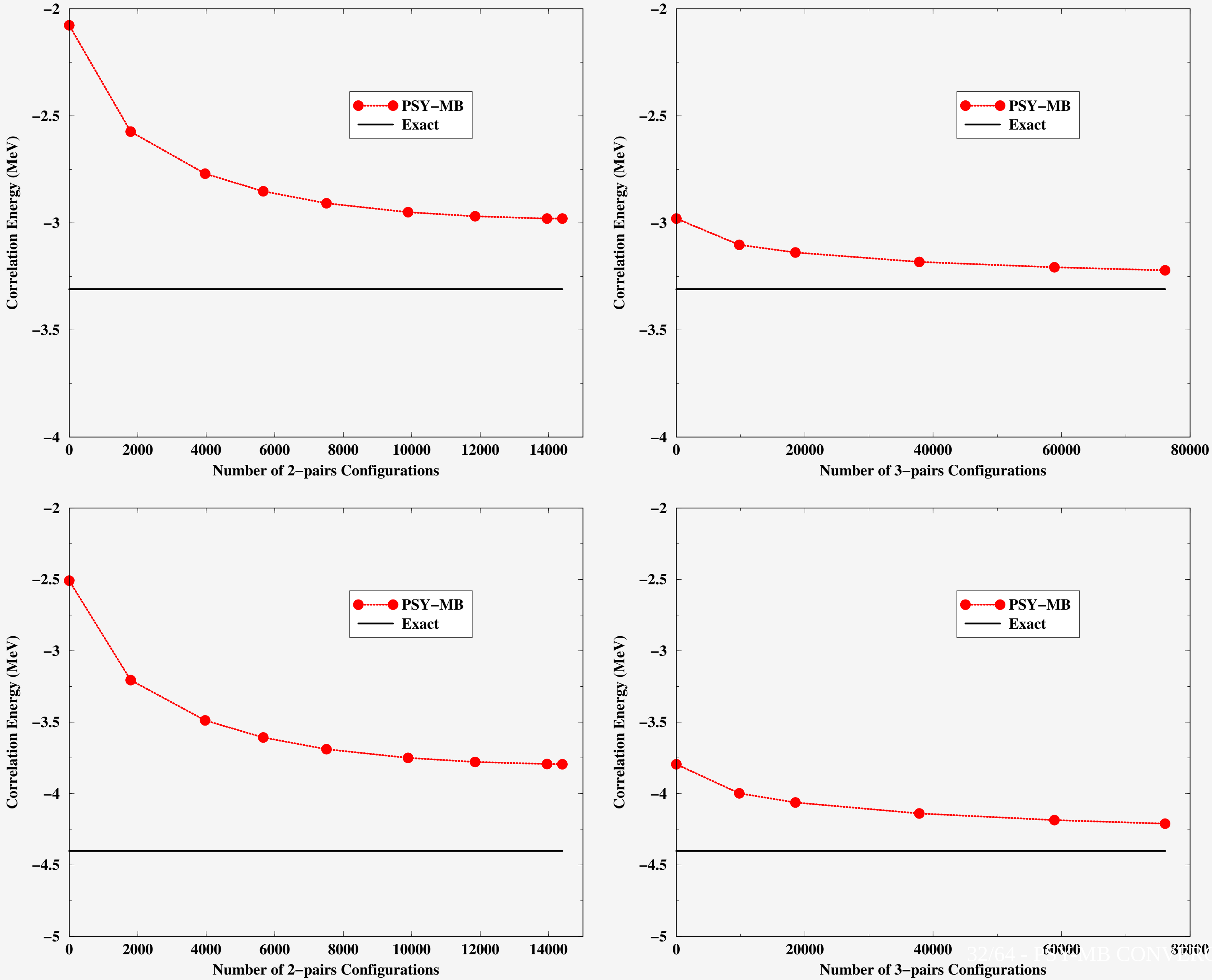
⋆ Excitation energies are given with respect to the ground-state of the 24 particles system..
⋆ Only small values of the pairing interation strength are considered.



⟶ Very similar behaviour of the pp-RPA, the r-RPA and the pp-TDA than for the first addition mode.
⟶ Results no longer good for the pphh-TDA case.
⟶ SCRPA and PSY-MB results are extremely close.

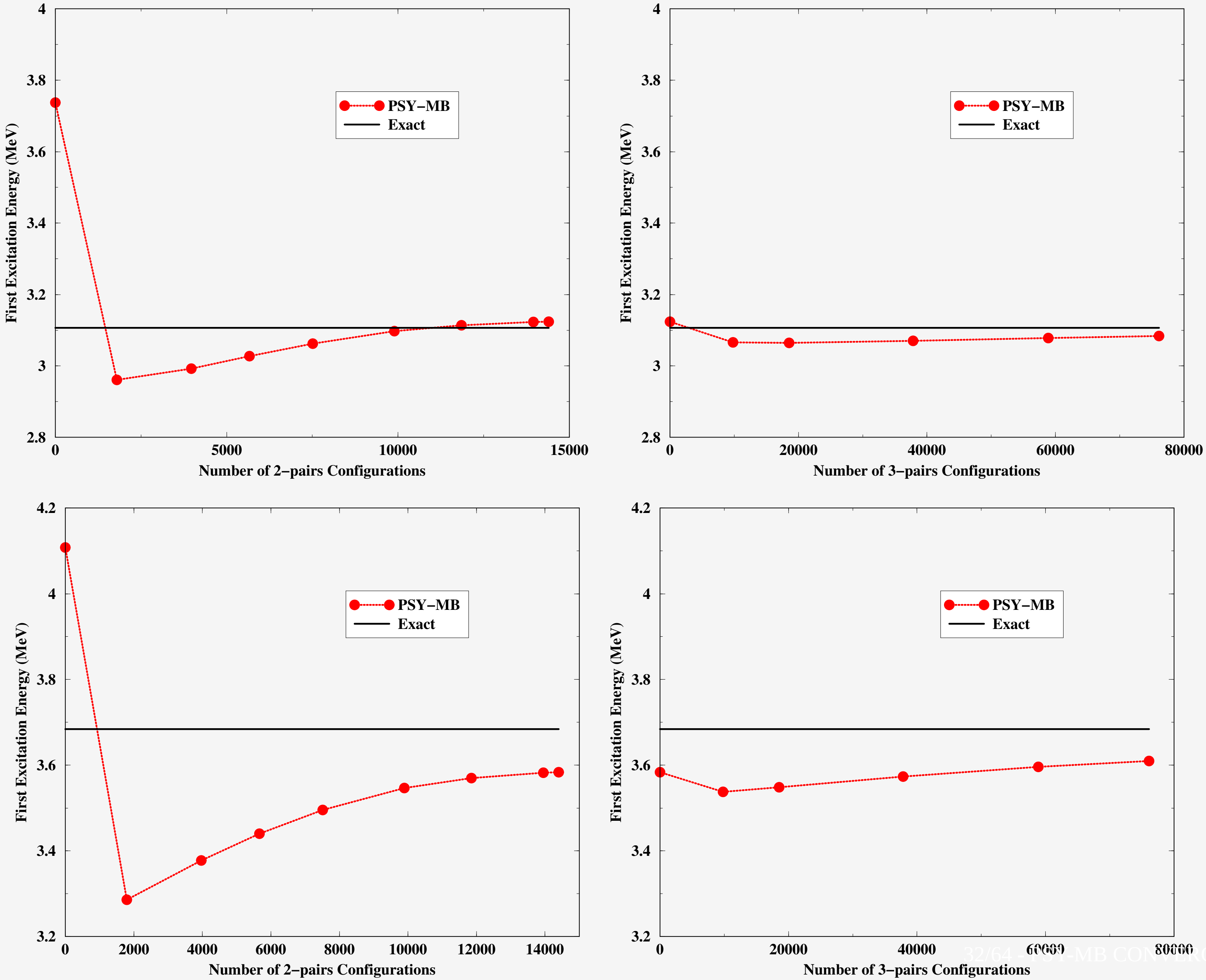
32/64 - PSY-MB CONVERGENCE

★ Top row: G=0.345 MeV. Bottom row: G=0.375 MeV.



32/64 - PSY-MB CONVERGENCE

⋆ Top row: G=0.345 MeV. Bottom row: G=0.375 MeV.



32/64 - RECALLING BCS EQUATIONS

⋆ We briefly recall the BCS equations (attention: here N counts the number of single-particle doublet-orbitals):

$$\begin{aligned} 1 &= \frac{G}{2} \sum_i \frac{1}{\tilde{e}_i} \\ N &= \sum_i v_i^2 \end{aligned}$$

where the quasi-particle energies are given by:

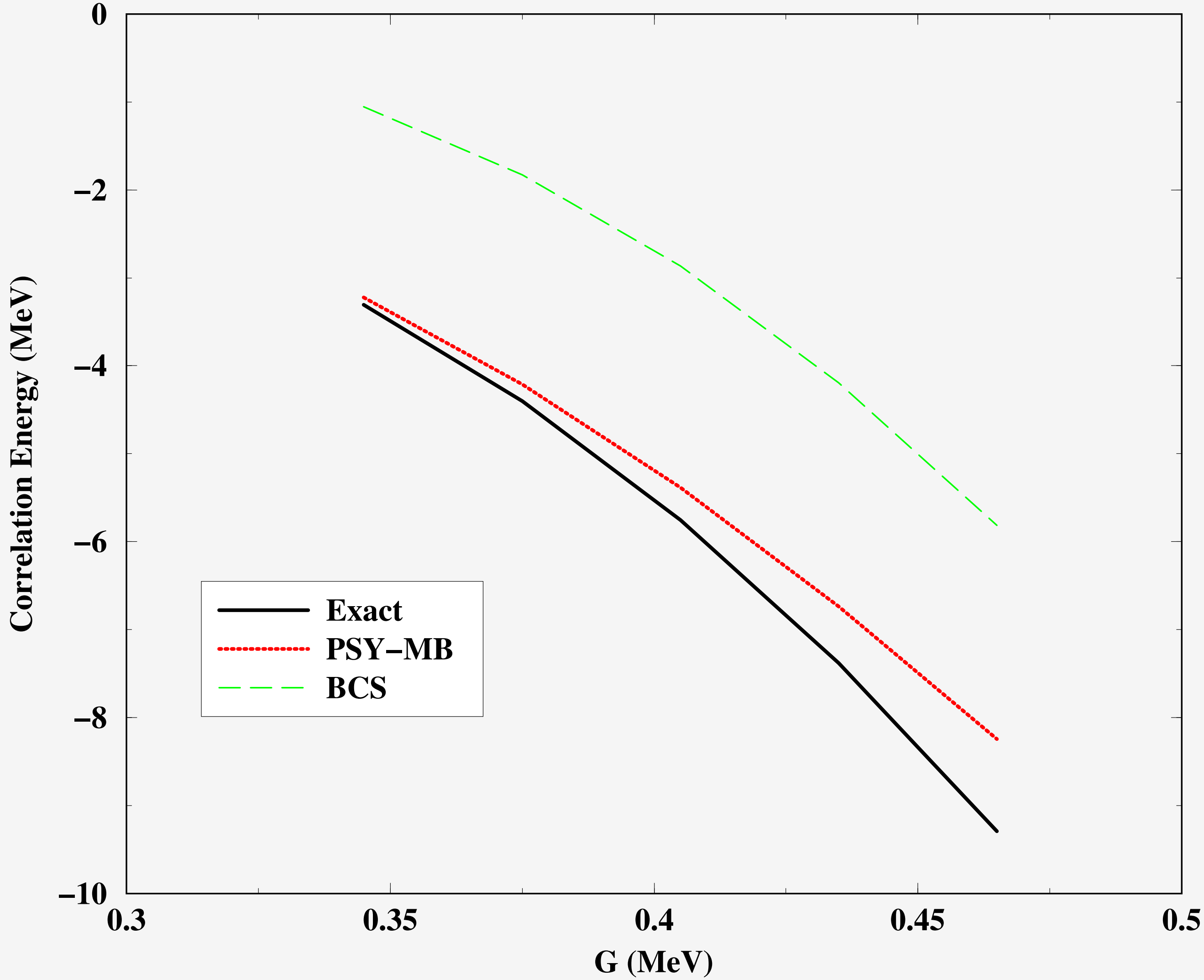
$$\tilde{e}_i = \sqrt{(\varepsilon_i - \lambda - G v_i^2)^2 + \Delta^2}$$

⋆ The BCS ground-state energy is given by:

$$E_{BCS} = \sum_i \left(2\varepsilon_i - G v_n^2\right) v_n^2 - \Delta^2 / G$$

32/64 - SUPERFLUID REGIME

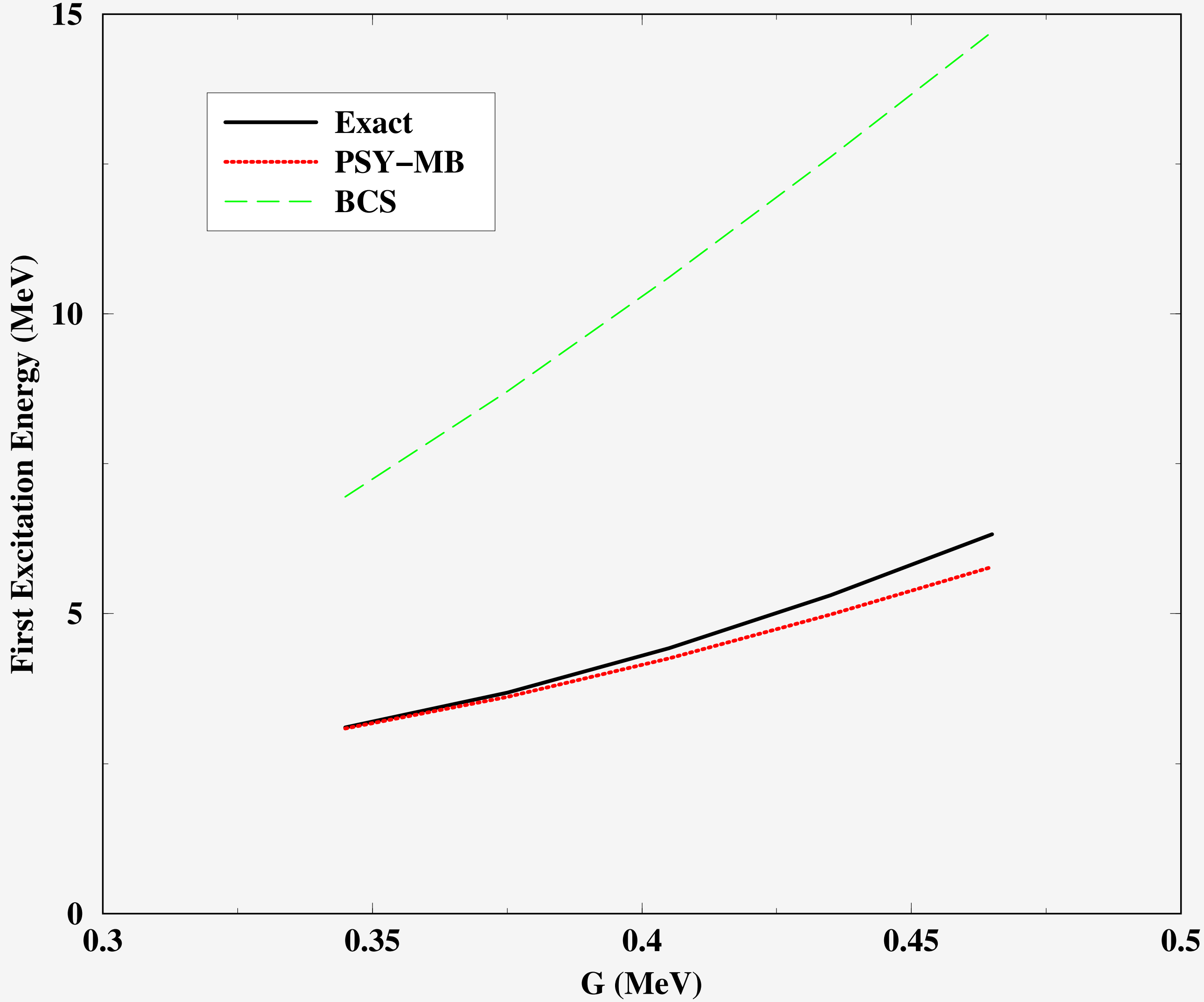
⟶ PSY-MB calculations are performed with less than 0.02 % of the basis configurations.



⟶ PSY-MB gives good correlation energies for the superfluid regime.

⟶ The BCS correlation energies are much too large and the results differ stronger from the exact results as G increases. This is also the case for the PSY-MB method.

32/64 - SUPERFLUID REGIME



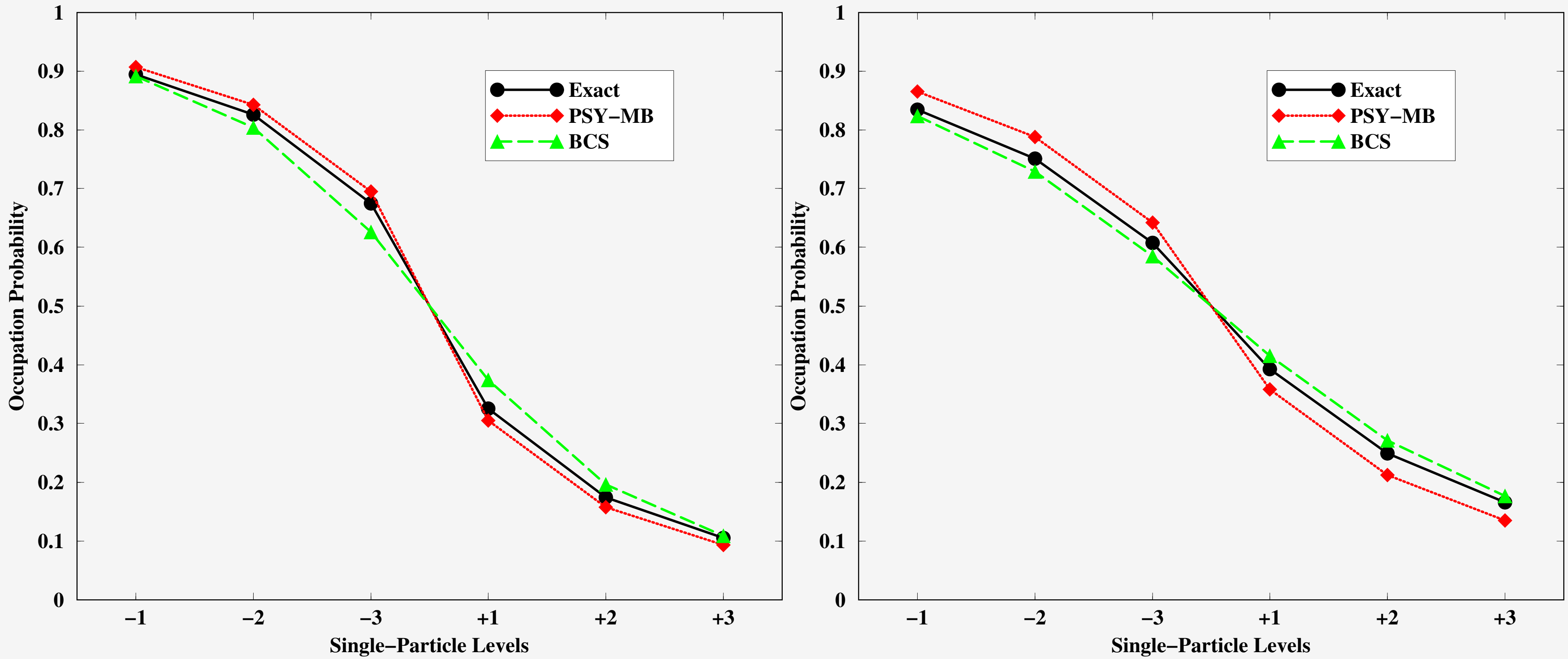
⟶ The s=0 excitations are described by 4 quasi-particles.

⟶ PSY-MB gives again good results, also for the first excitation energy of the s=0 system.

⟶ The BCS values are, here also, too large, and differ more for greater interaction strengths.

32/64 - SUPERFLUID REGIME

⋆ Left: G=0.375 MeV. Right: G=0.435 MeV.



⟶ As G increases the deviations between the exact results and the PSY-MB results get larger.

⟶ Conversely, the BCS occupation probabilities are in better agreement with the exact results, for the larger value of the pairing strength !

CONCLUSIONS

⋆ The half-filled picket fence model has been employed in order to test various methods for the nuclear pairing correlations.

⋆ A small system composed of 24 particles on 48 levels, as well as a large system of 32 particles on 64 levels has served as the model spaces.

⋆ An analysis in the normal and the superfluid regime has been performed. The crucial point is that no artificial abrupt phase transition has to be seen.

⋆ Very close results have been obtained in comparing the SCRPA and the PSY-MB methods in the normal regime. We look forward to see an extension of the SCRPA method to the superfluid regime (QPSCRPA ?).

⋆ The BCS approximation has been widely used, but has also received some criticism over the years. However, the conclusions may vary depending on which criteria the arguments are based.

⋆ The PSY-MB method provides a robust treatment for systems composed of about 30 particles on 60 levels, up to relatively large values of the pairing strength.

⋆ This gives a good hope for realistic calculations in the future.