Exact and Nearly Exact Pairing Treatment for Large Scale Calculations

H. Molique, J. Dudek

EXACT AND NEARLY EXACT PAIRING TREATMENT FOR LARGE SCALE CALCULATIONS*

Hervé MOLIQUE

IUFM d'Alsace and IPHC/IReS-ULP
23, rue du Loess B.P. 28 — F-67037 Strasbourg Cedex 2, France
Herve.Molique@IReS.in2p3.fr

and

Jerzy DUDEK

IPHC/IReS-ULP
23, rue du Loess B.P. 28 — F-67037 Strasbourg Cedex 2, France
Jerzy.Dudek@IReS.in2p3.fr

In this article we present an analysis of the practical applicability of the earlier introduced PSY-MB method in solving the nuclear pairing hamiltonian. In particular, we illustrate the convergence properties of the ground-state correlation energy, as well as the first excitation energy, in the case of the so-called picket-fence model where 32 particles are distibuted over 64 equispaced, doubly-degenerated levels. In order to illustrate the ability of the method, we compare the correlation energies of the ground-state to the exact solutions obtained with the Richardson formalism, as well as the BCS approach, in function of the increasing monopole pairing strength parameter.

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1. The PSY-MB Method

Some years ago the so-called PSY-MB (P-SYmmetries oriented Many Body) method has been introduced (cf. Ref. [1]); its aim is to solve the eigenvalue problem of the state-dependent pairing hamiltonian composed of the mean-field term $\hat{H}_{mf}$ and the pairing term $\hat{H}_{pair}$, which can be written

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as

$$\hat{H} = \hat{H}_{mf} + \hat{H}_{pair} = \sum_{\alpha=1}^{\Omega} (\varepsilon_\alpha - \lambda)\, \hat{N}_\alpha - \sum_{\alpha,\beta=1}^{\Omega} G_{\alpha\beta}\, \hat{P}_\alpha^+ \hat{P}_\beta, \qquad (1)$$

where $\hat{N}_\alpha = a_\alpha^+ a_\alpha + a_{\bar{\alpha}}^+ a_{\bar{\alpha}}$ and $\hat{P}_\alpha^+ = a_\alpha^+ a_{\bar{\alpha}}^+$ represent the number- and the pair-operators, respectively. In this expression, the states α and $\bar{\alpha}$ denote a pair of conjugated single-particle levels with respect to time-reversal, signature, simplex, or any other dichotomic symmetry.

The PSY-MB method is a procedure based on the analytical block-diagonalization of the original Hamiltonian. More precisely, three mutually commuting operators, say P_1, P_2 and P_{12}, can be built up out of the appropriately constructed unitary-group generators. They can be shown also to commute with the Hamiltonian of the problem, the latter conveniently expressed in terms of the same generators. The implied blocks of the Hamiltonian can be treated using the Lanczos method up to the largest limits acceptable by the computer at hand. Today the spaces corresponding to 18-20 particle on 36-40 levels can be treated. Above that limit, an extremely effective pre-selection of some many-body configurations adapted to the nature of the pairing interaction, in conjunction with a given energy cut-off are used before the final diagonalization employing the Lanczos method.

The configurations are classified as n-pair configurations if, starting from the ground-state configuration, one excites n pairs of particles from below to above the Fermi level. For simplicity, we concentrate here on calculations of the seniority zero solutions, but other seniorities can be studied in the same way. In order to be useful in realistic nuclear physics calculations, a single-particle space needs to be chosen sufficiently large, and the convergence of the obtained solution has to be investigated with respect to the increase of the selected many-body configurations. In this paper we focus our attention on the space composed of 32 particles distributed over 64 equispaced (the level-spacing being equal to 1 MeV) single-particle states (picket-fence model). By construction, the PSY-MB method can be applied in the case of any state-dependent pairing, but in this paper we shall restrict ourselves to the case of a constant pairing interaction.

2. Convergence of the Ground-State Correlation Energy and the First Excitation Energy

In this Section, we study the convergence properties of the correlation energy of the ground state for two different values of the pairing strength parameter G. The results are plotted in Figs. 1 and 2 for $G = 0.345$ and $G = 0.375$, respectively. On the left hand sides of the Figures, the ground-state basis configuration and all the 256 1-pair states are considered, and then the number of 2-pair configurations is increased until the maximum value of 14 400 configurations has been reached. On the right hand sides of the Figures we plot the convergence in function of the number of 3-pair states. In this case the number of 1-pair configurations is also equal to 256, and the number of 2-pair configurations is kept equal to 14 400 all the way through. We compare the results with the exact solution given by the Richardson procedure [2]. We can see from these figures that in both cases the convergence seems to be very similar: the calculated correlation energy decreases steadily to come very close to the exact results.

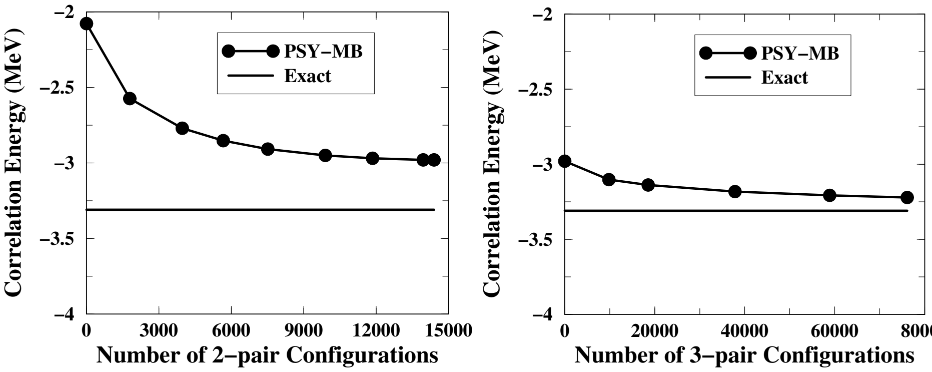

Fig. 1. Correlation energy of the ground state solution of a system of 32 particles distributed over 64 equispaced doubly degenerate levels, in function of the number of 2-pair configurations (left) and the number of 3-pair configurations (right). The value of the pairing strength parameter is G=0.345 MeV.

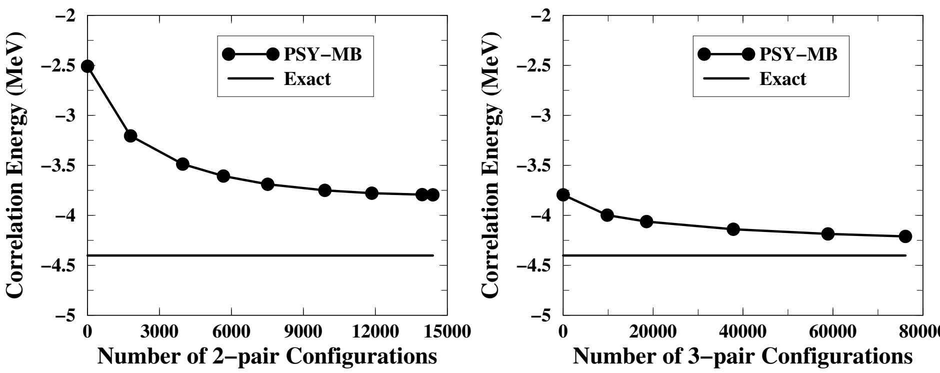

Fig. 2. Similar as in Fig. 1, but for the pairing strength G=0.375 MeV.

Similarly to the case of the correlation energy of the ground-state, we

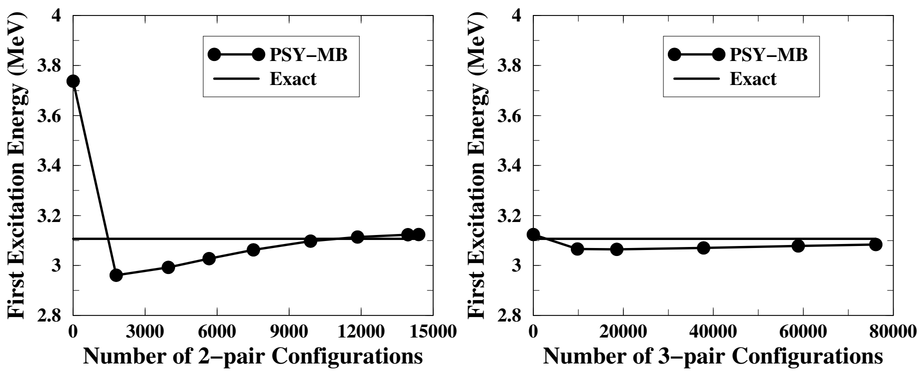

Fig. 3. Similar to Fig. 1, but for the energy of the first excited state. The value of the pairing strength parameter is G=0.345 MeV.

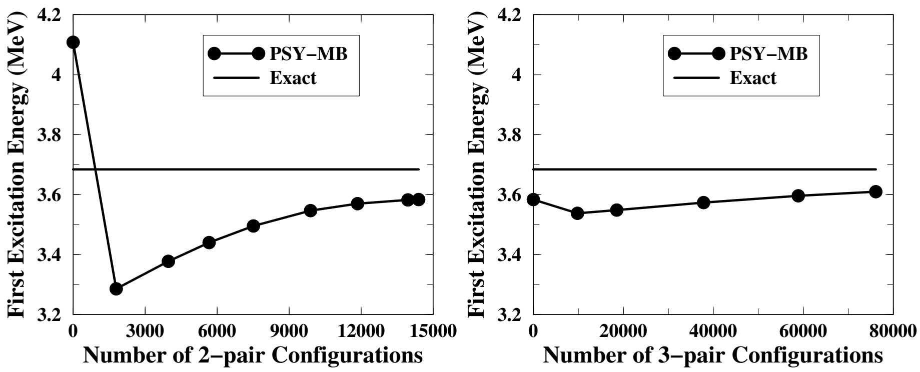

Fig. 4. The same as in Fig. 3, but for the pairing strength G=0.375 MeV.

illustrate the convergence properties of the first excitation energy in Figs. 3 and 4. From these Figures, it is clear that one cannot generaly conclude that a monotone convergence can be achieved as the number of 2-pair configurations is increased. In the case of $G = 0.345$ MeV, we see that if all the 2-pair configurations are taken into account, the solution may be further away from the exact value than if not all the configurations are included. Furthermore, if all the 2-pair configurations are included, adding some 3-pair configurations may lead to a result again further away from the exact value.

3. Comparison between the PSY-MB, BCS and the Exact Results

As an illustration for the use of the PSY-MB method, we plot in Fig. 5 the ground-state correlation energies in function of the pairing strength parameter G, for the PSY-MB, the BCS and the exact calculations. In the PSY-MB case, the ground-state configuration, all the 256 1-pair, all the 14 400 2-pair and 76 113 3-pair configurations are taken into account, which means that less than 0.02 % of the 601 080 390 seniority zero states are considered. (Remark: the number of 3-pair states taken here, namely 76 113, comes as a result of the fact that there are many basis configurations which have the same energy because of the somehow trivial structure of the picket-fence model. In the selection procedure of the configurations one is fixing a given energy cut-off, and it seems a priori natural to select all the configurations with the same energy). We see from this Figure that the agreement of the PSY-MB results with the exact ones is very satisfying, whereas the BCS solutions lie too far above. Of course, other quantities of interest such as single-particle occupation probabilities are accessible within the PSY-MB framework, and the overall agreement with the exact quantities has been checked in the same way.

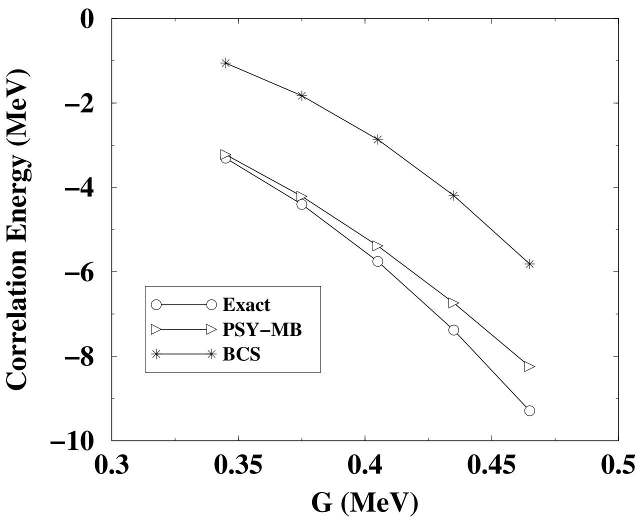

Fig. 5. Correlation energy of the ground state solution of a system of 32 particles distributed over 64 equispaced doubly degenerate levels, in function of the pairing interaction strength parameter.

4. Conclusions and Outlook

In this paper we have illustrated the use of the PSY-MB method in the case of the so-called picket-fence model composed of 32 particles distributed over 64 doubly-degenerated equidistant single-particle levels. Special attention has been payed to the convergence properties of the ground-state correlation energy and the energy of the first excited state in function of the increase of the pre-selected many-body configurations.

In recent detailed investigations we have performed a comparison, cf. Ref. [3], with other many-body techniques such as the Self-Consistent RPA treatment (see Ref. [4]) and a natural interpretation of the PSY-MB procedure that goes beyond a simple TDA treatment of the pairing correlation has been underlined.

REFERENCES

[1] H. Molique and J. Dudek, *Phys. Rev.* **C56**, 1795 (1997).

[2] R.W. Richardson, *Phys. Rev.* **141**, 949 (1966).

[3] H. Molique and J. Dudek, submitted to *Int. J. of Modern Physics, 2006.*

[4] J.G. Hirsh, A. Mariano, J. Dukelsky and P. Schuck, *Ann. Phys.* **296**, 187 (2002).