

Description of pairing in finite like-particle systems in a formalism of quartets

M Sambataro¹ and N Sandulescu²

¹ Istituto Nazionale di Fisica Nucleare - Sezione di Catania, Via S. Sofia 64, I-95123 Catania, Italy

² National Institute of Physics and Nuclear Engineering, P.O. Box MG-6, Magurele, Bucharest, Romania

E-mail: michelangelo.sambataro@ct.infn.it, sandulescu@theory.nipne.ro

Abstract. We provide a description of the ground state correlations induced by a general pairing Hamiltonian in a finite system of like fermions in terms of four-body correlated structures (quartets). These are real superpositions of products of two pairs of particles in time-reversed states. Quartets are determined variationally through an iterative sequence of diagonalizations of the Hamiltonian in restricted model spaces and are, in principle, all distinct from one another. The ground state is represented as a product of quartets to which, depending on the number of particles (supposed to be even, in any case), an extra collective pair is added. The extra pair is also determined variationally. We show some realistic applications of the quartet formalism in the case of Sn isotopes.

1. Introduction

Pairing plays a crucial role in the comprehension of a large variety of quantum many-body systems ranging from very small, like nuclei, to very large, like stars. In a mean-field treatment of nuclei, pairing mimics the short range part of the effective nucleon-nucleon interaction. Its action basically consists in scattering the nucleons between pairs of time-reversed single-particle levels. The eigenstates of the pairing Hamiltonian for a finite system of like fermions can be constructed in a (semi)analytical form in the simplifying hypothesis that the interaction strength is independent of the single-particle levels [1, 2]. One finds in this case that, for an even number of particles ($2N$), these eigenstates are a product of distinct, collective pairs of particles in time-reversed states. These pairs can be either real or complex, with reference to their mixing amplitudes, depending on the value of the pairing strength. Complex pairs, in particular, always occur in a complex-conjugate form. It is possible to show [3], that the product of two such complex-conjugate pairs forms a four-body correlated structure with real mixing amplitudes (quartet) irrespective of the pairing strength. The exact ground state of the constant pairing Hamiltonian can therefore be equivalently formulated as a product of real quartets. Quartets are expected to be all distinct from one another and, for odd values of N , they are joined in by an extra collective pair also characterized by real amplitudes. Such a representation of the ground state in terms of quartets holds exactly only for a constant pairing Hamiltonian. We have extended this representation in an approximate form to the case of a general pairing Hamiltonian by resorting to a numerical procedure [4]. In the following we will shortly illustrate how this procedure has been implemented and we will present some of the



results that have been obtained. A comparison with a representation of the pairing ground state in terms of independent pairs [5] will also be discussed.

2. The quartet formalism

The general pairing Hamiltonian has the form

$$H = \sum_i \epsilon_i \mathcal{N}_i - \sum_{ii'} g_{ii'} L_i^\dagger L_{i'}, \quad (1)$$

where

$$\mathcal{N}_i = \sum_{m_i} a_{im_i}^\dagger a_{im_i}, \quad L_i^\dagger = \sum_{m_i > 0} P_{im_i}^\dagger, \quad P_{im_i}^\dagger = a_{im_i}^\dagger \tilde{a}_{im_i}^\dagger. \quad (2)$$

The operator $a_{im_i}^\dagger$ creates a particle on the single particle level i , with energy ϵ_i and degeneracy Ω_i , $\tilde{a}_{im_i}^\dagger$ being the time reversed operator. In the case of pairing in a spherically symmetric mean field, $i \equiv n_i, l_i, j_i$ (adopting the standard notation), $\Omega_i = 2j_i + 1$ and $\tilde{a}_{im_i}^\dagger = (-1)^{j_i - m_i} a_{i, -m_i}^\dagger$, m_i being the projection of j_i . In this case, the operator L_i^\dagger creates a pair of particles on the level i with total angular momentum $J = 0$. In the absence of spherical symmetry, L_i^\dagger simply creates a pair of particles with opposite projections of the intrinsic spin on the doubly degenerate level i ($m_i = \pm$ and $\Omega_i = 2$ in this case).

We begin by considering a system with an even number N of pairs and we assume a ground state of the form

$$|\Psi_{gs}\rangle = \prod_{\nu=1}^{N/2} Q_\nu^\dagger |0\rangle, \quad Q_\nu^\dagger = \sum_{k < k'}^{(1, \Omega)} q_{kk'}^{(\nu)} P_k^\dagger P_{k'}^\dagger. \quad (3)$$

The operator Q_ν^\dagger is a linear superposition of products of two P_k^\dagger operators (each operator creating a pair of particles in time-reversed states) and the amplitudes $q_{kk'}^{(\nu)}$ are assumed to be real. In the following, we will refer to a four body correlated structure with these general properties as a quartet. $|\Psi_{gs}\rangle$ is therefore a product of quartets which are, in principle, all distinct from one another. In order to search for the most appropriate $q_{kk'}^{(\nu)}$'s we make use of an iterative variational procedure that resorts to diagonalizations of the Hamiltonian in spaces of a rather limited size. This procedure draws inspiration from an analogous technique previously developed for a treatment of pairing correlations in terms of a set of independent pairs [5] and works as follows. Let us suppose that, at a given stage of the iterative process, one knows the state (3) and let us construct the space

$$F^{(\rho)} = \left\{ P_k^\dagger P_{k'}^\dagger \prod_{\nu=1(\nu \neq \rho)}^{N/2} Q_\nu^\dagger |0\rangle \right\}_{1 \leq k < k' \leq \Omega}. \quad (4)$$

The states of $F^{(\rho)}$ are generated by acting with the operators $P_k^\dagger P_{k'}^\dagger$ ($k < k'$) on the product of all the quartets Q_ν^\dagger but the ρ -th one. The dimension of each space (4) is therefore $\Omega(\Omega-1)/2$ and one can form at most $N/2$ such spaces. By diagonalizing the Hamiltonian in $F^{(\rho)}$ and searching for the lowest eigenstate, one constructs the state

$$|\Psi_{gs}^{(new)}\rangle = Q_\rho^{\dagger(new)} \prod_{\nu=1(\nu \neq \rho)}^{N/2} Q_\nu^\dagger |0\rangle. \quad (5)$$

This differs from $|\Psi_{gs}\rangle$ only for the new quartet $Q_\rho^{\dagger(new)}$ and its energy is by construction lower than (or, at worst, equal to) that of $|\Psi_{gs}\rangle$. As a result of this operation, then, the quartet $Q_\rho^{\dagger(new)}$

has updated Q_ρ^\dagger while all the other quartets have remained unchanged. At the same time the energy of $|\Psi_{gs}\rangle$ has been driven towards its minimum. Performing a series of diagonalizations of H in $F^{(\rho)}$ for all possible ρ values ($1 \leq \rho \leq N/2$) exhausts what we define an iterative cycle. At the end of a cycle all the quartets Q_ν^\dagger have been updated and a new cycle can then start. The sequence of iterative cycles goes on until the difference between the ground state energy at the end of two successive cycles becomes vanishingly small.

The case of an odd number N of pairs proceeds along the same path but one now assumes that the ground state is formed by $(N-1)/2$ quartets and one extra pair. One has, then,

$$|\Psi_{gs}\rangle = B^\dagger \prod_{\nu=1}^{(N-1)/2} Q_\nu^\dagger |0\rangle, \quad B^\dagger = \sum_{k=1}^{\Omega} \beta_k P_k^\dagger, \quad (6)$$

the quartets Q_ν^\dagger being defined as in equation (3) and the amplitudes β_k being supposed to be real. In this case, the iterative cycle consists of two different steps. In the first one, one performs a series of diagonalizations in the spaces

$$R^{(\rho)} = \left\{ P_k^\dagger P_{k'}^\dagger B^\dagger \prod_{\nu=1(\nu \neq \rho)}^{(N-1)/2} Q_\nu^\dagger |0\rangle \right\}_{1 \leq k < k' \leq \Omega} \quad (7)$$

for all possible ρ values. These diagonalizations update the $(N-1)/2$ quartets while leaving unchanged the pair. Once these have been completed, as a second step, one performs a diagonalization in the space

$$S = \left\{ P_k^\dagger \prod_{\nu=1}^{(N-1)/2} Q_\nu^\dagger |0\rangle \right\}_{1 \leq k \leq \Omega} \quad (8)$$

which updates the pair B^\dagger with the quartets acting as spectators. Also in this case, the sequence of iterative cycles goes on up to the convergence of the ground state energy.

3. Ground state results for Sn isotopes

As an application of the procedure just described, we have considered a case of pairing in a spherically symmetric mean field. This application has concerned, in particular, the Sn isotopes with the valence neutrons in the 50-82 neutron shell. As customary for these nuclei, the model space has been restricted to the five neutron orbitals $g_{7/2}$, $d_{5/2}$, $d_{3/2}$, $s_{1/2}$, and $h_{11/2}$. Single-particle energies ϵ_j and pairing strengths $g_{ii'}$ have been taken from the work of Zelevinsky and Volya [6].

In figure 1, we have plotted the relative error in the ground state correlation energy (i.e., the energy of the ground state relative to the lowest uncorrelated many-body configuration) as a function of the number N of pairs. Results obtained with the procedure of section 2 are shown at various levels of approximation, each level corresponding to a different number of iterative cycles (indicated by the number next to each solid line). Already at the lowest level of approximation (1 cycle), the approach is seen to provide a remarkably good agreement with the exact results. This agreement progressively improves with increasing the number of iterative cycles up to becoming basically exact. We remark that the quartets Q_ν^\dagger of equation (3) are defined in an uncoupled formalism and so they are not characterized by a good angular momentum J . The same is true for the pair B^\dagger of equation (6). In spite of that, $J=0$ pair and quartets naturally arise from the calculations due to the assumed spherical symmetry of the mean field.

It is of interest to compare these results with those which can be obtained in a formalism of independent $J=0$ pairs [5]. The dot-dashed line in figure 1 refers to a calculation in which the pairing ground state has been assumed to be a product of real, collective, distinct, $J=0$ pairs. The approach based on quartets appears to be considerably more effective than the corresponding one with $J=0$ pairs.

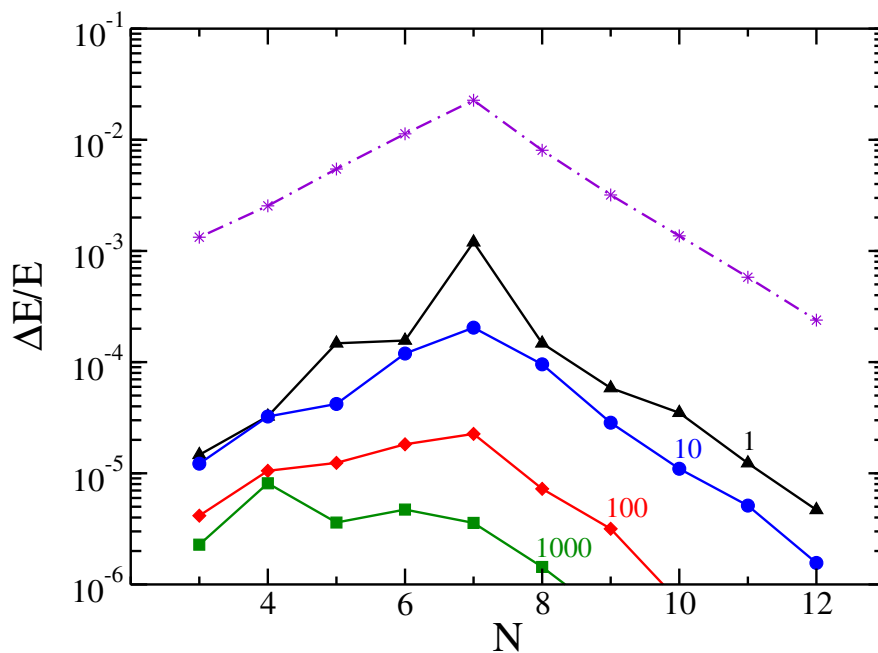


Figure 1. Relative errors in the ground state correlation energy of Sn isotopes with $2N$ active neutrons. Solid lines refer to the procedure of section 2 at various levels of approximations: the number next to each line indicates how many iterative cycles have been carried out in each calculation (see text). The dot-dashed line shows the same quantity calculated with the approach of [5] based on independent $J = 0$ pairs.

4. Conclusions

We have provided a description of the ground state of a general pairing Hamiltonian for a finite system of like particles in a formalism of quartets. We have shown that a product of distinct $J = 0$ quartets (and, in case, an extra $J = 0$ pair) can provide a basically exact representation of the pairing ground state. The quartet formalism has also been extended to excited states [4].

It has been recently observed that the ground state of the proton-neutron isovector pairing Hamiltonian can be very effectively described as a condensate of isospin $T=1$ quartets [7, 8]. An extension of this quartet condensation model in a formalism of independent quartets constructed with a procedure of the type discussed in section 2 is under way.

Acknowledgments

N.S acknowledges the support from UEFISCDI of Romanian Ministry of Education and Research through Grant IDEI No 57

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