Equations-of-motion treatment of pairing correlations: Seniority-one states

F. Andreozzi, A. Covello, A. Gargano, and A. Porrino
Dipartimento di Scienze Fisiche, Università di Napoli, 80125 Napoli, Italy
and Istituto Nazionale di Fisica Nucleare, 80125 Napoli, Italy
(Received 5 January 1988)

In prior work we have developed an equations-of-motion method for treating seniority-one states in pairing-force theory. Here we present a new and simpler version of that method. Some numerical applications to Sn isotopes show its considerable practical value.

In a previous paper[1] (hereafter referred to as I) we proposed an equations-of-motion method to treat pairing correlations in odd nuclei. The essence of the method is to solve the equations of motion for single-particle operators making use of the solution of the seniority-zero problem which can be obtained through a chain calculation involving only even nuclei. The formalism necessary to treat the latter problem is based on the use of the equations of motion for pair operators and is described in detail in Ref. 2. The explicit form of the equations of motion used in I is

$$[H,a^{\dagger}_{jm}]=(\epsilon_j-G_j)a^{\dagger}_{jm}-\sum_{j'}G_{jj'}a_{j\bar{m}}A^{\dagger}_{j'}\ , \tag{1}$$

$$[H,a_{j\bar{m}}]=-\epsilon_j a_{j\bar{m}}-\sum_{j'}G_{jj'}a^{\dagger}_{jm}A_{j'}\ , \tag{2}$$

where H is the pairing Hamiltonian,

$$H=\sum_j \epsilon_j\hat{N}_j-\sum_{jj'}G_{jj'}A^{\dagger}_j A_{j'}\ , \tag{3}$$

and the notation is the same as that adopted in I.

In contrast to some earlier approaches to the pairing-force problem based on the full treatment[3,4] of the equations of motion (1) and (2), our method completely decouples the problem of even nuclei from that of odd nuclei. This is indeed a key element for its practical usefulness. The reader is referred to Ref. 5 for a detailed discussion of this important point.

The object of this paper is to present a new version of the method developed in I which provides an even simpler (and more clearly formulated) treatment of seniority-one states in pairing-force theory.

The wave function for a seniority-one state with $(N+1)$ particles can be related either to the seniority-zero states of the system with N particles or to the seniority-zero states of the system with $(N+2)$ particles. That is, we write

$$|N+1,pjm\rangle=\sum_{\beta}c_{pj\beta}(N+1)a^{\dagger}_{jm}|N,\beta\rangle \tag{4}$$

and

$$|N+1,pjm\rangle=\sum_{\alpha}g_{pj\alpha}(N+1)a_{j\bar{m}}|N+2,\alpha\rangle\ , \tag{5}$$

where, as before, the notation is the same as that of I.

In I we made use of Eq. (1) in conjunction with the wave function (5) and of Eq. (2) in conjunction with the wave function (4). In fact, given the arrangement of the creation and annihilation operators on the right-hand side of Eqs. (1) and (2), this option is the one which leads to the best approximation scheme. The complete description of this approach is to be found in I.

Here, we start by recasting the equations of motion (1) and (2) into the form

$$[H,a^{\dagger}_{jm}]=\epsilon_j a^{\dagger}_{jm}-\sum_{j'}G_{jj'}A^{\dagger}_j a_{j\bar{m}}\ , \tag{6}$$

$$[H,a_{j\bar{m}}]=(G_j-\epsilon_j)a_{j\bar{m}}-\sum_{j'}G_{jj'}A_{j'}a^{\dagger}_{jm}\ . \tag{7}$$

This seemingly trivial change in the exact statement of the equations of motion provides what we consider to be the most convenient way of solving the seniority-one problem within the framework of our approach.

We now make use of the equations of motion for the creation operators $a^{\dagger}_{jm}$ in conjunction with the wave function (4). Taking matrix elements of (6) we then obtain the eigenvalue equation

$$\sum_{\beta'}M_{j\beta\beta'}S_{pj\beta'}(N+1)=E_{pj}(N+1)S_{pj\beta}(N+1)\ , \tag{8}$$

where

$$M_{j\beta\beta'}=[E_{\beta}(N)+\epsilon_j]\delta_{\beta\beta'}+\frac{1}{\Omega_j}\sum_{\gamma\gamma'}\bar{d}^{-1}_{j\gamma\gamma'}(N-2)\Delta_{j\beta'\gamma}(N)X_{j\beta\gamma'}(N)\ , \tag{9}$$

and where we have used the closure relations

$$\sum_{q}|N-1,qjm\rangle\langle N-1,qjm|=\hat{1}\ ,$$
$$\sum_{\beta}|N,\beta\rangle\langle N,\beta|=\hat{1}\ . \tag{10}$$

The various quantities occurring in (8) and (9) have the following definitions:

$$X_{j\beta\gamma}(N)=\langle N,\beta|A^{\dagger}_j|N-2,\gamma\rangle\ , \tag{11a}$$

$$\Delta_{j\beta\gamma}(N)=\sum_{j'}G_{jj'}X_{j'\beta\gamma}(N)\ , \tag{11b}$$

$$S_{pj\beta}(N+1)=\langle N+1,pjm|a^{\dagger}_{jm}|N,\beta\rangle\ , \tag{11c}$$

and $\Omega_j=j+\frac{1}{2}$. The quantities $\bar{d}^{-1}_{j\gamma\gamma'}(N-2)$ are the ele-

ments of the inverse of the "reduced metric matrix" of the states $a^{\dagger}_{jm} \mid N-2,\gamma\rangle$. This reduced metric matrix can be obtained from the metric matrix

$$d_{j\gamma\gamma'}(N-2)=\langle N-2,\gamma \mid a_{jm}a^{\dagger}_{jm} \mid N-2,\gamma'\rangle = \delta_{\gamma\gamma'}-\rho_{j\gamma\gamma'}(N-2) , \quad (12)$$

through the procedure described in Ref. 6. Here $\rho_{j\gamma\gamma'}(N-2)$ are the elements of the density matrix for the $(N-2)$-particle system:

$$\rho_{j\gamma\gamma'}(N-2)=\langle N-2,\gamma \mid a^{\dagger}_{jm}a_{jm} \mid N-2,\gamma'\rangle . \quad (13)$$

The spectroscopic amplitudes $S_{pj\beta}(N+1)$ are related to the coefficients $c_{pj\beta}(N+1)$ of (4) through

$$S_{pj\beta}(N+1)=\sum_{\beta'} c_{pj\beta'}(N+1)d_{j\beta\beta'}(N) . \quad (14)$$

From the normalization condition for the states $\mid N+1,pjm\rangle$, it follows that

$$\sum_{\beta} c_{pj\beta}(N+1)S_{pj\beta}(N+1)=1 . \quad (15)$$

Clearly, the preceding equations allow one to solve the seniority-one problem in terms of the solutions of the seniority-zero problem. The formalism set up thus far is exact in the sense that all the existing seniority-zero states of the N-particle system are taken into account. As in our previous treatment,[1] however, the use of an overcomplete set of basis vectors $a^{\dagger}_{jm} \mid N,\beta\rangle$ in (4) gives rise to spurious solutions. We refer the reader to Ref. 6 for a detailed account of how to remove the redundant states within the framework of our formalism.

In the above, we have given the formulation of the theory in terms of particles. The hole formalism can be readily derived by proceeding precisely as before. In this case, one has to use the equations of motion (7) in conjunction with the wave function (5). This leads to the eigenvalue equation

$$\sum_{\alpha'} M_{j\alpha\alpha'}T_{pj\alpha'}(N+1)=E_{pj}(N+1)T_{pj\alpha}(N+1) . \quad (16)$$

with

$$M_{j\alpha\alpha'}=[E_{\alpha}(N+2)+G_j-\epsilon_j]\delta_{\alpha\alpha'} + \frac{1}{\Omega_j}\sum_{\omega\omega'} \bar{h}^{-1}_{j\omega\omega'}(N+4)\tilde{\Delta}_{j\alpha'\omega}(N+2)\tilde{X}_{j\alpha\omega'}(N+2) , \quad (17)$$

where

$$\tilde{X}_{j\alpha\omega}(N+2)=\langle N+2,\alpha \mid A_j \mid N+4,\omega\rangle , \quad (18a)$$

$$\tilde{\Delta}_{j\alpha\omega}(N+2)=\sum_{j'} G_{jj'}\tilde{X}_{j'\alpha\omega}(N+2) , \quad (18b)$$

$$T_{pj\alpha}(N+1)=\langle N+1,pjm \mid a_{j\bar{m}} \mid N+2,\alpha\rangle , \quad (18c)$$

and $\bar{h}^{-1}_{j\omega\omega'}(N+4)$ are the elements of the inverse of the reduced metric matrix of the basis states $a_{j\bar{m}} \mid N+4,\omega\rangle$.

Of course, when the sums on β and α run over all existing core states [seniority-zero states of the N- or the $(N+2)$-particle system], both formalisms permit one to solve the seniority-one problem exactly. In the approximate versions of the method, however, one has to use the appropriate formalism depending on the considered j and on the number of valence particles. We shall discuss this point in detail in the context of the lowest order of approximation.

The exact statement of our method provides the framework for a sequence of approximations depending on the number of core states which are included in the expansion (4) [or (5)]. In the following we shall focus attention on the simplest stage of approximation, which we call first-order theory, wherein the core states are restricted to a single state, the seniority-zero ground state $\mid N,0\rangle$ (or $\mid N+2,0\rangle$).

In this case, the wave function (4) becomes (from now on we drop the index p)

$$\mid N+1,jm\rangle=c_j(N+1)a^{\dagger}_{jm} \mid N,0\rangle , \quad (19)$$

and the eigenvalue problem (8) reduces to

$$E_j(N+1)=E_0(N)+\Gamma_j , \quad (20)$$

with

$$\Gamma_j=\epsilon_j+\frac{X_j(N)}{\Omega_j[1-\rho_j(N-2)]}\Delta_j(N) . \quad (21)$$

The wave function (5) is written as

$$\mid N+1,jm\rangle=g_j(N+1)a_{j\bar{m}} \mid N+2,0\rangle , \quad (22)$$

TABLE I. Values of the energies E_j (in MeV) of the various seniority-one states for the Sn isotopes. The columns labeled I, III, and VIII list the results obtained from the first-, third-, and eighth-order calculations, respectively.

j \ A	111			115			119		
	I	III	VIII	I	III	VIII	I	III	VIII
$\frac{5}{2}$	−1.67	−1.57	−1.57	2.56	2.63	2.62	10.22	10.27	10.26
$\frac{7}{2}$	−1.83	−1.69	−1.69	2.36	2.45	2.43	10.02	10.08	10.07
$\frac{1}{2}$	−0.87	−0.90	−0.89	1.53	1.51	1.51	8.79	8.80	8.80
$\frac{3}{2}$	−0.62	−0.62	−0.63	1.64	1.76	1.77	8.66	8.73	8.74
$\frac{11}{2}$	−0.07	−0.07	−0.08	2.18	2.31	2.30	8.79	8.96	8.99

TABLE II. Values of the spectroscopic factors S_j^2 for the Sn isotopes.

j \ A	111			115			119		
	I	III	VIII	I	III	VIII	I	III	VIII
$\frac{5}{2}$	0.283	0.275	0.275	0.088	0.070	0.070	0.051	0.055	0.055
$\frac{7}{2}$	0.419	0.384	0.384	0.094	0.088	0.087	0.060	0.065	0.065
$\frac{1}{2}$	0.901	0.921	0.921	0.754	0.874	0.874	0.433	0.418	0.419
$\frac{3}{2}$	0.921	0.939	0.939	0.859	0.911	0.910	0.606	0.592	0.593
$\frac{11}{2}$	0.947	0.962	0.961	0.909	0.949	0.949	0.786	0.823	0.823

and it is easy to verify that the analog of Eq. (20) for holes is

$$E_j(N+1)=E_0(N+2)+\tilde{\Gamma}_j \ , \tag{23}$$

where

$$\tilde{\Gamma}_j=(G_j-\epsilon_j)+\frac{\tilde{X}_j(N+2)}{\Omega_j\rho_j(N+4)}\tilde{\Delta}_j(N+2) \ . \tag{24}$$

We now give the criterion of how to decide, for each N and for each j, whether to use the particle or the hole formalism. This criterion, which is essentially the same as that used in I, stems from the fact that either of the two wave functions (19) and (22) may contain components which violate the Pauli principle. Therefore, we have to choose the one which is less affected by the lack of antisymmetrization between the core and the added particle. A measure of the violation of the Pauli principle in the states $a_{jm}^{\dagger} \mid N,0\rangle$ and $a_{j\bar{m}} \mid N+2,0\rangle$ is given by the values of their norms. In fact, a large violation causes the norm of the corresponding vector to be close to zero. Consequently, we select as basis state the vector with the larger norm, namely, $a_{jm}^{\dagger} \mid N,0\rangle$ if $d_j(N)>h_j(N+2)$, and $a_{j\bar{m}} \mid N+2,0\rangle$ if $d_j(N)<h_j(N+2)$. In other words, we use the particle formalism if the quantity

$$\frac{d_j(N)}{h_j(N+2)}=\frac{1-\rho_j(N)}{\rho_j(N+2)} \tag{25}$$

is >1, and the hole formalism if it is <1. It should be mentioned that this criterion may be extended to higher-order approximations by considering the ratio of the determinants of the reduced metric matrices $\bar{d}$ and $\bar{h}$.

To illustrate the practical value of our approach, we now give the results of a numerical application to the odd Sn isotopes. The single-particle energies and the coupling strength G (we consider a constant pairing force, $G_{jj'}=G$) are the same as those of Ref. 7.

In Table I and II we give the energies and the spectroscopic factors S_j^2 for the various seniority-one states of ^{111}Sn, ^{115}Sn, and ^{119}Sn obtained from the first-, third-, and eighth-order applications of the theory (the results of the eighth-order calculation may be considered exact). In the first-order calculation we have used as input data the results obtained from the first-order theory for the even isotopes according to the method of Ref. 2. In the third- and eighth-order calculations [the $v=0$ core states in (4) and (5) are restricted to the lowest three and eight states, respectively] we have used the solutions of the seniority-zero problem obtained from the highest-order approximation considered in Ref. 5, to which we refer the reader for details.

From the results obtained, it appears that the accuracy of the lowest-order approximation is already very good, while the third-order calculation suffices to obtain results which are practically exact.

It should be noted that expression (20) [and (23)] is formally similar to that giving the energies of the one-quasiparticle states in the Bardeen-Cooper-Schrieffer (BCS) theory. Thus, we may conclude that our approach retains the main attractive feature of this theory, namely, its calculational simplicity, while being free from the drawback of particle-number violation. It can be easily verified that our first-order results are considerably better than the BCS ones.

Finally, it should be mentioned that the formalism given here for the seniority-one states can be generalized to treat states of any seniority $v>0$ ($v=\sum_j v_j$) in essentially the same way.[8] This will be the subject of a future publication.

This work was supported in part by the Italian Ministry of Education.

[1]F. Andreozzi, A. Covello, and A. Porrino, Phys. Rev. C **22**, 2555 (1980).

[2]F. Andreozzi, A. Covello, and A. Porrino, Phys. Rev. C **21**, 1094 (1980).

[3]M. Jean, Nuovo Cimento **40**, 1224 (1965).

[4]G. Do Dang and A. Klein, Phys. Rev. **143**, 735 (1966).

[5]A. Covello, in *Proceedings of the First International Spring Seminar on Nuclear Physics, Sorrento, 1986,* edited by A. Covello (Italian Physical Society, Bologna, 1987), p. 145.

[6]F. Andreozzi, A. Covello, A. Gargano, and A. Porrino, in *Proceedings of the International Symposium on Nuclear Shell Models, Philadelphia, 1984,* edited by M. Vallieres and B. H. Wildenthal (World-Scientific, Singapore, 1985), p. 610.

[7]L. S. Kisslinger and R. A. Sorensen, K. Dan. Vidensk. Selsk. Mat-Fys. Medd. **32**, No. 9 (1960).

[8]F. Andreozzi, A. Covello, A. Gargano, and A. Porrino, in *Proceedings of the International Nuclear Physics Conference, Harrogate, 1986,* edited by J. L. Durell, J. M. Irvine, and G. C. Morrison (Institute of Physics, London, 1986), Vol. 1, p. 54.