Equations-of-motion method and pairing correlations in doubly even nuclei

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An equations-of-motion method is presented for treating pairing correlations in doubly even nuclei. A simple technique is developed to overcome the problem of the spurious states arising from the use of an overcomplete set of basis vectors. The method yields very accurate ground-state energies, occupation numbers, and two-particle transfer amplitudes, as evidenced by comparison with the exact results for the case of the Ni isotopes.

[NUCLEAR STRUCTURE Equations-of-motion method in pairing-force theory.]

The equations-of-motion method has been applied to the pairing-force problem by many authors.[1] In particular, it has been shown[2,3] that approximate solutions to the pairing Hamiltonian can be found by a simple step-by-step procedure which involves iteration only across even nuclei. The main difficulty with this approach is the existence of spurious states arising from the violation of the exclusion principle. Such a problem has been tackled by Mauger and Evans,[4] who have developed a properly antisymmetrized theory. The usefulness of their treatment, however, is restricted to the lowest orders of approximation where the matrices to be diagonalized can be kept to manageable size. In this paper we report on a new formulation of the theory which is much simpler in application, as it allows a drastic reduction in the size of the matrices at any order of approximation. The main feature in which our approach differs from that of Mauger and Evans is the use of an angular-momentum coupled representation. This implies a different technique for the elimination of the spurious states.

We start with the pairing Hamiltonian

$$H = \sum_j \epsilon_j \hat{N}_j - \sum_{jj'} G_{jj'} A_j^\dagger A_{j'} , \tag{1}$$

where

$$\hat{N}_j = \sum_m a_{jm}^\dagger a_{jm} , \tag{2}$$

$$A_j^\dagger = \sum_{m>0} a_{jm}^\dagger a_{j\bar{m}}^\dagger , \tag{3}$$

and

$$a_{j\bar{m}}^\dagger = (-)^{j+m} a_{j-m}^\dagger .$$

The wave function for a system of an even number N of identical particles (we restrict ourselves to states with individual level seniorities of zero) is written as

$$|N,\beta\rangle = \sum_{j\gamma} c_{j\beta\gamma}(N) A_j^\dagger |N-2,\gamma\rangle , \tag{4}$$

where β and γ specify the states containing N and $(N-2)$ particles, respectively.

The equations of motion for $A_j^\dagger$ are

$$[H, A_j^\dagger] = 2\epsilon_j A_j^\dagger - \sum_{j'} G_{jj'} A_{j'}^\dagger (\Omega_j - \hat{N}_j) , \tag{5}$$

where $\Omega_j = j + \frac{1}{2}$. Taking matrix elements of (5), one has

$$\sum_{j'\gamma'} M_{j\gamma j'\gamma'} X_{j'\beta\gamma'}(N) = E_\beta(N) X_{j\beta\gamma}(N) , \tag{6}$$

with

$$M_{j\gamma j'\gamma'} = [2\epsilon_j + E_\gamma(N-2)]\delta_{jj'}\delta_{\gamma\gamma'} - G_{jj'}\Omega_j[\delta_{\gamma\gamma'} - 2\rho_{j\gamma'\gamma}(N-2)] , \tag{7}$$

where

$$X_{j\beta\gamma}(N) = \langle N,\beta | A_j^\dagger | N-2,\gamma\rangle , \tag{8}$$

$$\rho_{j\gamma'\gamma}(N-2) = \langle N-2,\gamma' | a_{jm}^\dagger a_{jm} | N-2,\gamma\rangle . \tag{9}$$

From the normalization condition $\langle N,\beta|N,\beta\rangle = 1$ it follows that

$$\sum_{j\gamma} c_{j\beta\gamma}(N) X_{j\beta\gamma}(N) = 1 . \tag{10}$$

The coefficients $c_{j\beta\gamma}(N)$ defined by (4) and the amplitudes $X_{j\beta\gamma}(N)$ are in turn related by

$$X_{j\beta\gamma}(N) = \sum_{j'\gamma'} c_{j'\beta\gamma'}^*(N) d_{j'\gamma' j\gamma}(N-2) , \tag{11}$$

where

$$d_{j'\gamma' j\gamma}(N-2) = \langle N-2,\gamma' | A_{j'} A_j^\dagger | N-2,\gamma\rangle \tag{12}$$

are the elements of the metric matrix.

As is clear from Eqs. (7) and (11), the calculation of the energies E_β and two-particle transfer

amplitudes for the N-particle system requires the knowledge of the density matrix (9) and of the metric matrix (12) for the $(N-2)$-particle system. It is straightforward, however, to express these matrices in terms of the $c_{j\gamma\delta}(N-2)$ and $X_{j\gamma\delta}(N-2)$. One finds

$$\rho_{j\beta\beta'}(N) = \frac{1}{\Omega_j}\sum_{\gamma} X_{j\beta\gamma}(N)c_{j\beta'\gamma}(N) + \sum_{j'\gamma\gamma'} X_{j'\beta\gamma'}(N)\rho_{j\gamma'\gamma}(N-2)c_{j'\beta'\gamma}(N), \quad (13)$$

$$d_{j\beta j'\beta'}(N) = \sum_{\gamma} X_{j'\beta\gamma}(N)X_{j\beta'\gamma}(N) + \Omega_j[\delta_{\beta\beta'} - 2\rho_{j\beta\beta'}(N)]\delta_{jj'}, \quad (14)$$

and hence the calculation can be carried out through a step-by-step procedure starting from $N=0$.

It is worth mentioning that the density matrix $\rho_{j\beta\beta'}(N)$ can also be calculated without using explicitly the coefficients $c_{j\beta\gamma}(N)$. In fact, taking matrix elements of the commutators $[\hat{N}_j, A^{\dagger}_{j'}]$ and $[H, \hat{N}_j]$, respectively, one obtains

$$\sum_{j'\beta'\gamma}\frac{1}{\Omega_{j'}}\rho_{j\beta\beta'}(N)X_{j'\beta\gamma}(N)X_{j'\beta'\gamma}(N) = \sum_{j'\gamma\gamma'}\frac{1}{\Omega_{j'}}\rho_{j\gamma'\gamma}(N-2)X_{j'\beta\gamma}(N)X_{j'\beta\gamma'}(N) + \frac{1}{\Omega_j^2}\sum_{\gamma}X^2_{j\beta\gamma}(N), \quad (15a)$$

$$\rho_{j\beta\beta'}(N) = \frac{1}{\Omega_j[E_{\beta}(N) - E_{\beta'}(N)]}\sum_{j'\gamma} G_{jj'}[X_{j\beta\gamma}(N)X_{j'\beta'\gamma}(N) - X_{j'\beta\gamma}(N)X_{j\beta'\gamma}(N)]. \quad (15b)$$

Clearly Eqs. (15) give all the quantities $\rho_{j\beta\beta'}(N)$, once the energies $E_{\beta}(N)$ and the amplitudes $X_{j\beta\gamma}(N)$ are known.

The use of a nonorthonormal and overcomplete set of basis vectors $A^{\dagger}_j|N-2,\gamma\rangle$ in (4) gives rise to spurious states. This problem is particularly serious when approximations are made (i.e., when one reduces the number of core states $|N-2,\gamma\rangle$), since the good solutions may mix strongly with the spurious ones.[4] We have worked out a procedure which leads to the elimination of the spurious states at any order of approximation. Our point of departure consists in diagonalizing the $n\times n$ (n is the number of vectors $A^{\dagger}_j|N-2,\gamma\rangle$) metric matrix (12). Since the set of basis vectors is overcomplete, it follows that some eigenvalues must vanish. This implies (we employ the abbreviation $|j\gamma\rangle \equiv A^{\dagger}_j|N-2,\gamma\rangle$)

$$\sum_{j\gamma} b^{(i)}_{j\gamma}|j\gamma\rangle = 0, \quad i = 1 \text{ to } n_s, \quad (16)$$

where the $b^{(i)}_{j\gamma}$ are the coefficients of the decomposition of the ith eigenvector of vanishing norm on the overcomplete set $|j\gamma\rangle$, and n_s is the number of spurious states. Clearly the n_s relations (16) enable one to determine the coefficients of the expansion of the n_s spurious vectors $|(j\gamma)_s\rangle$ in terms of the n_g good vectors $|(j\gamma)_g\rangle$,

$$|(j\gamma)_s\rangle = \sum_{(j\gamma)_g} k_{(j\gamma)_s(j\gamma)_g}|(j\gamma)_g\rangle. \quad (17)$$

Each of the n vectors $|j\gamma\rangle$ may then be written as

$$|j\gamma\rangle = \sum_{j'\gamma'}\xi_{j\gamma j'\gamma'}|j'\gamma'\rangle, \quad (18)$$

where the $n\times n$ matrix ξ is defined by

$$\xi_{j\gamma j'\gamma'} = \begin{cases} \delta_{jj'}\delta_{\gamma\gamma'} & \text{if } |j\gamma\rangle \text{ is nonspurious,} \\ k_{j\gamma j'\gamma'} & \text{if } |j\gamma\rangle \text{ is spurious and } |j'\gamma'\rangle \text{ nonspurious,} \\ 0 & \text{if both } |j\gamma\rangle, |j'\gamma'\rangle \text{ are spurious.} \end{cases} \quad (19)$$

Assuming now that the pair of indices $(j\gamma)$ refers to nonspurious states, the eigenvalue problem (6) can be reformulated as follows:

$$\sum_{j'\gamma'}\bar{M}_{j\gamma j'\gamma'}X_{j'\beta\gamma'}(N) = E_{\beta}(N)X_{j\beta\gamma}(N), \quad (20)$$

where $\bar{M}$ is the $n_g\times n_g$ matrix

TABLE I. Values of the ground-state energy (in MeV) for the Ni isotopes.

E_0 \ N	$2(^{58}\text{Ni})$	$4(^{60}\text{Ni})$	$6(^{62}\text{Ni})$	$8(^{64}\text{Ni})$	$10(^{66}\text{Ni})$
Exact	−1.49	−2.10	−1.75	−0.50	1.70
Mauger and Evans	−1.49	−2.07	−1.72	−0.45	1.86
Present work	−1.49	−2.07	−1.73	−0.53	1.60

TABLE II. Values of the occupation numbers $\rho_j(N)$ for the Ni isotopes.

j \ N	2		4		6		8		10	
	Exact	P.W.	Exact	P.W.	Exact	P.W.	Exact	P.W.	Exact	P.W.
$\frac{3}{2}$	0.343	0.343	0.629	0.596	0.764	0.729	0.859	0.812	0.934	0.876
$\frac{5}{2}$	0.082	0.082	0.198	0.213	0.404	0.413	0.631	0.632	0.856	0.833
$\frac{1}{2}$	0.036	0.036	0.081	0.090	0.153	0.169	0.252	0.278	0.408	0.466
$\frac{9}{2}$	0.007	0.007	0.013	0.016	0.021	0.027	0.027	0.040	0.031	0.057

$$\bar{M}_{j\gamma j'\gamma'} = [2\epsilon_j + E_\gamma(N-2)]\delta_{jj'}\delta_{\gamma\gamma'} - \Omega_j \sum_{j''\gamma''} G_{jj''}\xi_{j''\gamma''j'\gamma'}[\delta_{\gamma\gamma''} - 2\rho_{j\gamma''\gamma}(N-2)] . \tag{21}$$

Clearly the matrix $\bar{M}$ is not symmetric. It can be shown,[5] however, that all eigenvalues E_β are real. It should be noted that Eq. (21) gives only n_g amplitudes $X_{j\beta\gamma}(N)$. The remaining $(n-n_g)$ amplitudes can be obtained from the relation

$$X_{j'\beta\gamma'}(N) = \sum_{j''\gamma''} \xi_{j'\gamma'j''\gamma''} X_{j''\beta\gamma''}(N) . \tag{22}$$

We come now to consider the first-order theory in which the core states are restricted to one state, the ground state $|N-2\rangle$ (the quantum numbers γ drop out in all of the above equations). In this case no eigenvalue of the metric matrix is exactly zero, but we can assume that Eq. (16) is approximately valid for any eigenvector corresponding to an eigenvalue $\lambda \ll 1$. It should be mentioned that in the first-order theory the occupation numbers are best obtained by using Eqs. (15) which reduce to the very simple formula (we omit the index β)

$$\rho_j(N) = \rho_j(N-2) + \frac{X_j^2(N)}{\Omega_j^2 \sum_{j'} \frac{X_{j'}^2(N)}{\Omega_{j'}}} . \tag{23}$$

As an illustration and application of the above theory, we calculate the ground-state energies, occupation numbers and two-particle transfer amplitudes for the even Ni isotopes in the case of constant pairing force $G_{jj'} = G$. The single-particle energies and the coupling strength G are the same as those used in Ref. 6. In Tables I–III we compare the results obtained from the first-order theory with the exact ones; in Table I we also give the energies obtained by Mauger and Evans[4] using their first-order theory.

We conclude with the following remarks.

(i) The numerical results obtained for the first-order theory indicate that our equations-of-motion formalism, with a proper treatment of the spurious states, provides an effective way of treating pairing correlations in a number conserving manner.

(ii) It is straightforward to carry the calculations to higher orders of approximation proceeding along the same lines of the first-order theory. An increase in the number of core basis states is certainly required to obtain an adequate description of the excited states. The results of higher-order calculations will appear in a future paper.[5]

(iii) The amount of computational labor involved in practical applications of the theory is very limited. The matrices to be diagonalized at each step of the iteration procedure are of order $\mathfrak{N}_\gamma n_j$, where $\mathfrak{N}_\gamma$ is the number of core states (i.e., the order of the theory) and n_j is the number of single-

TABLE III. Values of the two-particle transfer amplitudes $X_j(N)$ for the Ni isotopes.

j \ N	2		4		6		8		10	
	Exact	P.W.	Exact	P.W.	Exact	P.W.	Exact	P.W.	Exact	P.W.
$\frac{3}{2}$	1.171	1.171	1.283	1.246	1.061	0.995	0.891	0.800	0.709	0.649
$\frac{5}{2}$	0.857	0.857	1.279	1.348	1.706	1.827	1.835	1.946	1.673	1.730
$\frac{1}{2}$	0.189	0.189	0.279	0.288	0.373	0.383	0.460	0.458	0.551	0.558
$\frac{9}{2}$	0.413	0.413	0.578	0.589	0.711	0.723	0.810	0.799	0.862	0.829

particle levels.

(iv) The present equations-of-motion treatment can be applied at any order of approximation to nonconstant pairing forces with no increase in complexity. This is in contrast to what happens in the BCS theory, where the energy gap Δ is no longer a constant.

(v) The procedure for the elimination of the spurious states described above may profitably be extended to the more complicated case of the spurious states arising in the equations-of-motion treatment of neutron-proton pairing correlations.[3] Work in this direction is in progress.

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[1]See, e.g., A. Covello in *Proceedings of the Latin American School of Physics, Mayaguez, Puerto Rico, 1978* (University Press, Mayaguez, Puerto Rico), and references therein.

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