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A SIMPLIFIED GENERATOR COORDINATE TREATMENT WITH ANALYTICAL PROJECTED-BCS SOLUTIONS FOR ISOVECTOR PAIRING COLLECTIVE MOTIONS*

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ABSTRACT

Analytical expressions for the projected-BCS energies and reaction transition rates among the isovector pairing collective states are obtained by the recognition of symmetry properties in a class of BCS wave functions. As a consequence, a simplified generator coordinate treatment is suggested.

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Recently, two methods, namely, the projected-BCS approximation and the Generator Coordinate Method (GCM), both of which conserve the nucleon number and the isospin, have been developed to treat the isovector pairing collective states in medium weight nuclei (Chen et al 1978). The most elaborate and time-consuming part of the calculations lies in the restoration of the broken symmetries appearing in the generating BCS wave functions. To damp the fluctuations both in the nucleon number and the isospin in question obliges one to face a four dimensional Hill-Wheeler projection integral which carries an integration over the gauge angle and all the three Euler angles in isospin space. Therefore the calculations in general become considerably more involved than that of angular momentum projection for deformed nuclei where a traditional simplification was made such that only one of the Euler angles was taken into account in the case of axial symmetry. One is thus very tempted to seek a possible counterpart of such an axial symmetry in the isospin case. It is the purpose of this letter to report that our searching effort in this direction proves to be fruitful. In recognizing the existence of a class of wave functions which show some kind of axial symmetry in isospin space we have been able to achieve a great simplification of formerly heavy computations and been furnished with a key to attack the problem of projected-BCS analytically. As a consequence, time and cost are considerably saved in performing projection. For some interesting cases, we even arrived at some closed forms for energies and reaction transition rates by which some physical features begin to show transparently.

It has been recognized for some time in the literature (Ginochio and Weneser 1968) that in the generalized treatment of isovector pairing with quasi-particle approximation, the solution for the proton-neutron gap parameter, $\Delta_{\pi\nu}$, is always zero for the lowest 0^+ states of even-even nuclei. This implies that the quasi-particle vaccum state wavefunction is always reduced to the following BCS product for the neutrons and protons separately:

$$|BCS\rangle = \prod_{jm>0} \left[U_{1\pi}(j)+(-)^{j-m}V_{1\pi}(j)a^{+}_{jm\pi}\ a^{+}_{j-m\pi}\right] \quad x$$

$$\left[U_{2\nu}(j)+(-)^{j-m}V_{2\nu}(j)a^{+}_{jm\nu}\ a^{+}_{j-m\nu}\right]|0\ \rangle \qquad (1)$$

where U and V are defined by the quasi-particle transformation

$$\alpha^{+}_{jm\sigma} = \sum_{\tau=\pi,\nu} \left[U_{\sigma\tau}(j)\ a^{+}_{jm\tau} + V_{\sigma\tau}(j)(-)^{j-m}\ a_{j-m\tau}\right] \qquad (2)$$

from the basis states $a^{+}_{jm\tau}$ to the quasi-particles $\alpha^{+}_{jm\sigma}$ in a orbit with space-spin quantum number jm, and $\tau=\pi$ for proton and $\tau=\nu$ for neutron. Here σ is a label that would distinguish between the two kinds of quasi-particles.

Now the simplicity of the BCS theory is revisited. However, the price one has to pay for this is that no way may one assume any kind of axial symmetry which would simplify the performance of the Hill-Wheeler projection to restore the lost symmetries in the wave functions. On the other hand, in keeping with the hope of finding such axial symmetry in the isospin case, we have noticed that for self-conjugate nuclei, the solution $\Delta_{\pi\pi}=\Delta_{\nu\nu}=\Delta$; $\Delta_{\pi\nu}=0$ can not be unique for the simple reason that the wave function (1) is only valid for even-even nuclei.

There must be another solution which would apply to both even-even and odd-odd. It is easy to prove that such a solution does exist and leads to

$$\Delta_{\pi\pi} = \Delta_{\nu\nu} = 0 \; ; \; \Delta_{\pi\nu} = \Delta \tag{3}$$

The corresponding wave function is then given by

$$|BCS> = C \prod_{jm>0} \Big[U^2_{1\nu}(j) V^2_{1\pi}(j) + (-)^{j-m} U_{1\nu}(j) V_{1\pi}(j) V^2_{2\nu}(j) \; (a^+_{j-m\nu} a^+_{jm\pi} + a^+_{j-m\pi} a^+_{jm\nu}) - - V^2_{1\pi} V^2_{2\nu} (a^+_{j-m\pi} a^+_{jm\pi} a^+_{j-m\nu} a^+_{jm\nu}) \Big] \; |0> \tag{4}$$

If we apply the rotation operator $\hat{R}(\alpha)=e^{i\alpha\hat{T}_z}$ to this type of wave functions with any value of $\Delta_{\pi\nu}$, we find $\hat{R}|BCS>=|BCS>$ which implies that this class of wave function does have the symmetry properties which we have searched for.

Of course, for the nuclei other than self-conjugate ones these properties no longer hold true. However, due to the charge independence of the Hamiltonian, the fact remains that there are degeneracies in energy among the members of the isospin multiplet and so it suffices to merely calculate the energy of one of its members, namely $T_z=0$, the self-conjugate nucleus. As for the reaction transition rates, owing to the Wigner-Eckart Theorem it is enough to calculate the reaction rates for a proton -neutron pair transfer from one conjugate nucleus to another. For these reasons we would not lose any generality if we formulate the theory by considering only self-conjugate nuclei. In doing so, we are fully utilizing the symmetry property of the class of wave functions which we have found. The analytical results thus obtained are therefore the most general ones.

In the framework of the projected-BCS approximation, our energy expression for a 2N-particle seniority zero state with isospin T is obtained as follows:

$$E_{NT} = \frac{\int_0^{\pi} d\beta \sin\beta \; P_T(\cos\beta) \int_0^{2\pi} d\theta \; e^{-iN\theta} \langle BCS|\hat{H} \; \hat{R}(\beta) \; \hat{S}(\theta)|BCS\rangle}{\int_0^{\pi} d\beta \sin\beta \; P_T(\cos\beta) \int_0^{2\pi} d\theta \; e^{-iN\theta} \langle BCS| \; \hat{R}(\beta) \; \hat{S}(\theta)|BCS\rangle} \qquad (5)$$

where $\hat{H}$ is the nuclear Hamiltonian. In arriving at this expression we have applied to the wave function, $|BCS\rangle$, according to eq.(4), the Hill-Wheeler projection integral which carries the integration over gauge angle θ and one of the Euler angles β. The corresponding transformations in gauge space and isospin space are $\hat{S}(\theta)$ and $\hat{R}(\beta)$ respectively. $P_T(\cos\beta)$ is the Legendre Polynomial.

If one uses the charge independent T=1 pairing Hamiltonian and adopts the notations $v_j(\theta)=V_{1\pi}(j)\exp(\frac{i\theta}{2})=V_{2\nu}(j)\exp(\frac{i\theta}{2})$ $u_j=U_{1\nu}(j)=U_{2\pi}(j)$ then the overlap functions $\langle BCS|\hat{R}(\beta)\hat{S}(\theta)|BCS\rangle$ and $\langle BCS|\hat{H}\hat{R}(\beta)\hat{S}(\theta)|BCS\rangle$ in eq.(5) can be evaluated by the procedure describe in (Chen et al 1978). The results are:

$$\langle BCS|\hat{R}(\beta)S(\theta)|BCS\rangle=\prod_j \{X_j(\beta,\theta)\}^{\Omega_j}$$

$$\frac{\langle BCS|\hat{H}\hat{R}(\beta)\hat{S}(\theta)|BCS\rangle}{\langle BCS|\hat{R}(\beta)\hat{S}(\theta)|BCS\rangle} = \sum_j \{\frac{\Omega_j v_j^2(\theta)}{X_j(\beta,\theta)}\left[(4\varepsilon_j-3G)v_j^2(\theta)+2(2\varepsilon_j-G\Omega_j)u_j^2\cos\beta\right] +$$

$$+ 4G\frac{\Omega_j(\Omega_j-1)}{X_j^2(\beta,\theta)} u_j^4 v_j^4(\theta)\sin^2\beta \}$$

$$-4G \sum_{j<j'} \frac{\Omega_j\Omega_{j'}u_j u_{j'} v_j(\theta) v_{j'}(\theta)}{X_{j'}(\beta,\theta)\ X_j(\beta,\theta)} \Big[(v_{j'}^2(\theta)u_j^2 + u_{j'}^2 v_j^2(\theta)\ ) + \tag{6}$$

$$+ (u_{j'}^2 u_j^2 + v_{j'}^2(\theta) v_j^2(\theta)\ )\cos\beta \Big]$$

where $X_j(\beta,\theta) = u_j^4 + v_j^4(\theta) + 2u_j^2 v_j^2(\theta)\cos\beta$ and ε_j are the single particle energies, Ω_j pair degeneracies and G is the pairing strength.

It is interesting to note that in general we can rewrite these overlap functions in the form of a polynomial in $v_j^2(\theta)$ and cos β by repeated applications of the binomial theorem. After introducing such expressions into eq.(5) the calculations of energy are then reduced to the evaluation of the following elementary integrals

$$I_{NT}(m,\ell) = \int_0^{\pi} d\beta\ \sin\beta\ P_T(\cos\beta)\ \cos^m\beta \int_0^{2\pi} d\theta\ e^{i(\ell-N)\theta} \tag{7}$$

This is the obvious result of applying the projection integral in eq.(5) to a term of the above mentioned overlap polynomials, say, $(v_j^2(\theta))^{\ell}(\cos\beta)^m$.

After some long and pain-taking labours, we finally arrived at the following form for the energies

$$E_{NT} = -N\sum_j \Omega_j G + \frac{1}{2}\Big[N(N-3) + T(T+1)\Big]G +$$

$$+ \chi_T \sum_{n=T}^{N} \Big[A_n(N,\Omega,U,V) + B_n(N,\Omega,U,V)\ T(T+1)\Big]\ F_T(n) \tag{8}$$

with

$$\chi_T = \frac{1}{\sum_{n=T}^{N} C_n(N,\Omega,U,V)\; F_T(n)}$$

where we have used the collective labels such as Ω, U and V for $\Omega_1, \Omega_2, \ldots, U(1), U(2) \ldots$ and $V(1), V(2), \ldots$. The isospin function $F_T(n)$ in the energy formula, is given by:

$$F_T(n) = \frac{n!}{2^T (n+T+1)!!(n-T)!!} \tag{9}$$

with

$$n = T,\ T+2,\ T+4,\ \ldots,\ N$$

from which the recursion formula for the F-function is obtained as

$$F_T(n-2) = \frac{n(n+1) - T(T+1)}{n(n-1)} F_T(n) \tag{10}$$

The isospin-independent coefficients A,B and C in eq.(8) written in terms of U and V form an extensive expression which can be found in (Kyotoku-1979). Here we only present the results for the degenerate model:

$$C_n = \frac{2^n\ \Omega!}{(\Omega - \frac{n+N}{2})!(\frac{N-n}{2})!n!}$$

$$A_n = C_n\left[(2\Omega+1)(\frac{n-N}{2}) - \frac{N(N-1)}{2}\right] \quad \text{and} \quad B_n = \frac{C_n}{2}G$$

It is interesting to see that in this simple case by using eq.(10) we are able to prove that the last term of eq.(8) vanishes thus reproducing the exact solution with isospin.

To see the functional dependence of the energy on $T(T+1)$, we simply write $F_T(n)$ in eq.(8) in terms of $F_T(N)$ using eq.(10) and by so doing we eventually end up with the expression of a quotient of two polynomials in $T(T+1)$ if we limit ourselves to the case of $T<<N$ or we approximate our formula by replacing the lower limit, of the summation in eq.(8) by some T-independent number. If in addition, the Taylor expansion of the above quotient is carried out, we finally would reach the form $a+bT(T+1)+cT^2(T+1)^2+$ .... which immediatly reminds us of rotation-vibration model.

In order to test our formula we have performed some numerical calculations with a semi-realistic four level model which stands for the states of the pf shell. As expected we did reproduce the results obtained by the previous method (Chen et al 1978) where the BCS wave functions were not chosen to be axially symmetric in isospin space and, as a consequence, we have been able to reduce the computational time considerably. Because of this reduction in time the FBCS calculations with isospin which implies variation after projection become as practical as those without isospin. This observation has been numerically confirmed by our FBCS results which prove comparable with the exact solutions.

In order to calculate the transition rates for pair transfer reactions we need to evaluate the reduced matrix elements of the operator $A_j^+=\left[a_j^+ \times a_j^+\right]^{J=0\ T=1}$. Noting that this operator no longer commutes with $\hat{R}(\alpha,\beta,\gamma)$, $\hat{S}(\theta)$, we have the following expression for the matrix elements between the projected state with isospin T and nucleon number 2N and that with T' and 2(N+1):

$$\langle P_T P_N BCS;T'N+1 || A_j^+ || P_T P_N BCS;TN\rangle = \frac{(2T'+1)(2T+1)}{16\pi^3} \sqrt{\chi_{T'}\chi_T} \sum_{\substack{MM' \\ t}} \begin{pmatrix} T' & 1 & T \\ -M' & t & M \end{pmatrix}$$

$$\int_0^{2\pi} d\theta e^{-iN\theta} \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} d\beta \sin\beta D_{MM'}^{T*}(\alpha\beta\gamma) \times \tag{11}$$

$$\langle P_T P_N BCS;T'M_{T'}=0 \; N+1 | A_{jt}^+ R(\alpha\beta\gamma)\hat{S}(\theta) | P_T P_N BCS;TM_T=0 \; N\rangle$$

where $D_{MM'}^{T*}$, is the Wigner D-function. One should note that the integration in eq.(11) is now over all the three Euler angles α, β and γ.

After utilizing the same trick that was used to reach eq. (8), we obtain

$$\langle P_T P_N BCS;T'N+1 || A_j^+ || P_T P_N BCS;TN\rangle = (2T'+1)(2T+1)\sqrt{\chi_{T'}\chi_T} \times$$

$$\sum_{n=T}^{N} \left\{ D_n^{(1)} \begin{pmatrix} T' & 1 & T \\ 0 & 0 & 0 \end{pmatrix} + D_n^{(2)} \begin{pmatrix} T' & 1 & T \\ 0 & 1 & -1 \end{pmatrix} \sqrt{T(T+1)} \right\} F_T(n) \tag{12}$$

The T-independent coefficients $D_n^{(1)}$ and $D_n^{(2)}$ are in general expressed in terms of N, Ω, U and V as found in (Kyotoku 1979). For degenerate model, they are simply given by

$$D_n^{(1)} = \frac{(2\Omega-N)}{2} C_n \qquad \text{and} \qquad D_n^{(2)} = -C_n \; .$$

In this simple model, one is able to verify, with the little effort, that for the transition, say, $T \to T+1$ our expression is then reduced to $\sqrt{T(T+1)(2\Omega-N-T)(T+N+3)/2}$, that of the exact solution (Hecht 1965).

So far we have been considering only the seniority zero isospin yrast states. It is very tempting to treat the higher excited states using the generator coordinate method with the generating functions obtained by projecting out sharp isospin and nucleon number from our axial symmetric BCS wave function (4). The gap parameter $\Delta_{\pi\nu}$ in $U(j)$ and $V(j)$ is now used as the only generator coordinate under the present assumption that the axial symmetry is preserved even for the excited states. The energy kernel $\langle P_T P_N BCS;\Delta^A_{\pi\nu}|\hat{H}|P_T P_N BCS;\Delta^B_{\pi\nu}\rangle$ and overlap $\langle P_T P_N BCS;\Delta^A_{\pi\nu}|P_T P_N BCS;\Delta^B_{\pi\nu}\rangle$ involved in the Hill-Wheeler equations can be evaluated analytically, as shown in detail in (Kyotoku-1979) by the method described above. We are thus adding one more interesting example to those few cases (de Toledo Piza et al 1977) where one is tempted to solve the Hill-Wheeler equation analytically. However, we choose to test the validity of the present approximation with GCM by solving the problem for four level model. Our preliminary results do agree reasonably well with the former one (Chen et al 1978). However further investigation in all cases is needed to draw some definite conclusions as to symmetry properties of the excited seniority zero states.

The great simplicity of the present methods, as compared with their earlier complicated versions suggests that they might prove powerful in the study of isovector pairing collective states which are strongly populated by pair transfer reactions in the medium weight nuclei.

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