Broken pair approach to rotating nuclei: Formalism

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A broken pair approach is developed to describe the high-spin band structures in rotating nuclei. The alignment processes are tacitly considered by including the higher angular momentum broken pairs.

I. INTRODUCTION

The backbending phenomena observed[1,2] in rotating nuclei is now well established to arise from the crossing of the paired ground-state band with the aligned configuration in which a pair of particles (or quasiparticles) is decoupled from the paired state with the angular momentum aligned along the rotational axis.[3] The properties of the nuclei in the high-spin regime such as this backbending phenomena have invariably been described in terms of the cranked-shell-model (CSM) approach.[4] In this CSM theory the influence of the strong pairing force between the identical nucleons is taken into account through the quasiparticle transformation. It is the system of noninteracting quasiparticles which is cranked around an axis perpendicular to the symmetry axis of the deformed nucleus to describe the intrinsic structures in a rotating coordinate system. While the CSM approach has been successful in providing a qualitative understanding of the backbending and predicts the bandcrossing frequencies fairly well,[5] it has also exhibited serious drawbacks. For example, the level interaction (repulsion) between the ground-state band and the two-particle aligned configuration (the AB interaction) is underpredicted.[6] Also a fully self-consistent CSM approach predicts a vanishing of the pair gap immediately after the first (AB) crossing. This in any situation is unrealistic. It has been suggested that these deficiencies in CSM are related to the fact that the particle number is conserved only on the average in the model.[7] The number fluctuation becomes exceedingly large at a band crossing. The improvement upon the conventional CSM can be achieved through the explicit particle-number projection.

Recently,[8] attempts have been made to develop a cranked-deformed-shell-model (CDSM) approach in which the particle number is built in the theory. In this model a system of interacting particles in a deformed mean field is cranked around an axis perpendicular to the symmetry axis of the mean field. The eigenstates of a system are determined by an exact diagonalization of the Hamiltonian. So far these investigations have been restricted only for the case of the valence particles in a single high-j intruder orbitial. Even in this simpler problem the dimensionality of the configuration space is quite large, and this is expected to grow rapidly in a realistic multi-j shell configuration space. To retain the advantages of the method with a definite particle number, one needs to truncate the basis in such a manner that the low-lying states of the deformed system are reproduced faithfully. The feasibility of the truncation scheme has been investigated[9] in a single-j shell with $j = \frac{11}{2}$ where the first few low-lying states of the system were very accurately reproduced with a basis which represented a severe truncation of the full space. Here we try to generalize the truncation scheme in a multi-j shell configuration space in the context of the broken pair approach (BPA).[10]

The usefulness of the BPA is now well established in the domain of low-spin spectroscopy.[10,11] The BPA reduces the intractable matrices in the shell-model configuration space to a manageable form and at the same time retaining all the basic features of the shell model. In its application to spherical nuclei the BPA ground state is a polynominal of collective bifermion excitations, all coupled to angular momentum (J) equal to zero. The degree of the polynominal is equal to the number of fermion pairs (p). In this sense the particle-number conservation is intrinsic in the formalism.

In its application to deformed nuclei the collective bifermion excitations with angular momentum greater than zero also need to be considered. For example, in the case of quadrupole deformation the collective bifermion excitations with $J=0$, 2, and 4 need to be considered.[12,13]

In order to describe the high-spin spectroscopy the inclusion of only low angular momentum collective excitations is inadequate. This is clearly indicated by a model study.[9,14] It is seen that before the AB crossing $J=0$, 2, and 4 are sufficient to reproduce the yrast configuration. But above this band crossing the yrast band is mainly composed of states with maximum alignment along the rotational axis. The AB band crossing is interpreted as due to the alignment of two particles. Thus in order to describe this band crossing a pair of particles is to be broken from the ground-state condensate. This broken pair should be allowed to carry all the possible angular momenta. The remaining (p−1) pairs are still in the condensed state of the collective bifermion excitations with angular momentum coupled to $J=0$, 2, and 4. In order to describe the higher-order band crossings more pairs

need to be broken from the ground-state condensate.

The purpose of the present investigation is to present the broken pair formalism in a very general form. A generalized BPA subspace is discussed in Sec. II. The Hamiltonian is presented in antinormal-ordered form (all the creation operators on the left) in Sec. III. The general overlap integral between the BPA basis is derived in Sec. IV. In Sec. V, the expressions for matrix elements needed are expressed in terms of the overlap integral. Finally, the summary and the conclusions are presented in Sec. VI.

II. BROKEN PAIR SUBSPACE

We start with a most general intrinsic state for p pairs of identical valence nucleons

$$|\Phi\rangle = N_p(\Gamma^\dagger)^p|0\rangle, \tag{1}$$

with

$$\Gamma^\dagger = \sum_{JM} Y_{JM} Q^\dagger_{JM}, \tag{2}$$

$$Q^\dagger_{JM} = \frac{1}{2}\sum_{ab} X_{JM}(ab) A^\dagger_{JM}(ab), \tag{3}$$

and

$$A^\dagger_{JM}(ab) = \sum_{\alpha\beta} \begin{bmatrix} j_\alpha & j_\beta & J \\ m_\alpha & m_\beta & M \end{bmatrix} C^\dagger_\alpha C^\dagger_\beta. \tag{4}$$

The operators $C^\dagger_\alpha$ ($C^\dagger_\beta$) are the fermion creation (annhilation) operators satisfying the following anticommutation relations:

$$[C_\alpha, C_\beta]_+ = [C^\dagger_\alpha, C^\dagger_\beta]_+ = 0, \quad [C_\alpha, C^\dagger_\beta]_+ = \delta_{\alpha\beta}. \tag{5}$$

The quantum numbers $\alpha, \beta, \ldots$ denote the single-particle shell-model states $nljm$. The quantum numbers $a, b, \ldots$ denote the same states but without the projection m. The square brackets in Eq.(4) denote a Clebsch-Gordan coefficient. The coefficients Y_{JM} are the weight factors for various angular momenta and the coefficients $X_{JM}(ab)$ are the collective coefficients defining the correlated fermion pairs Q_{JM}. In other words, the coefficients Y_{JM} reflect the importance of the various angular momenta and $X_{JM}(ab)$ reflect the collective features of the system under consideration. We reexpress Eq.(2) in terms of the single-particle operators

$$\Gamma^\dagger = \frac{1}{2}\sum_{\alpha\beta JM} Z_{JM}(\alpha\beta) C^\dagger_\alpha C^\dagger_\beta, \tag{6}$$

with

$$Z_{JM}(\alpha\beta) = \begin{bmatrix} j_\alpha & j_\beta & J \\ m_\alpha & m_\beta & M \end{bmatrix} X_{JM}(ab) Y_{JM}. \tag{7}$$

In Eq.(6) we have decoupled a two-particle state and the resulting Clebsch-Gordan coefficient is coupled with the expansion coefficients $X_{JM}(ab)$ and Y_{JM} to define the new expansion coefficient $Z_{JM}(ab)$. In this way the Racah recoupling algebra is bypassed which becomes quite involved for more than a one-broken pair configuration.[10] In the following all the algebraic expressions are therefore worked out in the m-scheme representation. The expansion coefficients are constrained to satisfy the following orthogonality relations:

$$\sum_{ab} X_{JM}(ab) X_{J'M'}(ab) = 2\delta_{JJ'}\delta_{MM'}, \tag{8}$$

$$\sum_{JM} Y^2_{JM} = 1, \tag{9}$$

with the following phase relationship:

$$X_{JM}(ab) = (-1)(-1)^{j_a+j_b+J} X_{JM}(ba). \tag{10}$$

It is to be pointed out that in the present work we are mainly interested in the various J truncations to Eq.(2) as explained in the following.

In the case of spherical nuclei it is believed that the ground state is to a good approximation a generalized seniority zero state,[15,16] thus implying that for spherical nuclei only J=0 is sufficient in Eq.(2). In the case of deformed nuclei, the higher angular momentum states also need to be included in Eq.(2). For example, in the case of nuclei with quadrupole deformation J=0, 2, and 4 terms need to be considered in Eq.(2) to reproduce[12,13] the low-lying excitation spectrum. For high-spin states, as mentioned in the Introduction, J=0,2,4 are inadequate. As an illustration, in a simple case of a Hamiltonian with monopole pairing (no deformation) and Coriolis forces,[17] the yrast line before the AB crossing is essentially a seniority (ν) zero state. But above this band crossing the yrast band is composed of states with maximum alignment along the rotational axis. The AB interaction in this model case[17] is due to the crossing of $\nu = 0, J = 0$ state [or zero broken state in the spherical limit of Eq.(1)] with $\nu = 2, J = M = (2j - 1)$ state (or one broken pair state), where j is the intruder orbital under consideration. Therefore, in order to describe the yrast band above the AB crossing, the state $M = J = (2j - 1)$ also needs to be included in the ground-state condensate for the model Hamiltonian.[17] In a realistic situation where the Hamiltonian also contains a deformation force, the ground state can be represented by

$$|\Phi_0\rangle = N_0 \sum_{abJM} \gamma_{JM}(ab) A^\dagger_{JM}(ab)(\Gamma^\dagger)^{p-1}|0\rangle. \tag{11}$$

In the above equation a pair has been broken from the condensate Eq.(1). The broken-pair angular momentum J in Eq.(11) is allowed to carry all the possible values. In contrast, the pairs in the condensate $(\Gamma^\dagger)^{p-1}$ are restricted to carry only J=0, 2, and 4 angular momenta. In order to describe the higher-order band crossings more pairs need to be broken from Eq.(1). Finally, if all the pairs are broken, one spans a space equivalent to the complete shell-model space and consequently one may obtain the exact ground state (as well as all the other states) by

diagonalization of the Hamiltonian in that space.

A general b-broken pair state can be written as

$$|\Phi(\alpha_1\alpha_2\cdots\alpha_{2b})\rangle = N(\alpha_1\alpha_2\cdots\alpha_{2b})\left(\prod_{i=1}^{2b} C^\dagger_{\alpha_i}\right)(\Gamma^\dagger)^{p-2b}|0\rangle, \quad (12)$$

where $N(\alpha_1\alpha_2\cdots\alpha_{2b})$ is the orthogonalization coefficient. It is to be noted that b-broken pair state has to be orthogonal to all states with less broken pairs. The spectrum is obtained by diagonalizing the Hamiltonian in the BPA basis Eq.(12) .

The ground-state parameters X and Y in Eq.(12) are obtained by minimizing the energy of the ground state

$$\delta\frac{\langle\Phi_0|H|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle} = 0, \quad (13)$$

which can be rewritten in the following form:

$$\langle\Phi_0|\Phi_0\rangle\langle\Phi_0|H|\delta\Phi_0\rangle - \langle\Phi_0|\delta\Phi_0\rangle\langle\Phi_0|H|\Phi_0\rangle = 0. \quad (14)$$

The above variation leads to a set of nonlinear coupled equations that determine the ground-state parameters. The variation of $|\Phi_0\rangle$ is given by

$$|\delta\Phi_0\rangle = N_0\frac{\partial}{\partial X_{JM}(ab)}(\Gamma^\dagger)^p|0\rangle \quad (15)$$

and

$$|\delta\Phi_0\rangle = N_0\frac{\partial}{\partial Y_{JM}}(\Gamma^\dagger)^p|0\rangle. \quad (16)$$

The differential of $(\Gamma^\dagger)^p$ is given by

$$\frac{\partial}{\partial X_{JM}(ab)}(\Gamma^\dagger)^p|0\rangle = \frac{\partial}{\partial X_{JM}(ab)}\left(\frac{1}{2}\sum_{\alpha'\beta'J'M'}\begin{bmatrix} j_{\alpha'} & j_{\beta'} & J' \\ m_{\alpha'} & m_{\beta'} & M'\end{bmatrix} Y_{J'M'}X_{J'M'}(a'b')C^\dagger_{\alpha'}C^\dagger_{\beta'}\right)^p|0\rangle, \quad (17)$$

or

$$\frac{\partial}{\partial X_{JM}(ab)}(\Gamma^\dagger)^p|0\rangle = pY_{JM}A^\dagger_{JM}(ab)(\Gamma^\dagger)^{p-1}|0\rangle, \quad (18)$$

where the orthogonality relation of the X's has been employed, i.e.,

$$\frac{\partial}{\partial X_{JM}(ab)}X_{J'M'}(a'b') = \delta_{JJ'}\delta_{MM'}[\delta_{aa'}\delta_{bb'} - (-1)^{j_a+j_b+J}\delta_{ab'}\delta_{ba'}]. \quad (19)$$

We also have

$$\frac{\partial}{\partial Y_{JM}}(\Gamma^\dagger)^p|0\rangle = \frac{p}{2}\sum_{\alpha\beta}\begin{bmatrix} j_\alpha & j_\beta & J \\ m_\alpha & m_\beta & M\end{bmatrix} X_{JM}(ab)C^\dagger_\alpha C^\dagger_\beta(\Gamma^\dagger)^{p-1}|0\rangle. \quad (20)$$

It is evident from Eqs.(18) and (20) that the variation of $|\Phi_0\rangle$ is essentially a one-broken pair state. Therefore, the overlap integral $\langle\Phi|\delta\Phi\rangle$ is an overlap between a zero-broken pair state and a one-broken state. In the next section the Hamiltonian is expressed in the antinormal-ordered form. This is quite useful as all the matrix elements can be expressed in terms of the overlaps between the BPA states.

III. HAMILTONIAN

The general Hamiltonian containing one- and two-body terms is written as

$$H = H_1 + H_2, \quad (21)$$

$$H = \sum_{\alpha\beta}\epsilon_{ab}C^\dagger_\alpha C_\beta + \frac{1}{4}\sum_{abcdJ}\sqrt{(1+\delta_{ab})(1+\delta_{cd})}\hat{J}\langle ab|v|cd\rangle_J \times[A^\dagger_J(ab)\times\tilde{A}_J(cd)]_{00},$$

with

$$\tilde{A}_{JM}(ab) = (-1)^{J-M}[A^\dagger_{J-M}(ab)]^\dagger = (-1)^{J-M}A_{J-M}(ab). \quad (22)$$

The first term of the Hamiltonian Eq.(21) contains the single-particle energies ϵ_{ab} obtained from a choosen average potential. The second term of Eq.(21) contains the coefficients $\langle ab|v|cd\rangle_J$, denoting the anti-symmetric normalized two-particle matrix elements of the assumed residual nucleon-nucleon interaction. We rewrite the two-body interaction as

$$H_2 = \frac{1}{4}\sum_{abcdJ}\hat{J}G_J(abcd)[A^\dagger_J(ab)\times\tilde{A}_J(cd)]_{00}, \quad (23)$$

where $G_J(abcd)$ are still antisymmetric but now unnormalized matrix elements given by

$$G_J(abcd) = \langle ab|v|cd\rangle_J\sqrt{(1+\delta_{ab})(1+\delta_{cd})}. \quad (24)$$

We now rewrite the Hamiltonian Eq.(21) in such a way that all the annihilation operators occur on the right. It is quite useful since all the matrix elements can be expressed in terms of the overlaps between the BPA states. The antinormal-ordered Hamiltonian is given by

$$H = \sum_{\alpha\beta} \epsilon_{\alpha\beta} \left(\delta_{\alpha\beta} - C_\beta C_\alpha^\dagger\right) + \frac{1}{4} \sum_{\alpha\beta\gamma\delta JM} \begin{bmatrix} j_\alpha & j_\beta & J \\ m_\alpha & m_\beta & M \end{bmatrix} \begin{bmatrix} j_\gamma & j_\delta & J \\ m_\gamma & m_\delta & M \end{bmatrix}$$
$$\times G_J(abcd)[\mathbf{P}(\alpha\beta)\delta_{\alpha\gamma}\delta_{\beta\delta} - \mathbf{P}(\alpha\beta)\mathbf{P}(\gamma\delta)\delta_{\beta\gamma}C_\gamma C_\alpha^\dagger + C_\delta C_\gamma C_\alpha^\dagger C_\beta^\dagger], \quad (25)$$

where

$$\mathbf{P}(\alpha\beta) = 1 - \alpha \leftrightarrow \beta. \quad (26)$$

IV. GENERAL OVERLAP INTEGRAL

The matrix elements of the Hamiltonian Eq.(25) between the BPA basis states Eq.(12) can be expressed in terms with $\prod_{i=1}^n C_{\beta_i} \prod_{j=1}^n C_{\alpha_j}^\dagger$ sandwiched between the pair condensate. In order to evaluate this matrix element it has to be brought to the normal-ordered form. We start with n=1,

$$C_{\beta_1} C_{\alpha_1}^\dagger = \delta_{\alpha_1\beta_1} - C_{\alpha_1}^\dagger C_{\beta_1}, \quad (27)$$

and for n=2

$$C_{\beta_1} C_{\beta_2} C_{\alpha_1}^\dagger C_{\alpha_2}^\dagger = \mathbf{P}(\alpha_1\alpha_2)\delta_{\alpha_1\beta_2}\delta_{\alpha_2\beta_1} - \mathbf{P}(\beta_1\beta_2)\mathbf{P}(\alpha_1\alpha_2)\delta_{\alpha_1\beta_2} C_{\alpha_2}^\dagger C_{\beta_1} + C_{\alpha_1}^\dagger C_{\alpha_2}^\dagger C_{\beta_1} C_{\beta_2} \quad (28)$$

where $\mathbf{P}(\alpha\beta)$ is defined in Eq.(26). For n=3 we have

$$C_{\beta_1} C_{\beta_2} C_{\beta_3} C_{\alpha_1}^\dagger C_{\alpha_2}^\dagger C_{\alpha_3}^\dagger = \mathbf{P}(\alpha_1, \alpha_2\alpha_3)\{\ \mathbf{P}(\alpha_2\alpha_3)[\delta_{\alpha_1\beta_3}\delta_{\alpha_2\beta_2}\delta_{\alpha_3\beta_1} - \mathbf{P}(\beta_1, \beta_2\beta_3)\delta_{\alpha_1\beta_3}\delta_{\alpha_2\beta_2} C_{\alpha_3}^\dagger C_{\beta_1}]$$
$$-\mathbf{P}(\beta_1, \beta_2\beta_3)\delta_{\alpha_1\beta_3} C_{\alpha_2}^\dagger C_{\alpha_3}^\dagger C_{\beta_2} C_{\beta_3}\} - C_{\alpha_1}^\dagger C_{\alpha_2}^\dagger C_{\alpha_3}^\dagger C_{\beta_1} C_{\beta_2} C_{\beta_3}, \quad (29)$$

with

$$\mathbf{P}(\alpha, \beta\gamma) = 1 - \alpha \leftrightarrow \beta - \alpha \leftrightarrow \gamma. \quad (30)$$

In a general case

$$\left(\prod_{i=1}^n C_{\beta_i}\right)\left(\prod_{j=1}^n C_{\alpha_j}^\dagger\right) = \prod_{i=1}^{n-1} \mathbf{P}\left(\alpha_i, \prod_{j=i+1}^n \alpha_j\right)\left(\prod_{i=1}^n \delta_{\alpha_i\beta_{n-i+1}}\right)$$
$$+\mathbf{P}\left(\beta_1, \prod_{j=2}^n \beta_j\right)\left[\sum_{p=1}^{n-1}(-1)^p \prod_{i=1}^{n-p} \mathbf{P}\left(\alpha_i, \prod_{j=i+1}^n \alpha_j\right)\right.$$
$$\left.\times \left(\prod_{i=1}^{n-p} \delta_{\alpha_i\beta_{n-i+1}}\right)\left(\prod_{i=1}^p C_{\alpha_{n-i+1}}^\dagger\right)\left(\prod_{i=1}^p C_{\beta_i}\right)\right]$$
$$+(-1)^n \left(\prod_{j=1}^n C_{\alpha_j}^\dagger\right)\left(\prod_{i=1}^n C_{\beta_i}\right), \quad (31)$$

where

$$\prod_{i=1}^{n-1} \mathbf{P}\left(\alpha_i, \prod_{j=i+1}^n \alpha_j\right) = \mathbf{P}\left(\alpha_1, \prod_{j=2}^n \alpha_j\right)\mathbf{P}\left(\alpha_2, \prod_{j=3}^n \alpha_j\right)\cdots\mathbf{P}(\alpha_{n-1}, \alpha_n) \quad (32)$$

and

$$\mathbf{P}\left(\alpha_i, \prod_j \alpha_j\right) = 1 - \sum_j \alpha_i \leftrightarrow \alpha_j. \quad (33)$$

In order to evaluate a general overlap integral between the BPA states we reexpress $(\Gamma^\dagger)^p$ as

$$(\Gamma^\dagger)^p = \left(\frac{1}{2}\sum_{\alpha\beta JM} Z_{JM}(\alpha\beta)C^\dagger_\alpha C^\dagger_\beta\right)^p$$
$$= \frac{1}{2}\sum_{\alpha_1\alpha_2 J_1 M_1} Z_{J_1M_1}(\alpha_1\alpha_2)C^\dagger_{\alpha_1}C^\dagger_{\alpha_2}\frac{1}{2}\sum_{\alpha_3\alpha_4 J_3 M_3} Z_{J_3M_3}(\alpha_3\alpha_4)C^\dagger_{\alpha_3}C^\dagger_{\alpha_4}$$
$$\vdots$$
$$\times\frac{1}{2}\sum_{\substack{\alpha_{n-1}\alpha_n\\ J_{n-1}M_{n-1}}} Z_{J_{n-1}M_{n-1}}(\alpha_{n-1},\alpha_n)C^\dagger_{\alpha_{n-1}}C^\dagger_{\alpha_n}, \tag{34}$$

or in a compact form,

$$(\Gamma^\dagger)^p = (\tfrac{1}{2})^p \sum_{\substack{\alpha_1,\alpha_2,\ldots,\alpha_n\\ J_{\alpha_1},J_{\alpha_3},\ldots,J_{\alpha_{n-1}}}} \prod_{\substack{i=1\\ \text{odd}}}^{n-1} Z_{J_{\alpha_i}}(\alpha_i,\alpha_{i+1})\prod_{i=1}^{n} C^\dagger_{\alpha_i}. \tag{35}$$

Using the above expression and Eq.(31) the general overlap integral between the BPA states is given by

$$O_n(\alpha_1\alpha_2\cdots\alpha_m;\beta_{m'}\beta_{m'-1}\cdots\beta_1) = \langle 0|(\Gamma)^{p'}\left(\prod_{i=1}^{m'} C_{\beta_{m'-i+1}}\right)\left(\prod_{i=1}^{m} C^\dagger_{\alpha_i}\right)(\Gamma^\dagger)^p|0\rangle$$
$$= (2)^{-(p+p')}\sum_{\substack{\alpha_{m+1},\alpha_{m+2},\ldots,\alpha_n\\ J_{\alpha_{m+1}},J_{\alpha_{m+3}},\ldots,J_{\alpha_{n-1}},J_{\beta_{m'+1}},J_{\beta_{m'+3}},\ldots,J_{\beta_{n-1}}}}\left(\prod_{\substack{i=m+1\\ \text{odd}}}^{n-1} Z_{J_{\alpha_i}}(\alpha_i,\alpha_{i+1})\right)$$
$$\times\left[\prod_{i=1}^{n-1}\mathbf{P}\left(\alpha_i,\prod_{j=i+1}^{n}\alpha_j\right)\right]\left(\prod_{\substack{i=m'+1\\ \text{odd}}}^{n-1} Z_{J_{\beta_i}}(\alpha_i,\alpha_{i+1})\right)\left(\prod_{i=1}^{m'}\delta_{\alpha_i\beta_i}\right), \tag{36}$$

with

$$n = 2p + m = 2p' + m', \tag{37}$$

and $m' \le m$ since in deriving Eq.(36) the variables $(\beta_{m'+1},\beta_{m'+2},\ldots,\beta_n)$ have been summed over. Equation (36) is a general overlap integral between the BPA states and is central to all the numerical calculations. Obviously an optimum algorithm is needed for the computation of this overlap integral. For instance, it is to be realized that most of the terms on the right-hand side of Eq.(36) when summed over the variables $(\alpha_{m+1},\alpha_{m+2},\ldots,\alpha_n)$ vanish since the terms with summation over any two repeated indices is not permitted by the Pauli principle. In the computer code the summation in Eq.(36) should therefore be restricted only to the antisymmetric combinations of the summed variables. For a fast processing of these antisymmetric configurations the bit manipulation technique as used in the Glasgow shell-model code[18] may need to be employed.

V. MATRIX ELEMENTS

In this section the various required matrix elements are expressed in terms of the overlap integral derived in the last section.

The overlap between the BPA ground state with n particles is given by

$$\langle\Phi_0|\Phi_0\rangle = N_0^2 O_n(0,0). \tag{38}$$

The overlap between the variational state $|\delta\Phi_0\rangle$ and the ground state $|\Phi_0\rangle$ is given by

$$\langle\Phi_0|\frac{\partial}{\partial X_{JM}(a_1a_2)}|\Phi_0\rangle = N_0^2\frac{n}{2}Y_{JM}\sum_{\alpha_1\alpha_2}\begin{bmatrix} j_{\alpha_1} & j_{\alpha_2} & J\\ m_{\alpha_1} & m_{\alpha_2} & M\end{bmatrix} O_n(\alpha_1\alpha_2,0) \tag{39}$$

and

$$\langle\Phi_0|\frac{\partial}{\partial Y_{JM}}|\Phi_0\rangle = N_0^2\frac{n}{4}\sum_{\alpha_1\alpha_2} X_{JM}(\alpha_1\alpha_2)O_n(\alpha_1\alpha_2,0). \tag{40}$$

Finally, we express the Hamiltonian matrix element

$\langle\Phi(\beta_{m'},\ldots,\beta_1)|H|\Phi(\alpha_1,\ldots,\alpha_m)\rangle$

$$
\begin{aligned}
&= N(\alpha_1\cdots\alpha_m)N(\beta_1\cdots\beta_m)\\
&\times\Bigg(\sum_{\alpha_{m+1}\beta_{m+1}}\epsilon_{a_{m+1}b_{m+1}}[\delta_{\alpha_{m+1}\beta_{m+1}}O_n(\alpha_1\cdots\alpha_m;\beta_1\cdots\beta_{m'})-O_{n+1}(\alpha_1\cdots\alpha_m\alpha_{m+1};\beta_1\cdots\beta_{m'}\beta_{m'+1})]\\
&\qquad\times\frac{1}{4}\sum_{\substack{\alpha_{m+1}\alpha_{m+2}\\ \beta_{m+1}\beta_{m+2}JM}}\begin{bmatrix} j_{\alpha_{m+1}} & j_{\alpha_{m+2}} & J\\ m_{\alpha_{m+1}} & m_{\alpha_{m+2}} & M\end{bmatrix}\begin{bmatrix} j_{\beta_{m+1}} & j_{\beta_{m+2}} & J\\ m_{\beta_{m+1}} & m_{\beta_{m+2}} & M\end{bmatrix}\\
&\qquad\times G_J(a_{m+1}a_{m+2}b_{m+1}b_{m+2})[\mathbf{P}(\alpha_{m+1}\beta_{m+1})\delta_{\alpha_{m+1}\beta_{m+1}}\delta_{\alpha_{m+2}\beta_{m+2}}O_n(\alpha_1\cdots\alpha_m;\beta_1\cdots\beta_{m'})\\
&-\mathbf{P}(\alpha_{m+1},\alpha_{m+2})\mathbf{P}(\beta_{m+1}\beta_{m+2})\delta_{\alpha_{m+2}\beta_{m+2}}O_{n+1}(\alpha_1\cdots\alpha_{m+1};\beta_1\cdots\beta_m\beta_{m+1})]\\
&+O_{n+2}(\alpha_1\cdots\alpha_m\alpha_{m+1}\alpha_{m+2};\beta_1\cdots\beta_m\beta_{m+1}\beta_{m+2})\Bigg).
\end{aligned}
\tag{41}
$$

VI. SUMMARY AND CONCLUSIONS

In the present work a broken pair approach has been developed to describe the high-spin band structures in rotating nuclei. This BPA space is a subspace of the full shell-model configuration space.

It is observed that the yrast configuration before the AB crossing is a fully paired state. For moderate deformations the dominant components in the paired state are the pairs coupled to angular momentum J=0, 2, and possibly 4. However, above the band crossings the yrast configuration is composed of the states with broken pairs. For example, in order to describe the AB crossing a pair is to be broken from the paired state. To take account of these facts a general broken pair state has been defined in Sec. II. The general overlap integral between the BPA basis states has been derived in Sec. IV, and the required matrix elements have been expressed in terms of this overlap in Sec. V.

To conclude we note that the present approach is an alternative shell-model formalism for studying the high-spin states in rotating nuclei. The present approach completely works in the real particle shell-model configuration space and therefore the particle number is intrinsic in the model.

It is to be added here that the general broken pair state defined in Eq.(12) does not have a definite angular momentum. The explicit angular momentum projection can be avoided by employing the cranking approximation. This is done simply by including a one-body term $-\omega J_x$ in the Hamiltonian. The problem of large angular momentum fluctuation[19] at the band crossings in the cranking approximation can be partially remedied in an angular momentum constrained cranking model.[20] This is achieved by using the cranking frequency ω as a Lagrangian multiplier in the Hamiltonian and varying it self-consistently with the constraint $\langle J_x\rangle = \sqrt{I(I+1)}$. The finer details, for example, the repulsion between the bands[21] may be sensitive to the approximation made for the angular momentum projection. Nevertheless, the angular momentum projection can be explicitly performed as in the MONSTER approach.[22] In the practical applications, however, the MONSTER basis is restricted to a condensate of pairs with axial symmetry, of which then only one or sometimes two pairs are broken. In contrast, in the present formalism no axial symmetry is assumed and hence explicit three-dimensional projection[23] is needed. Moreover, the number of broken pairs is not formally limited in the present approach. Of course, the possibility as to how many broken pairs are feasible in a particular problem is to be borne out of the calculations.

The explicit numerical calculations based on the present formulation are in progress and will be reported in the future.

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