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INS-Rep.-1046
Aug. 1994
W9437

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In order to describe collective rotational bands in the yrare region an approximate fixed configuration method is proposed within the Hartree-Fock-Bogoliubov (HFB) theory. It provides a HFB subspace to which variational principle is applied. An example of description of the ground- and S-bands of a deformed nucleus is shown.

Study of rotational bands of nuclei began along the *yrast line* [1], and now the study is developing to the *yrare region*. As a matter of course there are many excited states in the *yrare region*. Thus a problem arises how we can obtain efficiently wave functions of a rotational band which we want to understand. One of ways to treat this problem is to introduce some constraints, and it is emphasized that those constraints are deeply connected to physical understanding of the band, because the constraints influence output of calculation much.

One of such constraints to specify a rotational band is approximate fixed configuration which was developed in the cranked shell model [2]–[6]. That approach has also a merit that we can avoid at least phenomenologically a difficulty that ordinary solutions of the mean-field theory often give poor approximation in the neighborhood of band crossing or level crossing [7]–[9]. When such an approach is physically valid, it ought to be possible to define a HFB subspace which can be used as a trial space for variational calculation to obtain a rotational band in the *yrare region*. One of merits to define such a subspace is that it is straightforward to obtain self-consistent HFB wave functions without any significant modification for the conventional numerical method [10]. Thus the aim of this letter is to propose a new method of introducing a HFB subspace specified by an approximate fixed configuration, and to test its feasibility.

On the basis of the variational principle a collective rotational state in the constrained (C-) HFB theory [10] can be obtained by searching a HFB state which gives the minimum of an expectation value of Hamiltonian under the constraints for expectation values of the particle number and the component of the angular momentum along the rotational axis for which an axis perpendicular to a symmetry axis of a nucleus under consideration is usually used. When this approach is applied to a description of collective rotational states of a medium-heavy well-deformed even-even nucleus, usually a *yrast line* is obtained which consists of the ground band in a lower-angular-momentum region and the S-band in an upper-angular-momentum region. Difference in configuration of these two bands can be clearly seen in uv -factors which are calculated by applying the Bloch-Messiah theorem [11],[12] to a general Bogoliubov transformation from a ground state to another state in the *yrast line*. (An example will be shown later.) Thus our idea is to introduce a HFB subspace for each rotational band by considering a constraint to v -factors of a Bogoliubov transformation.

Next we explain a procedure. Here we take the ground band of a deformed even-even nucleus as an example. First of all we obtain the ground state $|\phi_0\rangle$ by use of the ordinary CHFB theory with the angular momentum $I=0$. Second we calculate the uv -factors of the transformation from $|\phi_0\rangle$ to another member of the band with $I\neq 0$, which is also obtained from the CHFB equation. Third we consider an upper limit $v_{\max}(I)$ to the v -factor $v_\alpha(I)$ and check whether an inequality

$$v_\alpha(I) \leq v_{\max}(I) , \quad (1)$$

is satisfied or not. How to determine this $v_{\max}(I)$ is the most important point in this method, and we shall discuss it in detail later. Fourth if the inequality (1) is not satisfied for one of single-particle levels α , then we resolve the variational equation of the CHFB theory under the additional constraint

$$v_\alpha(I) = v_{\max}(I) , \quad (2)$$

for the level α . Such a calculation can be done by making use of the gradient method [13],[14]. Detailed expressions will be given elsewhere. Thus the trial HFB subspace is defined by the constraint (1) in addition to usual constraints for the particle number and the angular momentum.

Our idea to determine $v_{\max}(I)$ is as follows: We consider a Bogoliubov transformation from the ground state to another CHFB state with $I \neq 0$ and make such a transformation that no clear configuration change is induced. Then we adopt a v -factor of the transformation for an intruder orbit close to the Fermi surface as $v_{\max}(I)$, because a significant change in an occupation probability of such an orbit is an origin of change in band structure of the yrast line. In order to make a transformation with such a property let us remind that a v -factor of the BCS transformation

$$V_{\alpha}^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\alpha} - \lambda}{\sqrt{(\epsilon_{\alpha} - \lambda)^2 + \Delta^2}} \right), \quad (3)$$

is a smooth and monotonically-decreasing function of a single-particle energy ϵ_{α} . Furthermore this property does not depend on a single-particle base used. Therefore as far as the property is concerned, distribution of V_{α}^2 for a cranked single-particle base with I which exceeds the band crossing region and that for a single-particle base with $I=0$ are expected to be similar to one another. Thus by combining a BCS transformation from a quasiparticle base associated with the ground state to the single-particle base and that from the single-particle base to a quasiparticle base associated with a CHFB state with $I \neq 0$, a transformation which induces no clear configuration change can be obtained. We define

$$\tilde{\epsilon}(I, j_{\text{intru}}^x) \equiv \epsilon_{j_{\text{intru}}^x} - \lambda(I) - I j_{\text{intru}}^x \hbar^2 / \mathcal{J}(I), \quad (4)$$

as a single-particle Routhian of an intruder orbit measured from the Fermi surface, where j_{intru}^x and $\epsilon_{j_{\text{intru}}^x}$ are a rotational-axis component of the angular momentum and an energy of the intruder orbit, respectively, and $\mathcal{J}(I)$ is a moment of inertia of the ground band. Using V_{α} with $\tilde{\epsilon}(0, j_{\text{intru}}^x)$ and that with $\tilde{\epsilon}(I, j_{\text{intru}}^x)$ and combining the two BCS transformations, we obtain

$$v_{\max}(I, j_{\text{intru}}^x)^2 = \frac{1}{2} \left(1 - \frac{\tilde{\epsilon}(0, j_{\text{intru}}^x) \tilde{\epsilon}(I, j_{\text{intru}}^x) + \Delta(I)^2}{\sqrt{(\tilde{\epsilon}(0, j_{\text{intru}}^x)^2 + \Delta(I)^2) (\tilde{\epsilon}(I, j_{\text{intru}}^x)^2 + \Delta(I)^2)}} \right). \quad (5)$$

Note that $v_{\max}(I, j_{\text{intru}}^x)$ in eq.(5) together with $\Delta(I)$, $\mathcal{J}(I)$ and $\lambda(I)$ should be determined self-consistently.

The starting point of the description of the S-band is chosen to be a CHFB state $|\phi(I_0)\rangle$ which has the minimum in fluctuation of the angular momentum of the S-band members. This means that the mean-field approximation is relatively good in $|\phi(I_0)\rangle$, and thus $|\phi(I_0)\rangle$ is suitable as the state to characterize the configuration of the S-band. The v -factor of the S-band is obtained for a transformation from $|\phi(I_0)\rangle$ to another state. $v_{\max}(I, j_{\text{intru}}^x)^2$ used for the S-band is generalized as

$$v_{\max}(I, I_0, j_{\text{intru}}^x)^2 = \frac{1}{2} \left(1 - \frac{\tilde{\epsilon}^S(I_0, I_0, j_{\text{intru}}^x) \tilde{\epsilon}^S(I, I_0, j_{\text{intru}}^x) + \Delta_S(I)^2}{\sqrt{(\tilde{\epsilon}^S(I_0, I_0, j_{\text{intru}}^x)^2 + \Delta_S(I)^2) (\tilde{\epsilon}^S(I, I_0, j_{\text{intru}}^x)^2 + \Delta_S(I)^2)}} \right), \quad (6)$$

$$\tilde{\epsilon}^S(I, I_0, j_{\text{intru}}^x) \equiv \epsilon_{j_{\text{intru}}^x}(I_0) - \lambda(I) - (I/\mathcal{J}_S(I) - I_0/\mathcal{J}_S(I_0)) j_{\text{intru}}^x \hbar^2, \quad (7)$$

where $\epsilon_{j_{\text{intru}}}^x(I_0)$ is defined in the same way as $\epsilon_{j_{\text{intru}}}^x$ except that $\epsilon_{j_{\text{intru}}}^x(I_0)$ is the single-particle Routhian with the angular velocity of $|\phi(I_0)\rangle$.

The Hamiltonian used here consists of the modified deformed harmonic oscillator [15] with $\delta = 0.29$, the doubly-stretched quadrupole force [16], the monopole and quadrupole pairing force. We modified to a small extent the theoretical value of the strength of the doubly-stretched quadrupole force of ref.[16] so as to reproduce the energy of the γ -vibration in the RPA. The strength of the monopole pairing force was determined from the odd-even mass difference [17]. As for the strength of the quadrupole pairing force we adopted the value of Hamamoto [18] multiplied by 0.9. Parameters of the modified harmonic oscillator were referred to from the textbook of Bohr and Mottelson [15]. For details of the Hamiltonian see ref. [17]. The space used in our calculation consists of 2 major shells with $N_{\text{osc}} = 4$ and 5 for the proton and 5 and 6 for the neutron, where N_{osc} is the total oscillator quantum number defined in the spherical harmonic oscillator.

Fig. 1 The energy of the ground- and S-bands of ^{164}Er as a function of the angular momentum I . Solid lines and open circles show the numerical and the experimental values [19],[20], respectively.

Fig. 2. Some v -factors squared for the positive parity neutrons, which are associated with the transformation from $|\phi_0\rangle$ to another HFB state. The upper shows those obtained by the ordinary CHFB theory for the yrast line. The middle illustrates $v_{\text{max}}(I, j_{\text{intru}}^x)^2$ of Eq. (5), and the lower is that obtained by our method for the ground band.

In Fig. 1 are shown the calculated and experimental energies of the ground- and S-bands of ^{164}Er . We show some $v_\alpha(I)^2$ in Fig. 2. The upper figure illustrates those for the positive parity neutrons obtained from the ordinary CHFB theory for the yrast line. It is clearly seen that a quasiparticle level is occupied almost completely around $I = 20$, and a configuration change takes place on the yrast line. The middle figure shows $v_{\max}(I, j_{\text{intru}}^x)^2$ given by Eq. (5). In the calculation of the ground band we imposed the constraint (1) on only the positive parity neutrons, because the other nucleons do not contribute to the band crossing. Actually we used two $v_{\max}(I, j_{\text{intru}}^x)$ for the positive parity neutrons in the ground band, i. e. one with $j_{\text{intru}}^x = 13/2$ and another one with $j_{\text{intru}}^x = 11/2$. This is because if we use only one $v_{\max}(I, j_{\text{intru}}^x)$, for $I \gtrsim 16$ degeneracy in the v -factor occurs. This causes a difficulty for convergence of the energy-minimum search under the constraints. $v_\alpha(I, j_{\text{intru}}^x)^2$ in the lower figure were obtained by our method for the ground band. By comparing these three figures it is seen that in the region of $I \lesssim 10$ our result is exactly the same as that of the ordinary CHFB theory. This is because in that region any of $v_\alpha(I, j_{\text{intru}}^x)^2$ of the ordinary CHFB theory does not exceed $v_{\max}(I, j_{\text{intru}}^x)^2$, while $v_{\max}(I, j_{\text{intru}}^x)^2$ plays a role to keep the configuration approximately in the region of $I \gtrsim 10$.

For the S-band I_0 was turned out to be 22. The “ v -constraint” is different for the regions of $I < 22$ and $I > 22$ in the S-band, because the band crossing with $I > 22$ is induced by the negative parity proton. Thus in the region of $I > 22$ the constraint (1) with $j_{\text{intru}}^x = 11/2$ was imposed on the negative parity protons, whereas in $I < 22$ the constraint with $j_{\text{intru}}^x = 13/2$ was imposed on the positive parity neutrons. For $\epsilon_{j_{\text{intru}}^x}(I_0)$ we averaged the two values of the positive and negative signature levels.

Fig. 3. The kinematical moment of inertia of the ground- and S-bands of ^{164}Er as a function of the angular velocity ω . Solid lines and open circles show numerical and experimental values, respectively. Upper and lower values are of the S-band and ground-band, respectively. A dashed line is calculated by using $v_{\max}(I, I_0, j_{\text{intru}}^x)$ multiplied by a factor 1.2 for $8 \leq I \leq 22$. The experimental data were obtained by using $J = (2I-1)\hbar^2/E_\gamma$ and $\hbar\omega = \sqrt{(I^2 - I + 1)}E_\gamma/(2I-1)$, [21] with an energy of in-band transition E_γ .

The kinematical moment of inertia of these bands are drawn in Fig. 3 as a function of the angular velocity ω . The lower curve and circles are those for the ground band, and the upper ones are for the S-band.

We have to mention a behavior of the kinematical moment of inertia of the S-band with $I = 8 - 10$. ($\omega \lesssim 0.10 \text{ MeV}/\hbar$) Calculated moment of inertia of the S-band at $I = 8$ is $156 \hbar^2/\text{MeV}$ with $\omega = 0.051 \text{ MeV}/\hbar$ and is much larger than the experimental data. For comparison we performed a calculation by use of $v_{\text{max}}(I, I_0, j_{\text{intru}}^x)$ multiplied by a factor 1.2 artificially and show a result in a dashed line in Fig.3. It is seen that an enhanced $v_{\text{max}}(I, I_0, j_{\text{intru}}^x)$ makes the moment of inertia of the S-band reduced. Thus in our method it is understood that configuration of states with $I = 8$ and 10 of the S-band is deviated from that of $I_0 = 22$.

In summary our method of introducing the HFB subspace specified by approximate fixed configuration supplies unperturbatively the HFB wave functions satisfying the self-consistency, which can well reproduce collective rotational bands. An investigation of collective rotational band on high- K isomer is in progress.

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