Rotational Symmetry and Collective Modes, in a Deformed Nucleus*

Lu LIN (林 騄)

Physics Department, National Central University, Chung-Li, Taiwan, Republic of China

(Received 10 April 1985)

A Microscopic approach is suggested which may be used to project good angular momentum states from a collective phonon type of wave-function.

*Work partially supported by the National Science Council of the Republic of China.

The eigenfunction of an isolated nuclear system must have a definite angular momentum, since the energy and the angular momentum of this system are commuting observables. Wave functions obtained in some well-known approximate methods do not have good angular momentum because of the violation of rotational symmetry. For instance, the single particle wave function obtained by the Hartree-Bogoliubov method does not possess the same symmetry property as the Hamiltonian of the system ’ , the microscopic phonon calculation using random-phase-approximation method based on Nilsson-BCS states ’ also does not conserve angular momentum.

A method for obtaining the wave function with good angular momentum was given by Peierls and Yoccoz[3] and has been discussed and applied to realistic calculations by many authors (see for instance, ref. 4, 5, 6, 7, 8). The Hartree-Bogoliubov theory with angular momentum projection developed by Onishi [4] results in an integral equation which is too difficult to solve. Other realistic calculations ’ [,6,7,8] are restricted to axially symmetrical wave functions or simply Nilsson BCS-type *wave* function. Also, they only considered the ground state band in a heavy deformed nucleus. Angular momentum projection for excited quasi-particle states was developed by Lin and Faessler[9,10,11], but the method can only be applied to calculations containing a small number of two-quasi-particle excited states, since the computing c.p.u. time increases in proportion to the square of the number of basic twoquasi-particle states (if $\psi = \sum_{i=1}^{N} \phi_i$ then $<\psi|H|\psi> = \sum_{i,j=1}^{N} <\phi_i|H|\phi_j>$). According to the method of Lin and Faessler[10], a single 2-quasi-particle excited state calculation will take four times the c.p.u. time needed for a ground state calculation with angular momentum projection, and even the ground state calculation is already known to be a time consuming program for the electronic computer. Because of this restriction, a largedimensional microscopic calculation, such as an angular momentum conserving calculation for an RPA phonon in a heavy deformed nucleus, vibrational states under strong rotational effect in the transition region, or a general Hartree-Bogoliubov calculation with angular momentum projection, is still numerically not feasible at the present day.

To resolve this difficulty, it would be ideal if we have two programs: a first program which can compute $<\phi|H|\phi>$ with a small amount of c.p.u. time, and a second program which can generate all the other $<\phi_i|H|\phi_k>$'s from a calculated $<\phi_0|H|\phi_0>$ with a small amount of c.p.u. time. In a recent paper[12]), the author has considered the first program and suggested a fast computational approximation method such that angular momentum projection can be easily and accurately performed for low-lying states with the Hartree-Bogoliubov type of wave function using a small amount of computer c.p.u. time. In the following, the method will extended to cover the second program assuming that the basic functions ϕ_i are Hartree-Bogoliubov wave functions with a canonical Nilsson BCS form, such that we can handle angular momentum projection for ,a collective state wave function $\psi = \Sigma\phi_i$ with a large number of components for low-lying states in a deformed nucleus.

In order to work out this method, we shall summarize the basic formalism for angular momentum projection (see for instance, ref. 10) and the main idea of ref. (12). In this work we assume that the nucleus has an axially symmetrical ground state with $K^\pi = 0^+$. The Hartree-Bogoliubov wave function can be written in the canonical representation as

$$|\phi> = \pi_{k>0} (u_k + v_k b_k^+ b_{\bar{k}}^+) |0> = (\pi_{k>0} u_k) \exp(\tfrac{1}{2} \Sigma f_{ik} b_i^+ b_k^+) |0> \quad (1)$$

where the f_{ik}'s can be expressed in matrix representation by the matrics U and V as

$$f_{ik} = (V \cdot U^{-1})_{ik} \quad (2)$$

The projected energy of state J is given as

$$E_J = \frac{\Sigma_{kk'} \int d\Omega\, D^{J*}_{kk'}(\Omega) <\phi|HR|\phi>}{\Sigma_{kk'} \int d\Omega\, D^{J*}_{kk'}(\Omega) <\phi|R|\phi>} = \frac{\Sigma_{kk'} \int d\Omega\, D^{J*}_{kk'}(\Omega)\, h(\Omega)}{\Sigma_{kk'} \int d\Omega\, D^{J*}_{kk'}(\Omega)\, n(\Omega)} \quad (3)$$

$$\left.\begin{aligned}
&\text{with } n(n) = (\det x(\Omega))^{1/2},\ x(\Omega) = U^T \cdot R(\Omega) \cdot U + V^T \cdot R(\Omega) \cdot V \\
&h(\Omega) = \frac{h(\Omega)}{n(\Omega)} \quad \Sigma_{k,i} T_{ki}\, \rho_{ik}(\Omega) + 1/2 \{ \Sigma_{i,j,k,l} V_{ijkl}\, \rho_{ji}(\Omega)\, \rho_{lk}(\Omega)\} \\
&\qquad + 1/4 \{ \Sigma_{i,j,k,l} V_{ijkl}\, \kappa_{lk}(\Omega)\, \sigma_{ji}(\Omega)\} \\
&\rho(\Omega) = R(\Omega) \cdot V \cdot X^{-1}(\Omega) \cdot V^T \\
&\kappa(\Omega) = \{R(\Omega) \cdot V \cdot X^{-1}(\Omega) \cdot U^T\}^T
\end{aligned}\right\} \quad (4)$$

$$\sigma(\Omega) = R(\Omega) \cdot U \cdot X^{-1}(\Omega) \cdot V^T$$

For an axially symmetric state with K = 0, all the expressions reduce to a dependence only on one Eulerian angle β(if $K \neq 0$, the projection method can be slightly modified by the method of Lin et al.[10] With K = 0, the matrix X can be easily shown to have the following form ·

$$X = \begin{pmatrix} \chi & \bar{\chi} \\ -\chi & \chi \end{pmatrix}, \text{ with } \chi_{ik} = (u_i u_k + v_i v_k) R_{ik}(\beta), \bar{\chi}_{ik} = \chi_{ik} \qquad (5)$$

$$X^{-1} \equiv Z = \begin{pmatrix} z & z \\ -\bar{z} & z \end{pmatrix}, \text{ with } z_{ik} = (\chi_{ik} + \bar{\chi}_{ij} \chi^{-1}_{jl} \bar{\chi}_{lk})^{-1} \qquad (6)$$

$$\text{and } \bar{z}_{ik} = - \bar{\chi}^{-1}_{ij} \bar{\chi}_{jl} z_{lk}$$

$$\text{and } \det X = (\det \chi) \det (\chi + \bar{\chi} \chi^{-1} \chi) \qquad (7)$$

The most time consuming part in the calculation is calculating $X^{-1}(\beta)$ and det(X) for many values of β. Usually, five values of β are calculated and an interpolation technique is introduced (see for instance, ref. 5,8). The first simplification introduced in this method is to approximate n(p) and $h(\beta)$ by

$$n(\beta) = n_o e^{-\alpha \sin^2 \beta}$$
$$n(\beta) = h_o e^{-\alpha' \sin^2 \beta} \qquad (8)$$

and then perform the integration in eq. (3) exactly. The result of the calculation reported in ref. (12) shows that this is a good approximation for low-lying states in a heavy deformed nucleus. Note that if the rotation operator and the $P_J(\cos\beta)$ in eq. (3) are expanded in β up to second order terms and then we integrate to get E_J, we can only obtain a spectrum of a pure rotor as discussed by Peierls and Yoccoz[3]. Here $n(\beta)$ and $h(\beta)$ are calculated for two values of β using eq. (4) to determine the constants in eq. (8). In eq. (8), n_o and h_o are the values of $n(\beta)$ and $h(\beta)$ at rotation angle $\beta = 0$, which are $< \phi|\phi >$ and $< \phi|H|\phi >$ in the un-rotated intrinsic frame (at $\beta = 0$, X becomes idagonal). It only takes very little c.p.u. time to compute them. Therefore, in doing the whole calculation, we only need to spend time in computing $n(\beta)$ and $h(\beta)$ for just one value of $\beta \neq 0$. (This can reduce the computing time by a factor of four in comparison to calculations done by Grümmer et al.[8] and Lin et al.[10]). If we choose a small enough β, such as 10^{-4}, then a power series expansion for X(p) and det $x(\beta)$ in eq. (4) could be used. From eq. (8), it is seen that we only need, for the expansion of the quantities in eqs. (5), (6) and (7), terms up to second order in β(with $\beta \sim 10^{-4}$ and the dimensionality of x about 30 to 60 for one major shell). Thus, for the quantities in eqs. (5), (6) and (7), we have the general form for a determinant

$$\det(X) = \left(\prod_i X_{ii}\right)\left(1 - \sum_{\substack{i,j \\ i\neq j}} \frac{X_{ij}X_{ji}}{X_{ii}X_{jj}}\right), \tag{9}$$

and for a matrix

$$X^{-1} = (X_{ii} + X_{ij})^{-1} = X_{ii}^{-1} - X_{ii}^{-1}X_{ij}X_{jj}^{-1} + \frac{X_{ij}X_{jk}}{X_{ii}X_{jj}X_{kk}} \tag{10}$$

where $X_{ii} >> X_{ik}$ for $i \neq k$. In eq. (10), the last term may or may not be needed, it depends on the order of magnitude of the X_{ik}'s. This treatment reduces the c.p.u time used in computing $X^{-1}(\beta)$ and det $X(\beta)$ by a factor of about eight. Thus we have a time-saving method which can reduce computing time for $X^{-1}(p)$ and det $X(p)$ by a factor of about 32.

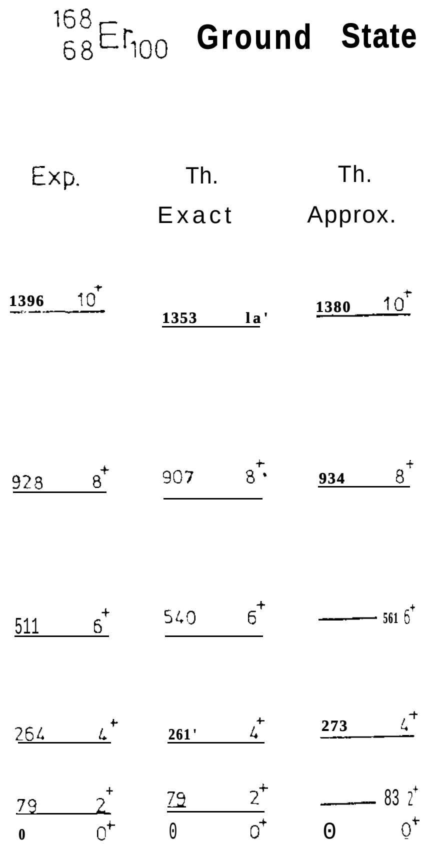

FIG. 1. The ^{168}Er ground state band energies from the approximation method compared with the exact calculation and with experiment.

results. To demonstrate this, we apply the method, without borrowing parameters from other calculations, to perform a larger calculation, repeating the work of ref. (1 1) including the ground state band and the two 0^+ excited bands in ^{168}Er. The calculated results are shown in Fig. 2 together with the experimental comparison. From this figure, we can see that the agreement between the calculated and experimental energies are almost as good as those in ref. (11) where the exact calculation was performed. On the other hand, the parameters used here differ only slightly from those used in ref. (1 1). More percisely, the constants used here are 17.5/A, 24/A, $80.5\alpha_\tau\alpha_{\tau'}A^{-1.4}$ and 18.533 for G_N, G_p, χ and $2\theta_0/\hbar^2$ (for the effective core) respectively, while in ref. (1 1), they are 17.41/A, 24/A, $76\alpha_\tau\alpha_{\tau'}A^{-1.4}$ and 16.5438.

The simple picture of the present approximation method can be understood in the following way: For the low-lying nuclear rotational states in deformed nuclei, the high-order terms in the expansion of the energy integral are small and do not produce a significant contribution to the calculation. The small effects introduced by neglecting these terms in the calculation can be absorbed in the slightly renormalized parameters" .

In considering the second part of this method, we write the total wavefunction with a good K as:

$$\psi = \sum_{A=1}^{M} f_A \phi_A \qquad (11)$$

where M is the number of excited quasi-particle states contained in ψ. An excited quasi-particle state is a state containing an even number of excited quasi-particles. Let us denote the set of Nilsson single-particle states by $(\alpha, \beta, \ldots.)$. Among them, we use $(\mu, \nu, \ldots.)$ for the excited slingle-particle states in a component ϕ_A, and (i, j, k,. ...) for those remained un-excited. (For instance, a two-quasi-particle excited state can be written as $a^+_\mu a^+_\nu|\phi_0\rangle$ with a^+ the quasi-particle creation operator.) The method of angular momentum for excited states with an even number of quasi-particles has been formulated by Lin et al.[9,10] simply by redefining the matrices U and V. The projected energy F of ψ can thus be written as

$$E_J = \frac{\int d\Omega\, D^{J*}_{kk}(\Omega)\langle\psi|HR|\psi\rangle}{\int d\Omega\, D^{J*}_{kk}(\Omega)\langle\psi|R|\psi\rangle} = \frac{\int d\Omega\, D^{J*}_{kk}(\Omega)\{\sum_{AB} f_A f_B\, n^{AB}(\Omega\, j\, h^{AB}(R)\}}{\int d\Omega\, D^{J*}_{kk}(\Omega)\{\sum_{AB} f_A f_B\, n^{AB}(\Omega)\}} \qquad (12)$$

From ref. (9),(10), we have

$$n^{AB}(\Omega) = \{\det(X^{AB}_{\alpha\beta})\}^{1/2} = \{\det(X_{ik})\cdot\det(X_{\mu\nu} - X_{\mu j}X^{-1}_{jl}X_{l\nu})\}^{1/2}$$
$$\equiv \{\det(X_{ik})/\det(Z_{\mu\nu})\}^{1/2} \qquad (13)$$

where and

$$X^{AB}_{\alpha\beta} = \begin{vmatrix} X_{ik} & X_{i\nu} \\ X_{uk} & X_{u\nu} \end{vmatrix} \qquad \left(X^{AB}_{\alpha\beta}\right)^{-1} \equiv Z^{AB}_{\alpha\beta} = \begin{pmatrix} Z_{ik} & Z_{i\nu} \\ Z_{\mu k} & Z_{\mu\nu} \end{pmatrix} \qquad (14)$$

In drder to determine the degree of accuracy of this approximation method, we applied it to a calculation of the ground statk band of ^{168}Er and compared the results with the exact calculation done by Lin et al. " . For the input parameters, we take exactly those from the work of ref. (11). The results of the two theoretical calculations together with the experimental data[13] for low-lying states are shown in Fig. 1. From the figure, it is seen that the moment of inertia calculated by the present approximation deviates from that of exact calculation only by a small amount (about 2.5% of the total moment of inertia). This shows that the method proposed here is a good approximation to the exact calculation for low-lying states in deformed nuclei.

In doing actual calculations, the coupling constants in a theoretical model are usually chosen to reproduce experimentally observed quantities such as the even-odd mass difference, the pairing gap energies and the energy of the first 2^+ state, etc. With this new method, we have an additional problem, namely that of determining the coupling constants. However, we do not want to perform an exact calculation to find the coupling constants every time we use the approximation method. That is, the new method should have a seif-consistent way of choosing reasonable parameters as well as producing good

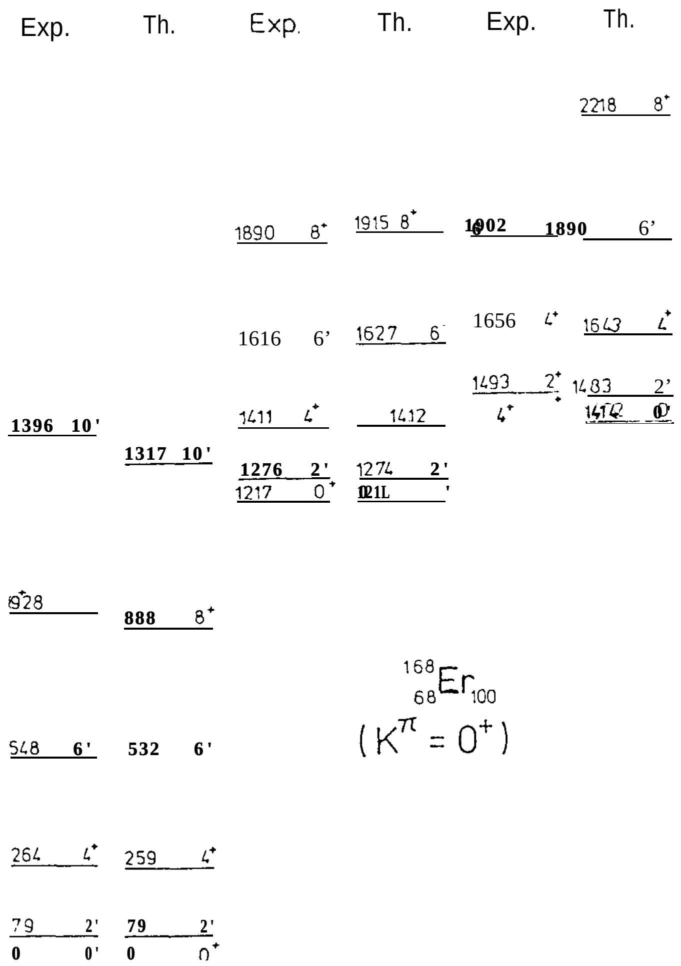

FIG. 2. Comparison of the calculated energies with experiment for the ground state band and $K=0^+$ excited bands in ^{168}Er.

we can write n^{AB} as

$$n^{AB}(\Omega) = n^{OO}(\Omega)\{\det(Z_{i'k'})/\det(Z_{\mu\nu})\}^{1/2} \equiv n^{OO}(\Omega)\bar{n}^{AB}(\Omega) \qquad (15)$$

where $n^{OO}(\Omega) = \langle\Phi_O|R(\Omega)|\Phi_O\rangle$ as defined in eq. (4), $Z_{i'k'}$ is a small matrix constructed from rows and columns in $Z^{OO}(\Omega)$ which correspond to those of $Z_{\mu\nu}$ in $Z^{AB}(\Omega)$. Therefore, $\bar{n}^{AB}(\Omega)$ contains only a small number of terms and can be easily computed out. Thus we have

$$\langle\psi|R(\Omega)|\psi\rangle = n^{OO}(\Omega)\{\sum_{AB} f_A f_B n^{AB}(\Omega)\} \qquad (16)$$

Concerning the energy kernel $\langle\psi|HR|\psi\rangle$, we shall only outline the main idea of the method here. The detailed formulation will be worked out in a seperated paper and published elsewhere. The criterion of treating this part is to seperate $\bar{h}^{AB}$ into the form

$$\bar{h}^{AB} = \bar{h}^{OO} + 2\bar{h}^{O}\bar{h}'^{AB} + (\bar{h}'^{AB})^2 \qquad (17)$$

where $\bar{h}'^{AB}$ contains only a small number of terms and can be computed easily. To do this, let us consider, for instance, the density matrix $\rho_{\alpha\beta}$, we have

$$\rho(\Phi,\Phi',\beta) = R(\beta)\, V'\, \{\tilde{U}R(\beta)U' + \tilde{V}R(\beta)V'\}^{-1}\, V\,. \qquad (18)$$

When the angle β is small, it is useful to write $R(\theta)$ in the form $R = 1\!\!1 + \epsilon$, where $\epsilon_{ii} = R_{ii} - 1$ and $\epsilon_{ij} = R_{ij}$ for $i \neq j$. Thererore we have

$$\rho(\Phi,\Phi',\beta) = R(\beta)V'\{(\tilde{U}U' + \tilde{V}V') + \tilde{U}\epsilon U' + \tilde{V}\epsilon V'\}^{-1}\tilde{V}$$
$$\equiv R(\beta)V\{S + \tilde{U}\epsilon U + \tilde{V}\epsilon V\}^{-1}\tilde{V} \qquad (19)$$

where S is a diagonal matrix, or can put into a diagonal form by changing some rows and columns. The order of magnitude of Sij is one, and all the other elements in ρ are small quantities. According to the arguments above, we can expand ρ in terms of β and we need to keep terms up to second order.

Next, we realize that $\rho(\Phi^A,\Phi^B,\beta)$ differs from $\rho(\Phi^O,\Phi^O,\beta)$ only by the matrices U, V and S. We can write

$$U(\Phi^A), V(\Phi^A), S(\Phi^A) = U(\Phi^O) + U'(\Phi^A), V(\Phi^O) + V'(\Phi^A), S(\Phi^O) + S'(\Phi^A) \qquad (20)$$

where $U(\Phi^A), V(\Phi^A), S(\Phi^A) = U(\Phi^A) - U(\Phi^O), V(\Phi^A) - V(\Phi^O), S(\Phi^A) - S(\Phi^O)$, all of these terms have small dimensionalities and contain only a few elements which are not zero. Thus we can write

$$\rho(\Phi^A, \Phi^B, \beta) = \rho(\Phi^o,\Phi^o,\beta) + \rho'(\Phi^A, \Phi^B, \beta) \tag{21}$$

where $\rho'(\Phi^A, \Phi^B, \beta)$ contains only a small number of terms, and we can easily compute them out with a small amount of effort. Terms involving κ and σ are easier than those for the p's and can be done in a similar manner. Finally we have

$$< \psi | HR(\beta) | \psi > = n^{oo}(\beta) \quad h^{oo}(\beta) \sum_{AB} n^{AB}(\beta) f_A f_B + 2 h^o(\beta) \sum_{AB} n^{AB} f_A f_B h'^{AB}$$

$$+ \sum_{AB} n^{AB} f_A f_B (h'^{AB})^2 \tag{22}$$

This looks promising that the calculation could be carried out without too much trouble.

REFERENCES

1. M. Baranger, The 1962 Cargèse Lectures in Theor. Physics, ed. M. Levy (Benjamin, N.Y., 1963)
2. T.S. Dumitrescu and I. Hamamoto, Nucl. Phys. A383 (1982) 205
3. R.E. Peierls and J. Yoccoz, Proc. Phys. Soc. 170 (1957) 381
4. N. Onishi, Prog. Theor. Phys. Jap. 40 (1968) 84
5. N. Onishi, R.K. Sheline and S. Yoshida, Phys. Rev. C2 (1970) 1304
6. K. Goeke, A. Faessler and H.H. Wolter, Nucl. Phys. Al83 (1972) 352
7. A. Faessler, L. Lin and F. Wittmann, Phys. Lett. 44B (1973) 366
   A. Faessler, F. Griimmer, L. Lin and J. Urbano, Phys. Lett 48B (1974) 87
8. F. Griimmer, K.W. Schmid and A. Faessler, Nùcl. Phys. A239 (1975) 289
9. L. Lin and A. Faessler, Phys. Lett. 78B (1978) 533
   L. Lin and A. Faessler, C.J. Phys. 19 (1981) 9
10. L. Lin, A. Faessler and R.M. Dreizler, Nucl. Phys. A318 (1979) 287
11. L. Lin, S.Y. Lee, S.F. Tsai and H.T. Chen, J. Phys. G:Nucl. Phys. 9 (1983) L223
12. L. Lin, Nucl. Phys. A431 (1984) 230
13. W.F. Davison, D.D. Warner, R.F. Casten, K. Schreckenbach, H.G. Borner, J. Simic, M. Stojanovic, M. Bogdanovic, S. Koicki, W. Gelletly, G.B. Orr and M.L. Stelts, J. Phys. G7 (1981) 455; 843