

## Self-Consistent Perturbation of Hartree-Fock-Bogoliubov Equations and Nuclear Rotational Spectra.\* I

EUGENE R. MARSHALEK

*Brookhaven National Laboratory, Upton, New York*

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The effect of a single-particle perturbation on the Hartree-Fock-Bogoliubov equations is considered. Corrections to the ground-state wave function, density matrix, and pairing tensor are obtained through third order, thus determining the energy through fourth order. The results are applied to rotational spectra of even-even atomic nuclei, in which the nucleons interact via pairing and quadrupole forces, and the single-particle perturbation is the Coriolis force in a rotating frame of reference. The energy levels of the ground-state band are obtained to order  $I^2(I+1)^2$  in the angular momentum. It is shown that the coefficient of the  $I^2(I+1)^2$  term contains contributions arising from centrifugal stretching of the self-consistent quadrupole field, and having the expected form of a rotation-vibration interaction. In addition, however, the coefficient contains terms arising from the Coriolis unpairing effect and also terms arising from the influence of the Coriolis force on independent quasiparticle motion. Approximate numerical estimates indicate that the contribution from the Coriolis unpairing is far greater than from the beta vibration-rotation interaction.

### I. INTRODUCTION

IT is well-known that the spectra of nonspherical atomic nuclei in the mass regions  $A \approx 24$ ,  $150 \leq A \leq 188$ ,  $A > 224$  display low-lying collective rotational bands.<sup>1,2</sup> The rotational interpretation is based on several criteria. For example, among the characteristics are the spin sequence and parity of the levels, such as  $I=0+$ ,  $2+$ ,  $4+$ ,  $\dots$ , for the ground-state band of even-even nuclei; the highly enhanced  $E2$  transition rates with branching ratios conforming approximately to ratios of Clebsch-Gordan coefficients; and other multipole radiation properties. But the prime characteristic is that energies within a band can be fitted by the expansion

$$E_I = (\hbar^2/2\mathcal{I})I(I+1) + \mathcal{B}I^2(I+1)^2 + \mathcal{C}I^3(I+1)^3 + \dots, \quad (1)$$

where  $I$  is the angular-momentum quantum number, and  $\mathcal{I}$  is called the moment of inertia. The higher powers of  $I(I+1)$  are expected for any quantized nonrigid rotating body.

Of course, one can fit almost any spectrum by choosing suitable values for the parameters  $\mathcal{I}$ ,  $\mathcal{B}$ ,  $\mathcal{C}$ , etc. But the expansion (1) characterizes a set of rotational states if the coefficient  $\hbar^2/2\mathcal{I}$  is much larger than  $\mathcal{B}$  and the higher order coefficients. This condition is generally satisfied, except, perhaps, at the boundaries of the regions of deformed nuclei.<sup>3</sup> As higher angular-momentum members of a band are found, additional terms must be added to Eq. (1) to obtain an exact fit, the coefficients of these terms being much smaller than preceding coefficients. Moreover, as additional terms are added to Eq. (1), the experimental estimates of the lower order coefficients are slightly modified.<sup>4</sup> Thus,

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<sup>1</sup> K. Alder, A. Bohr, T. Huus, B. Mottelson, and A. Winther, *Rev. Mod. Phys.* **28**, 432 (1956).

<sup>2</sup> B. R. Mottelson and S. G. Nilsson, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Skrifter* **1** (1959), No. 8.

<sup>3</sup> The parameter  $\hbar^2/(2\mathcal{I})$  is typically of the order of magnitude of 10 keV, and  $-\mathcal{B}$  is 10 eV, in the rare-earth region, for example.

<sup>4</sup> J. S. Greenberg, G. G. Seaman, E. V. Bishop, and D. A. Bromley, *Phys. Rev. Letters* **11**, 211 (1963).

high-angular-momentum members of a band must be known to get really accurate values of the lower order coefficients, and such data are now accumulating.<sup>5,6</sup>

At the present time, spins as high as  $I=20$  have been excited. It would be desirable, therefore, to have a theory which predicts the parameters in Eq. (1) and also tells us at what angular momentum the expansion (1) ceases to converge [and therefore fitting of data by means of Eq. (1) becomes meaningless].

In the present work, an expansion of the rotational energy in powers of the angular momentum is developed by studying rotating solutions of the Hartree-Fock-Bogoliubov (HFB) equations,<sup>7,8</sup> which combine Hartree-Fock averaging of two-body interactions together with superconductor pairing effects of the type considered by Bardeen, Cooper, and Schrieffer (BCS).<sup>9</sup> We shall focus particularly on the  $\mathcal{B}$  coefficient in Eq. (1), since the problem of obtaining  $\mathcal{I}$  has been widely studied. First, however, related work on the problem will be reviewed.

### Phenomenological Collective Model

The collective model of Bohr and Mottelson provides an expansion of the form (1).<sup>10</sup> The deviations from the  $I(I+1)$  term arise from vibration-rotation interactions between bands both in even-even and in odd nuclei, but in the latter case there are additional contributions due to Coriolis mixing of bands.<sup>11</sup> In the case of even-even spheroidal nuclei, to which we will restrict ourselves in this paper, a perturbation calculation of the

<sup>5</sup> F. S. Stephens, N. Lark, and R. M. Diamond, *Phys. Rev. Letters* **12**, 225 (1964).

<sup>6</sup> J. deBoer, G. Goldring, and H. Winkler, *Phys. Rev.* **134**, B1032 (1964).

<sup>7</sup> N. N. Bogoliubov, *Usp. Fiz. Nauk*, **67**, 549 (1959) [English transl.: *Soviet Phys.—Usp.* **2**, 236 (1959)].

<sup>8</sup> M. Baranger, *Phys. Rev.* **122**, 992 (1961).

<sup>9</sup> J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).

<sup>10</sup> A. Bohr and B. R. Mottelson, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **27**, No. 16 (1953).

<sup>11</sup> A. K. Kerman, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **30**, No. 15 (1956).

vibration-rotation interaction gives the following value for the  $\mathfrak{B}$  coefficient of the ground-state band to lowest order<sup>12</sup>:

$$\mathfrak{B} = -\frac{1}{8} \frac{\hbar^4}{g^4} \left( \frac{\partial g}{\partial \beta} \right)^2 \frac{1}{C_\beta} - \frac{1}{8} \frac{\hbar^4}{g^4} \left( \frac{\partial g}{\partial \gamma} \right)^2 \frac{1}{C_\gamma}. \quad (2)$$

The quantity  $C_\beta$  is the force constant for  $\beta$  vibrations, which have an angular momentum projection on the nuclear symmetry axis of  $K=0$ , and  $C_\gamma$  is the force constant for  $\gamma$  vibrations, for which  $K=2$  (for one-phonon vibrations). The first term in Eq. (2) arises from the interaction of the ground-state band with the one-phonon  $\beta$ -vibrational band, and the second from the interaction with the one-phonon  $\gamma$ -vibrational band. The derivatives of the moment of inertia are evaluated at the equilibrium distortions  $\beta=\beta_0$ ,  $\gamma=0$ .

It should be noted that a higher order perturbation calculation of the vibration-rotation interaction would give, not only the higher powers of  $I(I+1)$ , but also additional terms to the estimate (2), as well as to the moment of inertia, which is already slightly renormalized by the lowest order treatment of the vibration-rotation interaction. These renormalizations are expected to be small for the ground-state band, except possibly at the boundaries of regions of deformed nuclei.<sup>13</sup>

In Eq. (2), no assumptions have been made about the dependence of  $g$  on  $\beta$  and  $\gamma$ . In the early version of the collective model, the moment of inertia was given by<sup>10</sup>

$$g = 4B\beta^2 \sin^2(\gamma - 2\pi/3), \quad (3)$$

where  $B$  is the vibrational mass parameter, assumed to be the same for  $\beta$  and  $\gamma$  modes. Using Eq. (3) and the definition of the mass parameter

$$B = C_\beta / \omega_\beta^2 = C_\gamma / (\omega_\gamma^2 \beta_0^2), \quad (4)$$

where  $\omega_\beta$  and  $\omega_\gamma$  are the frequencies of  $\beta$  and  $\gamma$  vibrations, respectively, one gets for Eq. (2)<sup>10</sup>

$$\mathfrak{B} = -\frac{1}{18} \left( \frac{3\hbar^2}{g} \right)^3 (\hbar\omega_\beta)^{-2} - \frac{1}{54} \left( \frac{3\hbar^2}{g} \right)^3 (\hbar\omega_\gamma)^{-2}. \quad (5)$$

Equation (5) provides the correct trends and sign, and predicts that the  $\gamma$ -vibrational contribution to  $\mathfrak{B}$  is smaller than the  $\beta$ -vibrational one, which is consistent with present experimental data. However, the magnitudes predicted by Eq. (5) are always greater than experimental values, on the average by a factor of 2.5.

Faessler and Greiner have attempted to treat the vibration-rotation interaction within the framework of the phenomenological model, using assumptions (3)

and (4), by a nonperturbation method and claim good agreement with experimental energies.<sup>14,15</sup> Their energies can be expanded in the form (1) for sufficiently low values of  $I$ , and ostensibly can be applied to high angular-momentum states, when perturbation theory is not valid. Their equation for  $\mathfrak{B}$  contains corrections to Eq. (5), the aforementioned renormalizations which apparently are not so small *in toto*, as the magnitudes of  $\mathfrak{B}$  agree fairly well with experiment, in contrast to Eq. (5). However, the authors have inconsistently neglected higher order vibration-rotation terms arising from an expansion of the reciprocal moments of inertia in powers of  $\beta$  and  $\gamma$ , these terms possibly being of the same order of magnitude as those taken into account. Moreover, the validity of expanding the moments of inertia in powers of the deformation parameters is questionable for large values of  $I$ . Another deficiency is neglect of anharmonic terms in the vibrational Hamiltonian which would give rise to contributions to Eq. (1).

There are additional conceptual difficulties with the above, and other similar phenomenological treatments. First of all, Eqs. (3) and (4) are not correct for strongly deformed nuclei, but only for nuclei deviating slightly from a spherical shape, as is clear from the work of Bohr and Mottelson.<sup>10</sup> For strongly deformed nuclei, one has, in general, different mass parameters  $B_\beta$  and  $B_\gamma$  for  $\beta$  and  $\gamma$  vibrations.<sup>16</sup> If the equilibrium deformation parameter  $\beta_0$  is large, higher order terms may become important. Moreover, the identification of the constant  $B$  in Eq. (3) with a vibrational mass parameter cannot be correct when the vibrations are not adiabatic compared to single-particle excitations, which is often the case.<sup>17</sup>

One can attempt to deduce the mass parameters  $B_\beta$  and  $B_\gamma$  from measured reduced quadrupole transition probabilities by using the equations<sup>12</sup>

$$B(E2; 0 \rightarrow 2+)'_{\gamma \text{ band}} = \left( \frac{3}{4\pi} ZeR_0^2 \right)^2 \beta_0^2 \hbar (B_\gamma \omega_\gamma)^{-1} (1 - 2\hbar^2 / (g\hbar\omega_\gamma))^2, \quad (6a)$$

$$B(E2; 0 \rightarrow 2+'' )_{\beta \text{ band}} = \left( \frac{3}{4\pi} ZeR_0^2 \right)^2 \times \frac{1}{2} \hbar (B_\beta \omega_\beta)^{-1} (1 - 6\hbar^2 / (g\hbar\omega_\beta))^2. \quad (6b)$$

Equation (6a) is the reduced transition probability from the ground state to the  $2+$  member of the  $\gamma$ -vibrational band, and Eq. (6b) refers to the corresponding transition to the  $\beta$ -vibrational band.<sup>18</sup> These equations

<sup>12</sup> B. L. Birbrair, L. K. Peker, and L. A. Sliv, Zh. Eksperim. i Teor. Fiz. **36**, 803 (1959) [English transl.: Soviet Phys.—JETP **9**, 566 (1959)].

<sup>13</sup> The renormalizations involve quantal zero-point corrections, while Eq. (2) is valid even for a classical vibration-rotation interaction.

<sup>14</sup> A. Faessler and W. Greiner, Z. Physik **168**, 425 (1962).

<sup>15</sup> A. Faessler and W. Greiner, Z. Physik **177**, 190 (1964).

<sup>16</sup> A. K. Kerman, Ann. Phys. (N. Y.) **12**, 300 (1961).

<sup>17</sup> Equations (3) and (5) are not necessarily hydrodynamic, as is often stated, unless hydrodynamic values of  $B$  and  $\hbar\omega$  are used.

<sup>18</sup> The factor  $[(3/4\pi)ZeR_0^2]^2$  depends on the assumption of a uniform charge distribution, which is only approximately correct.

include a correction for vibration-rotation band mixing in lowest order, corresponding to Eq. (2).

One finds that the values of  $B_\beta$  and  $B_\gamma$  thus obtained exceed  $\mathcal{J}_0/3\beta_0^2$  [Eq. (3) is evaluated at  $\beta=\beta_0$ ,  $\gamma=0$ ] by a factor of 3 to 4. Direct theoretical calculations using a random phase approach (RPA) also yield values of  $B_\beta$  and  $B_\gamma$ , which are not equal and greatly exceed  $\mathcal{J}/3\beta_0^2$ , especially when the vibrations are not adiabatic.<sup>19</sup>

As a final point, it should be noted that additional corrections to Eq. (2) are expected which are unrelated to band mixing, even within the framework of the phenomenological model, if all the terms of the Hamiltonian to a given order are included. For example, Bohr and Mottelson omit anharmonic quartic terms in the collective dynamic variables defined relative to the laboratory system.<sup>10</sup> Since the quadratic terms in the time derivatives of these variables give rise to the term  $(\hbar^2/2\mathcal{J})(\hat{I}^2 - \hat{I}_3^2)$  in the Hamiltonian expressed in collective variables of the nuclear reference frame, the quartic terms in the time derivatives would be expected to give rise to terms proportional to  $(\hat{I}^2 - \hat{I}_3^2)^2$  which would contribute to the  $\mathcal{B}$  coefficient. These contributions, which do not arise from band mixing, will be called "intrinsic" contributions. They cannot be estimated without a microscopic description, unless irrotational hydrodynamics is assumed, which might be worthwhile for a rough estimate.

Since it is now possible to sort out the separate band-mixing contributions to the  $\mathcal{B}$  and other coefficients, by measuring branching ratios between members of the ground-state and vibrational bands,<sup>20,21</sup> it is important to have a satisfactory microscopic theory of collective rotation and vibration to complement the deficiencies of the phenomenological models.

### Previous Microscopic Approaches

The discussions of nuclear rotation are far too numerous to recount here. But the most successful approaches have been based on the cranking model, or on the time-dependent self-consistent field method, which is essentially a self-consistent cranking model. Beliaev first derived an expression for the moment of inertia, including BCS pairing effects, by cranking independent quasiparticles,<sup>22</sup> and Griffen and Rich<sup>23</sup> and Nilsson and Prior<sup>24</sup> showed that this formula agreed well with experimental moments of inertia.

Thouless and Valatin,<sup>25</sup> Valatin,<sup>26</sup> and Brown<sup>27</sup> dis-

cussed the self-consistent cranking model, showing that the Hartree-Fock equations contained solutions corresponding to a rotating deformed average field. Pairing correlations can be included by using the HFB equations which are applied to the rotational problem by Prange,<sup>28</sup> Beliaev,<sup>29</sup> Katz and Blatt,<sup>30</sup> Katz,<sup>31</sup> Thouless and Valatin,<sup>32</sup> and others.<sup>33</sup> These authors obtained additional, but apparently small, corrections to the original Beliaev cranking formula. The approach of the present paper is a systematic extension of this work to obtain higher order corrections to rotational spectra.

The first attempts at obtaining the  $\mathcal{B}$  coefficient were made by Grin',<sup>34</sup> Grin' and Pavlichenkov,<sup>35</sup> Hemmer,<sup>36</sup> and Radojević *et al.*<sup>37</sup>

Radojević *et al.* proposed that the  $\mathcal{B}$  coefficient should be calculated from Eq. (2) by substituting the cranking model expressions for  $\mathcal{J}$ ,  $C_\beta$ , and  $C_\gamma$ .<sup>37</sup> Pairing effects can be included by using Beliaev's moment of inertia, and the elasticity constants of the type calculated by Kisslinger and Sorensen<sup>38</sup> and Bes.<sup>39</sup> The moment of inertia depends on  $\beta$  and  $\gamma$  through the deformed single-particle potential. These authors calculated the  $\gamma$ -vibrational contribution to Eq. (2) by this prescription for a few cases and obtained fair agreement with experiment. However, no justification was given for this procedure, which will be shown later to be approximately correct for the vibration-rotation contribution to  $\mathcal{B}$ .

Hemmer presented a self-contained derivation of an  $I^2(I+1)^2$  correction to the rotational energy, by extending the cranking model.<sup>36,40</sup> In this derivation, the equilibrium deformation of the cranked potential is allowed to change until the centrifugal force balances the restoring force, which arises from an incompressibility constraint on the potential, of the type used by Nilsson.<sup>41</sup> The rotational stretching of the deformation parameter  $\beta$ , corresponding to a semiclassical descrip-

<sup>19</sup> J. G. Valatin, in *Lectures in Theoretical Physics* (Interscience Publishers, Inc., New York, 1962), Vol. IV, p. 1.

<sup>20</sup> G. E. Brown, in *Lectures on the Many-Body Problem from the First Bergen International School of Physics 1961*, edited by C. Fronsdaal (W. A. Benjamin, Inc., New York, 1962), p. 164.

<sup>21</sup> R. E. Prange, *Nucl. Phys.* **22**, 283 (1961).

<sup>22</sup> S. T. Beliaev, *Nucl. Phys.* **24**, 322 (1961).

<sup>23</sup> A. Katz and J. M. Blatt, *Nucl. Phys.* **23**, 612 (1961).

<sup>24</sup> A. Katz, *Nucl. Phys.* **26**, 129 (1961).

<sup>25</sup> D. J. Thouless and J. G. Valatin, *Nucl. Phys.* **31**, 211 (1962).

<sup>26</sup> The various authors used superficially different but, in fact, equivalent versions of the HFB theory.

<sup>27</sup> Yu. T. Grin', *Zh. Eksperim. i Teor. Fiz.* **41**, 445 (1961) [English transl.: *Soviet Phys.—JETP* **14**, 320 (1962)].

<sup>28</sup> Yu. T. Grin' and I. M. Pavlichenkov, *Zh. Eksperim. i Teor. Fiz.* **43**, 465 (1962) [English transl.: *Soviet Phys.—JETP* **16**, 333 (1963)].

<sup>29</sup> P. C. Hemmer, *Nucl. Phys.* **32**, 128 (1962).

<sup>30</sup> V. Radojević, A. Sobiczewski, and Z. Szymański, *Nucl. Phys.* **38**, 607 (1962).

<sup>31</sup> L. S. Kisslinger and R. A. Sorensen, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **32**, No. 9 (1960).

<sup>32</sup> D. R. Bés, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **33**, No. 2 (1961).

<sup>33</sup> A similar unpublished result is alluded to in Ref. 19.

<sup>34</sup> S. G. Nilsson, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **29**, No. 16 (1955).

<sup>19</sup> E. R. Marshalek, thesis, UCRL-10046, 1962 (unpublished).

<sup>20</sup> O. B. Nielsen, in *Proceedings of the Rutherford Jubilee International Conference, Manchester* (Heywood and Company, Ltd., London, 1961), p. 317.

<sup>21</sup> Y. Yoshizawa, B. Elbek, B. Herskind, and M. Olesen, *Nucl. Phys.* (to be published).

<sup>22</sup> S. T. Beliaev, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **31**, No. 11 (1959).

<sup>23</sup> J. J. Griffen and M. Rich, *Phys. Rev.* **118**, 850 (1960).

<sup>24</sup> S. G. Nilsson and O. Prior, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **32**, No. 16 (1961).

<sup>25</sup> D. J. Thouless and J. G. Valatin, *Phys. Rev. Letters* **5**, 509 (1960).

tion of vibration-rotation interaction, gives rise to a contribution to the  $\mathcal{B}$  coefficient, in addition to a pure fourth-order Coriolis term. The work of Hemmer, while on the right track, is limited by the use of a pure axially symmetric harmonic-oscillator potential, and by neglect of pairing effects.<sup>42</sup> Moreover, the relation of this model to a Hartree-Fock approach is somewhat obscure. In Hemmer's model, the total energy is a sum of single-particle energies, while in the Hartree-Fock approach one must subtract one-half of the total potential energy from the sum of single-particle energies to compute the total energy. It is just this correction which provides a restoring force against deformation in the Hartree-Fock case, while the restoring force in the Hemmer model arises from the *ad hoc* incompressibility constraint.

Another attempt at obtaining the  $\mathcal{B}$  coefficient was made by Grin<sup>34</sup> and Grin' and Pavlichenkov<sup>35</sup> who "cranked" the Gor'kov equations,<sup>43</sup> which are just a Green's function formulation of the HFB equations. These authors considered only a pairing interaction with constant matrix elements and neglected long-range components of the effective nuclear interaction. They were therefore unable to obtain centrifugal stretching of the average field, which is produced by the long-range force, but instead obtained terms arising from the Coriolis unpairing effect (to be discussed later),<sup>44</sup> and some fourth-order Coriolis perturbation terms. Unfortunately, the final results were marred by rough approximations which obscured the physical significance of the terms.

In the present work, the long-range force will be included so that stretching of the self-consistent field can be included simultaneously with Coriolis unpairing. It will be shown that the results can be written in a simple form which brings out their physical significance.

## II. SINGLE-PARTICLE PERTURBATION OF THE HFB EQUATIONS

Let us consider the effect of a single-particle perturbation on the HFB equations.<sup>45</sup> The original Hamiltonian, including the perturbation is assumed to have the second-quantized form

$$H' = \sum_l \epsilon_{kl} a_k^\dagger a_l + \sum_{kl} h_{kl}^{(1)} a_k^\dagger a_l + \frac{1}{4} \sum_{klmn} \mathcal{V}_{kl, mn} a_k^\dagger a_l^\dagger a_n a_m, \quad (7)$$

where  $a_k^\dagger$ ,  $a_k$  are fermion creation and annihilation operators, respectively.

<sup>42</sup> A sign error in Hemmer's Eq. (4) leads to his final result for the coefficient of the  $I^2(I+1)^2$  term being 9 times larger than the correct one.

<sup>43</sup> L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **36**, 1918 (1959) [English transl.: Soviet Phys.—JETP **9**, 1364 (1959)].

<sup>44</sup> B. R. Mottelson and J. G. Valatin, Phys. Rev. Letters **5**, 511 (1960).

<sup>45</sup> The perturbation of the ordinary Hartree-Fock equations has been considered by R. McWeeny, Phys. Rev. **126**, 1028 (1962).

The first term in Eq. (7), on the right-hand side, is a Hermitian, spherically symmetric shell-model potential. The second term is a single-particle perturbation, which is proportional to a parameter  $\xi$ , and is assumed to be Hermitian, and either even or odd under time reversal. That is,

$$h_{-k-l}^{(1)} = \pm h_{kl}^{(1)*} \theta_k \theta_l = \pm h_{lk}^{(1)} \theta_k \theta_l, \quad (8)$$

where the top sign holds when the perturbation is even under time reversal, and the bottom sign when it is odd under time reversal. This convention will hold in subsequent equations, whenever the  $\pm$  symbol appears. The symbol  $\theta_k$  means

$$\begin{aligned} \theta_k &= 1, & k > 0, \\ \theta_k &= -1, & k < 0. \end{aligned}$$

The index  $-k$  refers to a single-particle state which is the time reverse of the state denoted by  $k$ . The summations in Eq. (7), and in all the equations to follow, refer to all the indices, positive and negative.

The last term in Eq. (7) is a residual two-nucleon interaction, assumed to be spherically symmetric, with matrix elements obeying the conditions

$$\mathcal{V}_{kl, mn} = -\mathcal{V}_{kl, nm} = -\mathcal{V}_{lk, mn} = \mathcal{V}_{mn, kl}^*.$$

The HFB variational wave function for Eq. (7) is the ground state  $\psi_0$  of the linearized Hamiltonian given by (aside from a constant which will not be needed)<sup>26</sup>

$$\mathcal{H}\mathcal{C} = \sum_{kl} (\epsilon_{kl} - \lambda \delta_{kl}) a_k^\dagger a_l + \frac{1}{2} \sum_{kl} (\Delta_{k-l} a_k^\dagger a_{-l}^\dagger + \text{H.c.}) + \sum_{kl} h_{kl}^{(1)} a_k^\dagger a_l, \quad (9a)$$

where  $\epsilon_{kl}$  is the self-consistent field, defined by<sup>46</sup>

$$\epsilon_{kl} \equiv \epsilon_{kl} + \sum_{mn} \mathcal{V}_{kl, mn} \rho_{nm}, \quad (10)$$

with  $\rho_{nm}$  a one-particle density matrix element defined by

$$\rho_{nm} \equiv \langle \psi_0 | a_m^\dagger a_n | \psi_0 \rangle, \quad (11)$$

and  $\Delta_{k-l}$  is the pairing potential matrix element defined by

$$\Delta_{k-l} \equiv \frac{1}{2} \sum_{mn} \mathcal{V}_{k-l, m-n} \chi_{m-n}, \quad (12)$$

with  $\chi_{m-n}$  an element of the pairing tensor given by

$$\chi_{m-n} \equiv \langle \psi_0 | a_{-n} a_m | \psi_0 \rangle. \quad (13)$$

The Hamiltonian (9a) can be diagonalized by introducing quasiparticles  $\eta_\sigma$ ,  $\eta_\sigma^\dagger$  defined by the general Bogoliubov canonical transformation

$$\eta_\sigma = \sum_k (U_{k\sigma}^* a_k^\dagger + V_{k\sigma} a_k),$$

$$\eta_\sigma^\dagger = \sum_k (V_{k\sigma}^* a_k^\dagger + U_{k\sigma} a_k),$$

<sup>46</sup> In Ref. (26), the Lagrange multiplier was included in the definition of the self-consistent field.

so that, with a suitable choice of the  $U_{k\sigma}$  and  $V_{k\sigma}$ , (9a) takes the form of independent quasiparticles

$$\mathcal{H} = \sum_{\sigma} \mathcal{E}_{\sigma} \eta_{\sigma}^{\dagger} \eta_{\sigma}. \quad (9a')$$

From the definitions, it is clear that  $\mathfrak{g}$  and  $\mathfrak{e}$  are Hermitian matrices, and  $\mathfrak{z}$  and  $\mathfrak{A}$  are anti-Hermitian. That is,

$$\begin{aligned} \mathfrak{g}^{\dagger} &= \mathfrak{g}, \\ \mathfrak{e}^{\dagger} &= \mathfrak{e}, \\ \mathfrak{z}^{\dagger} &= -\mathfrak{z}^*, \\ \mathfrak{A}^{\dagger} &= -\mathfrak{A}^*. \end{aligned}$$

The Hamiltonian, Eq. (9), is obtained from a self-consistent linearization of

$$H'' = H' - \lambda N,$$

where  $N$  is the number operator  $N = \sum_k a_k^{\dagger} a_k$  and  $\lambda$  is a Lagrange multiplier introduced to give the correct expectation value  $n$  for the number of particles since the Hamiltonian, Eq. (9a), does not commute with  $N$ . Thus, we have

$$\langle \psi_0 | N | \psi_0 \rangle = \text{Tr} \mathfrak{g} = n. \quad (14)$$

The ground state of Eq. (9a) can be obtained by guessing values of  $\chi_{k-l}$ ,  $\rho_{kl}$ , and  $\lambda$ , computing the  $\epsilon_{kl}$  and  $\Delta_{k-l}$ , finding the corresponding eigenfunction  $\psi_0$  of Eq. (9a) and computing new input values of  $\chi_{k-l}$ ,  $\rho_{kl}$ , and  $\lambda$ , the process being continued until Eqs. (11) and (13) reproduce the input values, and Eq. (14) is satisfied. It will be assumed that this process has already been carried out with  $h_{kl}^{(1)} = 0$ , so that a complete set of zero-order wave functions,  $\mathfrak{g}^{(0)}$ ,  $\mathfrak{z}^{(0)}$ ,  $\mathfrak{e}^{(0)}$ ,  $\mathfrak{A}^{(0)}$ ,  $\lambda^{(0)}$  are all known. Then,  $h_{kl}^{(1)}$  will be treated as a perturbation and explicit corrections to the ground-state wave function, the matrices in question, and the ground-state energy can be obtained in terms of the zero-order solutions. Alternatively, the matrix equations of the HFB theory may be treated by perturbation theory,<sup>26</sup> but it turns out that considerable tedious algebra is required in higher order to bring the results into a tractable form. The use of the linearized Hamiltonian [Eq. (9a)] immediately gives the results in the desired form.

The matrices  $\mathfrak{e}$ ,  $\mathfrak{A}$ ,  $\mathfrak{g}$ ,  $\mathfrak{z}$ , and  $\lambda$  all depend on the perturbation parameter  $\xi$  and must be expanded in powers of this parameter:

$$\epsilon_{kl} = \epsilon_{kk}^{(0)} \delta_{kl} + \sum_{n=1}^{\infty} \epsilon_{kl}^{(n)}, \quad (15a)$$

$$\Delta_{k-l} = \Delta_{k-k}^{(0)} \delta_{kl} + \sum_{n=1}^{\infty} \Delta_{k-l}^{(n)}, \quad (15b)$$

$$\lambda = \lambda^{(0)} + \sum_{n=1}^{\infty} \lambda^{(n)}. \quad (15c)$$

In Eq. (15), it is assumed that  $\mathfrak{e}^{(0)}$  and  $\mathfrak{A}^{(0)}$  commute,

and that they are in canonical form in the chosen representation. It is convenient to choose a representation independent of  $\xi$ . Although it is straightforward to consider the case when  $\mathfrak{e}^{(0)}$  and  $\mathfrak{A}^{(0)}$  do not commute, the resulting equations would be more complicated and of little practical use. The commutation of  $\mathfrak{e}^{(0)}$  and  $\mathfrak{A}^{(0)}$  is believed to be a good approximation for nuclear interactions.

The density and pairing matrices are likewise expanded in powers of the perturbation parameter:

$$\rho_{kl} = \rho_{kk}^{(0)} \delta_{kl} + \sum_{n=1}^{\infty} \rho_{kl}^{(n)}, \quad (16a)$$

$$\chi_{k-l} = \chi_{k-k}^{(0)} \delta_{kl} + \sum_{n=1}^{\infty} \chi_{k-l}^{(n)}. \quad (16b)$$

Since  $\mathfrak{e}^{(0)}$  and  $\mathfrak{A}^{(0)}$  are in canonical form,  $\mathfrak{g}^{(0)}$  and  $\mathfrak{z}^{(0)}$  must also be in canonical form.

The zero-order part of Eq. (9a) takes the form

$$\begin{aligned} \mathcal{H}^{(0)} &= \sum_k (\epsilon_{kk}^{(0)} - \lambda^{(0)}) a_k^{\dagger} a_k \\ &\quad + \frac{1}{2} \sum_k (\Delta_{k-k}^{(0)} a_k^{\dagger} a_{-k}^{\dagger} + \text{H.c.}), \end{aligned} \quad (17a)$$

which can be diagonalized by the quasiparticle transformation

$$a_k^{\dagger} = U_k \alpha_k^{\dagger} + \theta_k V_k \alpha_{-k}, \quad (18)$$

$$a_{-k} = -\theta_k V_k \alpha_k^{\dagger} + U_k \alpha_{-k},$$

where

$$\rho_{kk}^{(0)} = V_k^2 = \frac{1}{2} (1 - \epsilon_{kk}^{(0)} / E_k), \quad (19a)$$

$$U_k^2 = 1 - V_k^2, \quad (19b)$$

$$\chi_{k-k}^{(0)} = U_k V_k \theta_k = -\frac{1}{2} \Delta_{k-k}^{(0)} / E_k, \quad (19c)$$

$$E_k = (|\epsilon_{kk}^{(0)}|^2 + |\Delta_{k-k}^{(0)}|^2)^{1/2}. \quad (19d)$$

By substituting Eq. (18) into Eq. (17a), we achieve an independent quasiparticle form,

$$\mathcal{H}^{(0)} = \sum_k E_k \alpha_k^{\dagger} \alpha_k. \quad (17b)$$

Substituting Eq. (18) into the full Hamiltonian, Eq. (9a), and using the expansions, Eq. (15), we obtain (apart from a constant which will not concern us)

$$\mathcal{H} = \sum_k E_k \alpha_k^{\dagger} \alpha_k + \mathcal{H}_{\text{pert}}, \quad (9b)$$

where the perturbation may be written as

$$\mathcal{H}_{\text{pert}} \equiv \sum_{n=1}^{\infty} H_{11}^{(n)} + \sum_{n=1}^{\infty} (H_{20}^{(n)} + \text{H.c.}), \quad (20a)$$

$$H_{11}^{(n)} \equiv \sum_{kl} A_{kl}^{(n)} \alpha_k^{\dagger} \alpha_l, \quad (20b)$$

$$H_{20}^{(n)} \equiv \sum_{kl} B_{kl}^{(n)} \alpha_k^{\dagger} \alpha_{-l}^{\dagger}, \quad (20c)$$

and where

$$A_{kl}^{(n)} \equiv \delta_{n1} h_{kl}^{(1)} (U_k U_l \mp V_k V_l) + (\epsilon_{kl}^{(n)} - \lambda^{(n)} \delta_{kl}) [U_k U_l - (\pm)^n V_k V_l] - \Delta_{k-l}^{(n)} \theta_l [U_k V_l + (\pm)^n U_l V_k], \quad (21a)$$

$$B_{kl}^{(n)} \equiv \delta_{n1} h_{kl}^{(1)} \theta_l (U_k V_l \pm U_l V_k) + (\epsilon_{kl}^{(n)} - \lambda^{(n)} \delta_{kl}) \theta_l [U_k V_l + (\pm)^n U_l V_k] + \Delta_{k-l}^{(n)} [U_k U_l - (\pm)^n V_k V_l], \quad (21b)$$

where the top sign of the  $(\pm)$  factors holds when the single-particle perturbation is even under time reversal, and the bottom sign holds when it is odd under time reversal, corresponding to Eq. (8). Equations (21) involve use of the properties

$$\begin{aligned} \rho_{-k-l}^{(n)} &= (\pm)^n \rho_{kl}^{(n)*} \theta_k \theta_l = (\pm)^n \rho_{lk}^{(n)} \theta_k \theta_l, \\ \chi_{-kl}^{(n)} &= -(\pm)^n \chi_{k-l}^{(n)*} \theta_k \theta_l = (\pm)^n \chi_{-lk}^{(n)*} \theta_k \theta_l, \\ \epsilon_{-k-l}^{(n)} &= (\pm)^n \epsilon_{kl}^{(n)*} \theta_k \theta_l = (\pm)^n \epsilon_{lk} \theta_k \theta_l, \\ \Delta_{-kl}^{(n)} &= -(\pm)^n \Delta_{k-l}^{(n)*} \theta_k \theta_l = (\pm)^n \Delta_{-lk}^{(n)*} \theta_k \theta_l. \end{aligned} \quad (22)$$

A straightforward proof of Eq. (22) can easily be obtained by perturbing the matrix equations and will not be given here.

The **A** and **B** matrices have the following properties:

$$\begin{aligned} A_{kl}^{(n)} &= A_{lk}^{(n)*}, \\ A_{-k-l}^{(n)} &= (\pm)^n A_{kl}^{(n)*} \theta_k \theta_l = (\pm)^n A_{lk}^{(n)} \theta_k \theta_l, \\ B_{-k-l}^{(n)} &= -B_{lk}^{(n)}, \\ B_{lk}^{(n)} &= (\pm)^n B_{kl}^{(n)*} \theta_k \theta_l = -(\pm)^n B_{-l-k}^{(n)*} \theta_k \theta_l. \end{aligned} \quad (23)$$

We now proceed to treat  $\mathcal{H}_{\text{pert}}$  by ordinary Rayleigh-Schrödinger perturbation theory.<sup>47</sup> The unperturbed ground-state, denoted by  $|0\rangle$  is defined by

$$\alpha_k |0\rangle = 0. \quad (24)$$

The perturbation will admix 2, 4, 6,  $\dots$ , etc., quasi-particle states, so that the ground state of the Hamiltonian [Eq. (9)] may be written in the form

$$\begin{aligned} \psi_0 = \left( b_0 + \frac{1}{2} \sum_{kl} b(k-l) \alpha_k^\dagger \alpha_{-l}^\dagger + \frac{1}{24} \sum_{klmn} b(k-lm-n) \right. \\ \left. \times \alpha_k^\dagger \alpha_{-l}^\dagger \alpha_m^\dagger \alpha_{-n}^\dagger + \dots \right) |0\rangle. \end{aligned} \quad (25)$$

The mixing amplitudes may be expanded in powers of  $\xi$ :

$$\begin{aligned} b_0 &= 1 + b_0^{(2)} + b_0^{(3)} + \dots, \\ b(k-l) &= b^{(1)}(k-l) + b^{(2)}(k-l) \\ &\quad + b^{(3)}(k-l) + \dots, \\ b(k-lm-n) &= b^{(2)}(k-lm-n) \\ &\quad + b^{(3)}(k-lm-n) + \dots. \end{aligned} \quad (26)$$

The mixing amplitudes for 2 and 4 quasiparticle states

<sup>47</sup> A. Dalgarno, in *Quantum Theory, I. Elements*, edited by D. R. Bates (Academic Press Inc., New York, 1961), p. 171.

have the property

$$\begin{aligned} b(k-l) &\equiv (0 | \alpha_{-l} \alpha_k | \psi_0) = -b(-lk), \\ b(k-lm-n) &\equiv (0 | \alpha_{-n} \alpha_m \alpha_{-l} \alpha_k | \psi_0) \\ &= -b(k-l-nm) = -b(-lkm-n) \\ &= b(-lk-nm). \end{aligned} \quad (27a)$$

In addition, the following properties can be proven from the perturbation formulas for the mixing amplitudes and Eqs. (22):

$$\begin{aligned} b^{(n)}(k-l) &= (-)^{n+1} (\mp)^n \theta_k \theta_l b^{(n)*}(-kl), \\ b^{(n)}(k-lm-n) &= (\pm)^n \theta_k \theta_l \theta_m \theta_n b^{(n)*}(-kl-mn). \end{aligned} \quad (27b)$$

Using the perturbed  $\psi_0$ , Eq. (25), one can calculate  $n$ th order corrections to  $\rho$  and  $\chi$  from Eq. (11) and Eq. (13), which therefore depend on  $\epsilon^{(n)}$ ,  $\Delta^{(n)}$ , and  $\lambda^{(n)}$ . The  $n$ th-order correction to  $\epsilon$  and  $\Delta$  are obtained from Eq. (10) and Eq. (12):

$$\epsilon_{kl}^{(n)} = \sum_{jm} \mathcal{U}_{kj,lm} \rho_{mj}^{(n)}(\epsilon^{(n)}, \Delta^{(n)}; \epsilon^{(n-1)}, \Delta^{(n-1)}; \dots; \lambda^{(n)}, \lambda^{(n-1)} \dots), \quad (28a)$$

$$\Delta_{k-l}^{(n)} = \frac{1}{2} \sum_{jm} \mathcal{U}_{k-l,j-m} \chi_{j-m}^{(n)}(\epsilon^{(n)}, \Delta^{(n)}; \epsilon^{(n-1)}, \Delta^{(n-1)}; \dots; \lambda^{(n)}, \lambda^{(n-1)}, \dots). \quad (28b)$$

Using Eq. (14), the  $n$ th order correction to  $\lambda$  is obtained from

$$\begin{aligned} \text{Tr} \rho^{(n)} = \sum_k \rho_{kk}^{(n)}(\epsilon^{(n)}, \Delta^{(n)}; \epsilon^{(n-1)}, \Delta^{(n-1)}; \dots; \\ \lambda^{(n)}, \lambda^{(n-1)}, \dots) = 0, \quad n \geq 1, \end{aligned} \quad (28c)$$

since  $\lambda^{(0)}$  is chosen to satisfy  $\text{Tr} \rho^{(0)} = n$ .

Let us abbreviate certain occupation amplitudes which occur frequently as follows:

$$\begin{aligned} f_{kl}^\pm &\equiv (U_k V_l \pm U_l V_k) \theta_l, \\ f_{kl}^{(\pm)n} &\equiv [U_k V_l + (\pm)^n U_l V_k] \theta_l, \\ g_{kl}^\mp &\equiv U_k U_l \mp V_k V_l, \\ g_{kl}^{(\mp)n} &\equiv U_k U_l - (\mp)^n V_k V_l. \end{aligned} \quad (29)$$

Energy denominators for two-quasiparticle excitations will be denoted by

$$E_{kl} \equiv E_k + E_l. \quad (30)$$

Applying standard  $n$ th-order formulas for Rayleigh-Schrödinger perturbation corrections to the wave function,<sup>47</sup> and using Eq. (11) and Eq. (13), the  $n$ th-order correction to the density matrix and pairing tensor have the form

$$\begin{aligned} \rho_{kl}^{(n)} &= R_{kl}^{(n)} - E_{kl}^{-1} [\epsilon_{kl}^{(n)} (f_{kl}^{(\pm)n})^2 \\ &\quad + \Delta_{k-l}^{(n)} f_{kl}^{(\pm)n} g_{kl}^{(\mp)n}], \end{aligned} \quad (31a)$$

$$\begin{aligned} \chi_{k-l}^{(n)} &= X_{k-l}^{(n)} - E_{kl}^{-1} [\epsilon_{kl}^{(n)} f_{kl}^{(\pm)n} g_{kl}^{(\mp)n} \\ &\quad + \Delta_{k-l}^{(n)} (g_{kl}^{(\mp)n})^2], \end{aligned} \quad (31b)$$

where  $R_{kl}^{(n)}$  and  $X_{k-l}^{(n)}$  depend on knowing  $\rho^{(n-1)}$  and  $\chi^{(n-1)}$  and lower orders. From Eqs. (28) it is clear that one may write linear integral equations for elements of  $\rho^{(n)}$  and  $\chi^{(n)}$  or alternatively for  $\epsilon^{(n)}$  and  $\Delta^{(n)}$ . Choosing the latter procedure, for example, one gets the coupled

integral equations

$$\begin{aligned} \epsilon_{kl}^{(n)} &= \sum_{ij} \mathcal{U}_{ki,ij} R_{ji}^{(n)} - \sum_{ij} E_{ij}^{-1} \mathcal{U}_{ki,ij} \\ &\quad \times (\epsilon_{ji}^{(n)} (f_{ji}^{(\pm)n})^2 + \Delta_{j-i}^{(n)} f_{ji}^{(\pm)n} g_{ji}^{(\mp)n}), \\ \Delta_{k-l}^{(n)} &= \frac{1}{2} \sum_{ij} \mathcal{U}_{k-l,j-i} X_{j-i}^{(n)} - \frac{1}{2} \sum_{ij} E_{ij}^{-1} \mathcal{U}_{k-l,j-i} \\ &\quad \times (\epsilon_{ji}^{(n)} f_{ji}^{(\pm)n} g_{ji}^{(\mp)n} + \Delta_{j-i}^{(n)} (g_{ji}^{(\mp)n})^2). \end{aligned} \quad (32)$$

Alternatively, one may write uncoupled integral equations for the elements of  $\mathbf{A}$  and  $\mathbf{B}$ . Using Eqs. (21) and the identity

$$(f_{kl}^{(\pm)n})^2 + (g_{kl}^{(\mp)n})^2 = 1,$$

the integral equations (32) may be written

$$\begin{aligned} B_{kl}^{(n)} &= (\delta_{n1} h_{kl}^{(1)} - \lambda^{(n)} \delta_{kl}) f_{kl}^{(\pm)n} + f_{kl}^{(\pm)n} \sum_{ij} \mathcal{U}_{ki,ij} [R_{ji}^{(n)} + (\delta_{n1} h_{ji}^{(1)} - \lambda^{(n)} \delta_{ji}) E_{ij}^{-1} (f_{ji}^{(\pm)n})^2] + \frac{1}{2} g_{kl}^{(\mp)n} \sum_{ij} \mathcal{U}_{k-l,j-i} \\ &\quad \times [X_{j-i}^{(n)} + (\delta_{n1} h_{ji}^{(1)} - \lambda^{(n)} \delta_{ji}) E_{ij}^{-1} f_{ji}^{(\pm)n} g_{ji}^{(\mp)n}] - \sum_{ij} E_{ij}^{-1} (\mathcal{U}_{ki,ij} f_{kl}^{(\pm)n} f_{ji}^{(\pm)n} + \frac{1}{2} \mathcal{U}_{k-l,j-i} g_{kl}^{(\mp)n} g_{ji}^{(\mp)n}) B_{ji}^{(n)} \\ A_{kl}^{(n)} &= (\delta_{n1} h_{kl}^{(1)} - \lambda^{(n)} \delta_{kl}) g_{kl}^{(\mp)n} + g_{kl}^{(\mp)n} \sum_{ij} \mathcal{U}_{ki,ij} [R_{ji}^{(n)} + (\delta_{n1} h_{ji}^{(1)} - \lambda^{(n)} \delta_{ji}) E_{ij}^{-1} (f_{ji}^{(\pm)n})^2] \\ &\quad - \frac{1}{2} f_{kl}^{(\pm)n} \sum_{ij} \mathcal{U}_{k-l,j-i} [X_{j-i}^{(n)} + (\delta_{n1} h_{ji}^{(1)} - \lambda^{(n)} \delta_{ji}) E_{ij}^{-1} f_{ji}^{(\pm)n} g_{ji}^{(\mp)n}] \\ &\quad - \sum_{ij} E_{ij}^{-1} (\mathcal{U}_{ki,ij} f_{ji}^{(\pm)n} g_{kl}^{(\mp)n} - \frac{1}{2} \mathcal{U}_{k-l,j-i} f_{kl}^{(\pm)n} g_{ji}^{(\mp)n}) B_{ji}^{(n)}. \end{aligned} \quad (33)$$

Note that the  $\mathbf{R}^{(n)}$  and  $\mathbf{X}^{(n)}$  depend on  $\lambda^{(n)}$ , which is obtained from Eq. (28c).

Expressions for  $\mathbf{g}^{(n)}$ ,  $\mathbf{z}^{(n)}$ , and  $\lambda^{(n)}$  are given through  $n=3$  in terms of  $\mathbf{A}$  and  $\mathbf{B}$  in Appendix A, since these may be of use in other applications.

The  $n$ th-order correction to the eigenvalues of the linearized Hamiltonian [Eq. (9)] can be obtained from the standard perturbation formulas.<sup>47</sup> However, the real interest lies in the expectation value of the Hamiltonian [Eq. (7)] using the state, Eq. (25). This expectation value can be expanded in powers of the perturbation parameter  $\xi$  as follows:

$$E' = \langle \psi_0 | H' | \psi_0 \rangle = E^{(0)'} + A_2 \xi^2 + A_3 \xi^3 + A_4 \xi^4 + \dots + A_n \xi^n + \dots \quad (34)$$

[*Note added in proof.* The  $A_n$  in Eq. (34) must not be confused with the  $A$ 's defined by Eq. (21a).]

We now use the fact that

$$\partial E' / \partial \xi = \langle \psi_0 | \partial H' / \partial \xi | \psi_0 \rangle,$$

which is a trivial consequence of the variational principle.

$$\begin{aligned} (\partial E' / \partial \xi) &= 2A_2 \xi + 3A_3 \xi^2 + 4A_4 \xi^3 + \dots + nA_n \xi^{n-1} \\ &\quad + \dots = \text{Tr}_{\mathbf{g}}(\partial \mathbf{h}^{(1)} / \partial \xi), \end{aligned} \quad (35)$$

where  $\mathbf{h}^{(1)}$  is the matrix corresponding to the single-particle perturbation defined by Eq. (8). Since  $\partial \mathbf{h}^{(1)} / \partial \xi$  is independent of  $\xi$  by definition, we have from Eq. (35)

$$A_n = n^{-1} \xi^{-n+1} \text{Tr}_{\mathbf{g}}^{(n-1)} \frac{\partial \mathbf{h}^{(1)}}{\partial \xi} = n^{-1} \xi^{-n} \text{Tr}_{\mathbf{g}}^{(n-1)} \mathbf{h}^{(1)}. \quad (36)$$

Thus, the  $n$ th-order correction to the expectation value of Eq. (7) is immediately obtained from the  $(n-1)$ th-order correction to the density matrix.

Suppose now that the single-particle perturbation  $\mathbf{h}^{(1)}$

arises from a constraint imposed during the variation, with  $\xi$  a Lagrange multiplier, expressed by

$$\text{Tr}_{\mathbf{g}}(\partial \mathbf{h}^{(1)} / \partial \xi) = X, \quad (37)$$

where  $X$  is a given constant. The true energy is the expectation value of  $H = H' - \sum_{kl} h_{kl}^{(1)} a_k^\dagger a_l$  given by

$$\begin{aligned} E = E' - \text{Tr}_{\mathbf{g}} \mathbf{h}^{(1)} &= E^{(0)} - A_2 \xi^2 - 2A_3 \xi^3 \\ &\quad - 3A_4 \xi^4 - \dots - (n-1)A_n \xi^n. \end{aligned} \quad (38)$$

It is desirable to express Eq. (38) as an expansion in powers of  $X$ . Equations (35) and (37) define  $X$  as an expansion in powers of  $\xi$ , which can be inverted to give, to third order in  $X$ ,

$$\begin{aligned} \xi &= \frac{1}{2} A_2^{-1} X - \frac{3}{8} A_3 A_2^{-2} X^2 \\ &\quad + \frac{1}{4} [(9/4) A_3^2 A_2^{-5} - A_4 A_2^{-4}] X^3 + \dots \end{aligned} \quad (39)$$

Substituting Eq. (39) into Eq. (38), we have to fourth order in  $X$

$$\begin{aligned} E &= E^{(0)} - \frac{1}{4} A_2^{-1} X^2 + \frac{1}{8} A_3 A_2^{-3} X^3 \\ &\quad - \frac{1}{16} [(9/4) A_3^2 A_2^{-5} - A_4 A_2^{-4}] X^4 + \dots \end{aligned} \quad (40)$$

### III. APPLICATION TO NUCLEAR ROTATIONAL SPECTRA

As was pointed out by Thouless and Valatin<sup>25</sup> and Valatin,<sup>26</sup> the time-dependent HFB equations may contain solutions corresponding to a uniformly rotating deformed average field (and a corresponding rotating density distribution). These solutions exist when the average single-particle field calculated from the time-independent HFB theory is already nonspherical. The above authors transformed the time-dependent HFB equations to a frame of reference rotating with the self-consistent field and then studied the time-independent solutions perturbed by the Coriolis force.

However, more general solutions can be obtained by

studying time-dependent equations in the rotating frame, since one can then describe intrinsic shape oscillations (such as  $\beta$  and  $\gamma$  oscillations) simultaneously with rotation. In lowest order, the case considered by Thouless and Valatin, the rotations, being decoupled from the vibrations, are adequately described by the perturbed time-independent theory. In higher order, however, there is a coupling between the rotational and vibrational modes which is more generally described by the fully time-dependent theory. Nevertheless, one can consider the effect of a Coriolis force on the time-independent HFB equations in higher order. This semiclassical description of the vibration-rotation interaction, whereby each nucleon in the rotating frame is subject to a static average field, additionally deformed by rotation, rather than a fluctuating (time-dependent) field, is expected to be valid in the adiabatic limit, when the frequency of the collective fluctuations is small compared to single-particle frequencies. In this paper, the mathematically simpler adiabatic case will be considered in detail.

In addition, it is assumed that the rotation is sufficiently slow so that the Coriolis force may be treated as a perturbation. This means that the angular velocity is much less than the critical value required to bring about the Mottelson-Valatin phase transition,<sup>44</sup> since near the critical point the pairing potential  $\Delta$  undergoes a large change and the expansion [Eq. (15b)] is probably not valid.

Finally, it is assumed, for the sake of simplicity, that the zero-order deformed field  $\epsilon^{(0)}$  is cylindrically symmetric, say about the  $z$  axis. It is then necessary to only consider rotation about an axis perpendicular to the  $z$  axis, say the  $x$  axis.<sup>48</sup> The perturbation theory of the previous section then applies to the Coriolis perturbation

$$h_{kl}^{(1)} \equiv -\Omega j_{kl}^x, \quad (41)$$

where  $\Omega$  is the angular velocity of the rotating frame and corresponds to the perturbation parameter  $-\xi$  of the previous section, and  $j_{kl}^x$  is a matrix element of the  $x$  component of the angular-momentum operator.

As noted by Beliaev,<sup>29</sup> our treatment of the Coriolis force is equivalent to minimizing the expectation value of the Hamiltonian [Eq. (7)] with  $h_{kl}^{(1)} = 0$ , subject to the constraint that the angular momentum have a given value. This constraint is necessary since the linearized Hamiltonian [Eq. (9)] is not spherically symmetric and therefore violates the condition of conservation of angular momentum. The Lagrange multiplier is thus  $\Omega$ . Corresponding to Eq. (37), it may be written

$$\langle \psi_0 | \sum_{kl} j_{kl}^x a_k^\dagger a_l | \psi_0 \rangle = \text{Tr} \mathbf{q} \mathbf{j}^x = R, \quad (42)$$

where the prescribed value of the angular momentum is

<sup>48</sup> The rotation induces, as will be seen, a small nonaxial deformation. Nevertheless, it is not necessary to consider rotation about the  $z$  axis since the expectation value of the  $z$  component of the angular momentum vanishes for the ground state band.

$R = \hbar[I(I+1)]^{1/2}$ . Since the energy cannot depend on the sense of rotation for the ground state of an even-even nucleus, odd powers of  $\Omega$  and  $R$  vanish in the expansions corresponding to Eqs. (34) and (40). The energy, Eq. (40), may be written in the form

$$E = R^2/(2\mathcal{J}) + \mathcal{B}R^4/\hbar^4 + \dots, \quad (43)$$

where, according to Eq. (36),

$$\mathcal{J} = \Omega^{-1} \text{Tr} \mathbf{q}^{(1)} \mathbf{j}^x \quad (44)$$

and

$$\mathcal{B} = -\frac{1}{4} \Omega^{-3} \hbar^4 \mathcal{J}^{-4} \text{Tr} \mathbf{q}^{(3)} \mathbf{j}^x. \quad (45)$$

It is interesting to note from Eqs. (39) and (40) that  $R$  and  $\Omega$  are related by the Hamilton-like equation

$$\partial E / \partial R = \Omega.$$

The angular momentum operators are odd under time reversal, i.e., the lower sign is chosen in Eq. (8), and in the equations in Appendix A. It is clear from (A1d), (A3d), and Eq. (29) that corrections to  $\lambda$  corresponding to odd powers of  $\Omega$  vanish for the odd time-reversal case. From Eqs. (A1c) and (21), one obtains for the moment of inertia, given by Eq. (44), the expression

$$\mathcal{J} = \sum_{kl} |j_{kl}^x|^2 (f_{kl}^-)^2 / E_{kl} - \Omega^{-1} \sum_{kl} \epsilon_{kl}^{(1)} j_{kl}^x (f_{kl}^-)^2 / E_{kl} - \Omega^{-1} \sum_{kl} \Delta_{k-l}^{(1)} j_{kl}^x f_{kl}^- g_{kl}^+ / E_{kl}. \quad (46)$$

The first term on the right-hand side in Eq. (46) is the original Beliaev cranking-model moment.<sup>22</sup> The other terms come from the first-order change in the self-consistent field and the pairing potential and have been previously derived by equivalent methods.<sup>27-32</sup> The  $\epsilon_{kl}^{(1)}$  and  $\Delta_{k-l}^{(1)}$  satisfy the integral equations given by Eq. (32) for the odd time-reversal case, with

$$\begin{aligned} R_{ji}^{(1)} &= \Omega j_{ji}^x (f_{ji}^-)^2 / E_{ji}, \\ X_{j-i}^{(1)} &= \Omega j_{ji}^x f_{ji}^- g_{ji}^+ / E_{ji}. \end{aligned} \quad (47)$$

One may go on and write similar expressions for the  $\mathcal{B}$  coefficient, valid for a general two-nucleon interaction. However, the physical meaning of the results is much clearer if a simplified interaction is chosen for which the integral equations can be solved in closed form.

### Pairing and Quadrupole Force

The formalism presented in the previous two sections applies to identical interacting fermions. However, the case of interacting neutrons and protons can be included if the single-particle states are made to depend on isotopic spin, and if two Lagrange multipliers  $\lambda_n$  and  $\lambda_p$  are introduced to give the correct expectation values  $n_n$  and  $n_p$  for the numbers of neutrons and protons, respectively. However, it is not really necessary to use the isotopic spin formalism since the linearized Hamiltonian [Eq. (9)] breaks up into a part acting only in



the neutron space and a part acting in the proton space

$$\mathcal{H} = \mathcal{H}_n + \mathcal{H}_p,$$

where the neutron Hamiltonian, for example, has the form

$$\mathcal{H}_n = \sum_{k_n, l_n} (\epsilon_{k_n l_n} - \lambda_n \delta_{k_n l_n}) a_{k_n}^\dagger a_{l_n} + \frac{1}{2} \sum_{k_n, l_n} (\Delta_{k_n - l_n} a_{k_n}^\dagger a_{-l_n}^\dagger + \text{H.c.}) + \sum_{k_n l_n} h_{k_n l_n}^{(1)} a_{k_n}^\dagger a_{l_n}.$$

Neutron single-particle states are denoted by the index  $k_n$  and proton single-particle states by  $k_p$ . The Hamiltonian  $\mathcal{H}_p$  is obtained by interchanging  $n$  and  $p$  subscripts. The trial wave function is a product of a neutron state and a proton state:

$$\psi_0 = \psi_{0n} \psi_{0p}.$$

The density matrix breaks up into a neutron subspace  $\rho_n$  and a proton subspace  $\rho_p$ , and similarly for the pairing tensor. The self-consistent field for neutrons  $\epsilon_n$  is given by

$$\epsilon_{k_n l_n} = \epsilon_{k_n l_n} + \sum_{i_n j_n} \mathcal{U}_{k_n i_n, l_n j_n} \rho_{j_n i_n} + \sum_{i_p j_p} \mathcal{U}_{k_n i_p, l_n j_p} \rho_{j_p i_p} \quad (48)$$

and the proton self-consistent field  $\epsilon_p$  is obtained by interchange of  $n$  and  $p$  subscripts. The pairing potential for neutrons  $\Delta_n$  is given by

$$\Delta_{k_n - l_n} = \frac{1}{2} \sum_{i_n j_n} \mathcal{U}_{k_n - l_n, i_n - j_n} \chi_{i_n - j_n}, \quad (49)$$

and  $\Delta_p$  is obtained by interchanging  $n$  and  $p$  subscripts. It is assumed that the contribution of the neutron-proton interaction to the pairing potentials is negligible, so that the formalism is applicable only to heavy nuclei. For light nuclei, neutron-proton pairing becomes important and some basic modification of the HFB theory, such as the one proposed by Brémond and Valatin, is needed.<sup>49</sup>

The total angular momentum, for example, is given by

$$R = \text{Tr}_{\rho_n} \mathbf{j}_n^x + \text{Tr}_{\rho_p} \mathbf{j}_p^x, \quad (50)$$

where the density matrices satisfy

$$\begin{aligned} \text{Tr}_{\rho_n} &= n_n, \\ \text{Tr}_{\rho_p} &= n_p. \end{aligned} \quad (51)$$

The two-body interaction considered in this section will be a sum of a quadrupole and a pairing force.<sup>50,51</sup>

<sup>49</sup> B. Brémond and J. G. Valatin, Nucl. Phys. 41, 640 (1963).

<sup>50</sup> M. Baranger, Phys. Rev. 120, 957 (1960).

<sup>51</sup> The quadrupole force is only one term in a multipole expansion of the two-body force. The other multipoles may also be included, and the equations will reduce to a finite set of inhomogeneous linear equations, provided that one restricts oneself to a finite number of multipoles with separable radial parts. The pairing force simulates effects of very high short-range multipoles. It is hoped that the quadrupole component is the most important long-range term in the expansion.

The quadrupole force  $V_Q$ , has the form

$$V_Q = -\kappa f(r_i) f(r_j) \sum_{\mu=-2}^2 Y_2^{(\mu)*}(\theta_i \varphi_i) Y_2^{(\mu)}(\theta_j \varphi_j), \quad (52a)$$

where the  $Y_2^{(\mu)}$  are spherical harmonics of order 2. Three positive strength parameters  $\kappa_n$ ,  $\kappa_p$ ,  $\kappa_{np}$  for neutron-neutron, proton-proton, and neutron-proton interactions, respectively, will be used for Eq. (52a). The separable radial part  $f(r_i) f(r_j)$  is chosen so as to reduce the integral Eqs. (32) to the exactly soluble degenerate kernel case. Since the exact form of  $f(r)$  does not appear to be important for collective nuclear properties, a convenient and popular choice is  $f(r) = r^2$ .

The pairing force is best defined by its matrix elements.<sup>50</sup>

$$\begin{aligned} \mathcal{U}_{i_n j_n, k_n l_n}^{\text{pair}} &= -G_n \zeta_{i_n} \zeta_{k_n} \theta_{i_n} \theta_{k_n} \delta_{j_n, -i_n} \delta_{l_n, -k_n}, \\ \mathcal{U}_{i_p j_p, k_p l_p}^{\text{pair}} &= -G_p \zeta_{i_p} \zeta_{k_p} \theta_{i_p} \theta_{k_p} \delta_{j_p, -i_p} \delta_{l_p, -k_p}, \end{aligned} \quad (52b)$$

with all other matrix elements vanishing, and  $G_n$ ,  $G_p > 0$ . The pairing force is operative only between nucleons scattering among single-particle states lying in an arbitrarily defined neighborhood of the Fermi surface. The magnitudes of  $G_n$  and  $G_p$  depend on how this "pairing neighborhood" is defined. The factors  $\zeta_i$  are therefore defined by

$$\begin{aligned} \zeta_i &= 0 \quad (i \text{ outside the pairing neighborhood}), \\ \zeta_i &= 1 \quad (i \text{ inside the pairing neighborhood}). \end{aligned}$$

This cutoff is necessary to insure solution of the integral equations (49) for  $\Delta_n^{(0)}$  and  $\Delta_p^{(0)}$ .

In addition to the choice of the total force, the following approximations are also made:

(1) The contributions of the long-range quadrupole force to the pairing potentials  $\Delta_n$  and  $\Delta_p$  is neglected on the grounds that these are incoherent and largely cancel out. Moreover, the empirically motivated choice of  $G_n$  and  $G_p$  already takes some of this contribution into account.

(2) The exchange contributions of the quadrupole force to the self-consistent fields  $\epsilon_n$  and  $\epsilon_p$  are neglected, since such contributions are expected to be small for a long-range force.

An additional approximation usually made is the neglect of the contribution of the pairing force to the self-consistent field, these contributions being of order  $G/2\Delta$  times the contribution of the quadrupole force or about 8% in the rare-earth region. However, as one goes to higher orders of perturbation theory, the error slowly accumulates. As no mathematical difficulties thereby occur, the contribution of the pairing force to the self-consistent field will be included. Since this contribution may involve some spurious self-energy effects, it can always be dropped afterwards if desired. On the other hand, approximations (1) and (2) above are absolutely necessary to insure mathematical tractability.

In the equations to follow, the density matrix, pairing

tensor, self-consistent field, and pairing potential for neutrons will be given. The corresponding quantities for protons can be obtained by interchanging  $n$  and  $p$  labels.

For the self-consistent solution of the pairing plus quadrupole problem with  $\Omega=0$ , the reader is referred to Ref. 50.

From Eqs. (48) and (52) and the approximations, the  $m$ th-order perturbation-theory correction to the neutron self-consistent field is

$$\epsilon_{k_n l_n}^{(m)} = - \sum_{\mu=-2}^2 q_{k_n l_n}^{(\mu)} [\kappa_n Q_{\mu}^{(m)*}(n) + \kappa_n p Q_{\mu}^{(m)*}(p)] - G_n \theta_{k_n} \theta_{l_n} \zeta_{k_n} \zeta_{l_n} \rho_{-l_n -k_n}^{(m)}, \quad (53a)$$

where  $q_{k_n l_n}^{(\mu)}$  is a matrix element of  $f(r)Y_2^{(\mu)}$ . The quantity  $Q_{\mu}^{(m)*}(n)$  is the  $m$ th-order perturbation correction to the mass quadrupole moment of the neutrons

$$Q_{\mu}^{(m)}(n) = \text{Tr} \rho_n^{(m)} \mathbf{q}_n^{(\mu)} = \sum_{k_n l_n} \rho_{k_n l_n}^{(m)} q_{l_n k_n}^{(\mu)}, \quad (53b)$$

and  $Q_{\mu}^{(m)}(p)$  is the mass quadrupole moment for protons. The first sum in Eq. (53a) comes from the quadrupole force, and the last term is the usually neglected contribution from the pairing force.

The  $Q_{\mu}^{(m)}$  vanish for odd  $m$  for a perturbation which is odd under time reversal. This is plausible since the quadrupole moments of an even-even nucleus cannot depend on the sign of  $\Omega$ . A direct proof of this is easily obtained from Eq. (22) and the property of the tensor operators,

$$q_{-l-k}^{(\mu)} = (-)^{\mu} q_{lk}^{(-\mu)*} \theta_l \theta_k = q_{kl}^{(\mu)} \theta_l \theta_k. \quad (54)$$

In fact, it is easily shown that the direct contribution of a general velocity-independent two-body interaction to  $\epsilon^{(m)}$  vanishes for odd  $m$  in the case of a perturbation odd under time reversal. Thus, for such an interaction, only exchange terms contribute to the second term on the right-hand side of the moment-of-inertia formula, Eq. (46).

The  $m$ th-order correction to the neutron pairing potential, using Eqs. (49) and (52b), is

$$\Delta_{k_n -l_n}^{(m)} = -\delta_{l_n, k_n} \zeta_{k_n} \theta_{k_n} \Delta_n^{(m)}, \quad (55a)$$

where

$$\Delta_n^{(m)} = \frac{1}{2} G_n \sum_{i_n} \zeta_{i_n} \theta_{i_n} \chi_{i_n -i_n}^{(m)}. \quad (55b)$$

Thus, the pairing potentials are "diagonal," and depend only on "diagonal" elements of the pairing tensors.

The density matrices and pairing tensors depend on the five unknown  $Q_{\mu}(n)$ , the five  $Q_{\mu}(p)$ ,  $\Delta_n$ ,  $\Delta_p$ ,  $\lambda_n$ , and  $\lambda_p$ . Substitution of  $\varrho_n$ ,  $\varrho_p$ ,  $\kappa_n$ , and  $\kappa_p$  into Eqs. (53b) and (55b), together with the conditions [Eq. (51)], gives 14 inhomogeneous linear equations for the 14 unknowns in each order of perturbation theory. Thus, the linear integral equations reduce to the degenerate kernel case due to the choice of a simple interaction together with some plausible approximations. When the perturbation is odd under time reversal, a further simplification occurs since the  $Q_{\mu}^{(m)}$ ,  $\Delta^{(m)}$ , and  $\lambda^{(m)}$  can all be made to vanish for odd  $m$ , and the linear equations need only to be solved in even orders of perturbation theory.

### The $\mathcal{I}$ and $\mathcal{B}$ Coefficients with Pairing and Quadrupole Forces

The derivation of the moment of inertia  $\mathcal{I}$  and the  $\mathcal{B}$  coefficient in the presence of the pairing and quadrupole force will be considered now. The first-order corrections to the quadrupole moments  $Q_{\mu}^{(1)}(n)$  and  $Q_{\mu}^{(1)}(p)$  vanish by previous arguments, as do  $\lambda_n^{(1)}$  and  $\lambda_p^{(1)}$ . From Eqs. (A1c) and (29), it is clear that  $\chi_{k_n -k_n}^{(1)} = \chi_{k_p -k_p}^{(1)} = 0$ , so that from Eq. (55),  $\Delta_n^{(1)} = \Delta_p^{(1)} = 0$ . The only correction to the self-consistent field  $\epsilon_n^{(1)}$ ,  $\epsilon_p^{(1)}$  come from the last term in Eq. (53a). Thus, from Eqs. (A1c) and (21), the first-order correction to, say, the neutron density matrix is

$$\rho_{k_n l_n}^{(1)} = \Omega j_{k_n l_n}^x (f_{k_n l_n}^-)^2 (E_{k_n l_n})^{-1} (1 + \phi_{k_n l_n}^-)^{-1}, \quad (56)$$

where

$$\phi_{k_n l_n}^{\pm} = G_n \zeta_{k_n} \zeta_{l_n} (f_{k_n l_n}^{\pm})^2 / E_{k_n l_n} \quad (57a)$$

and  $\rho_{k_p l_p}^{(1)}$  is obtained by interchanging  $n$  and  $p$  labels in Eqs. (56) and (57).

The moment of inertia [Eq. (46)] may be written

$$\mathcal{I} = \mathcal{I}_n + \mathcal{I}_p, \quad (58a)$$

where  $\mathcal{I}_n$  is the neutron contribution and  $\mathcal{I}_p$  the proton contribution and

$$\mathcal{I}_n = \sum_{k_n l_n} |j_{k_n l_n}^x|^2 |f_{k_n l_n}^-|^2 (E_{k_n l_n})^{-1} (1 + \phi_{k_n l_n}^-)^{-1}. \quad (58b)$$

The moment of inertia [Eq. (58)] differs from the original Beliaev value by an amount of the order of  $G/2\Delta$  of the Beliaev value.

Next, let us compute the  $\mathcal{B}$  coefficient [Eq. (45)]. It is first necessary to solve a set of inhomogeneous equations in second order.

From Eqs. (A2d), (21), (53), and (55), the neutron density matrix is given in second order by

$$\rho_{k_n l_n}^{(2)} = (1 - \phi_{k_n l_n}^+)^{-1} \left[ \Omega^2 \sum_{m_n} \frac{J_{k_n m_n} J_{m_n l_n} g_{k_n m_n}^+ f_{m_n l_n}^- f_{k_n l_n}^+}{E_{k_n l_n} E_{m_n l_n}} + \Omega^2 \sum_{m_n} \frac{J_{k_n m_n} J_{m_n l_n} f_{m_n k_n}^- g_{m_n l_n}^+ f_{l_n k_n}^+}{E_{k_n l_n} E_{k_n m_n}} \right. \\ \left. + \Omega^2 \sum_{m_n} \frac{J_{k_n m_n} J_{m_n l_n} f_{k_n m_n}^- f_{l_n m_n}^- g_{k_n l_n}^-}{E_{k_n m_n} E_{m_n l_n}} + \frac{(f_{k_n l_n}^+)^2}{E_{k_n l_n}} \sum_{\mu=-2}^2 q_{k_n l_n}^{(\mu)} (\kappa_n Q_{\mu}^{(2)*}(n) + \kappa_n p Q_{\mu}^{(2)*}(p)) \right. \\ \left. + \delta_{l_n k_n} \zeta_{k_n} \frac{\Delta_n^{(2)} f_{k_n k_n}^+ g_{k_n k_n}^- \theta_{k_n}}{2E_{k_n}} + \delta_{l_n k_n} \lambda_n^{(2)} \frac{(f_{k_n k_n}^+)^2}{2E_{k_n}} \right], \quad (59a)$$

where

$$J_{k_n l_n} \equiv j_{k_n l_n}^x - \Omega^{-1} \epsilon_{k_n l_n}^{(1)} = j_{k_n l_n}^x (1 + \phi_{k_n l_n}^-)^{-1}, \quad (60)$$

and the "diagonal" elements of the neutron pairing tensor are

$$\begin{aligned} \chi_{k_n - k_n}^{(2)} = & \Omega^2 \sum_{m_n} \frac{|J_{k_n m_n}|^2 f_{m_n k_n}^- g_{m_n k_n}^+ g_{k_n k_n}^-}{E_{k_n} E_{k_n m_n}} (1 - \phi_{k_n k_n}^+)^{-1} - \Omega^2 \sum_{m_n} \frac{|J_{k_n m_n}|^2 (f_{m_n k_n}^-)^2 f_{k_n k_n}^+}{(E_{k_n m_n})^2} (1 - \gamma_{k_n k_n}) \\ & + \frac{f_{k_n k_n}^+ g_{k_n k_n}^-}{2E_{k_n}} (1 - \phi_{k_n k_n}^+)^{-1} q_{k_n k_n}^{(0)} (\kappa_n Q_0^{(2)}(n) + \kappa_n p Q_0^{(2)}(p)) \\ & + \zeta_{k_n} \frac{(g_{k_n k_n}^-)^2 \theta_{k_n}}{2E_{k_n}} (1 - \phi_{k_n k_n}^+)^{-1} \Delta_n^{(2)} + \frac{f_{k_n k_n}^+}{2E_{k_n}} g_{k_n k_n}^- (1 - \phi_{k_n k_n}^+)^{-1} \lambda_n^{(2)}, \end{aligned} \quad (59b)$$

where

$$\gamma_{k_n l_n} \equiv \frac{G_n \zeta_{k_n} \zeta_{l_n} (g_{k_n l_n}^-)^2}{E_{k_n l_n}} \left( 1 - \frac{G_n \zeta_{k_n} \zeta_{l_n} (f_{k_n l_n}^+)^2}{E_{k_n l_n}} \right)^{-1}. \quad (57b)$$

In Eq. (59b), the assumption of cylindrical symmetry of the zero order single-particle potential has been used. The single-particle states are eigenfunctions of the  $z$  projection of the angular momentum, with corresponding quantum number  $K$ . According to the Wigner-Eckhardt theorem applied to the  $K$  quantum number,  $q_{kk}^{(\mu)}$  vanishes unless  $\mu = 0$ .

Substitution of Eqs. (59a) and (59b) into the definitions of  $Q_\mu^{(2)}(n)$ ,  $Q_\mu^{(2)}(p)$ ,  $\Delta_n^{(2)}$ ,  $\Delta_p^{(2)}$ , given by Eqs. (53b) and (55b), and use of the number conservation conditions [Eq. (51)], leads to the desired inhomogeneous equations for these quantities and the chemical potentials  $\lambda_n^{(2)}$ ,  $\lambda_p^{(2)}$ . Let us define certain coefficients of these linear equations as follows:

$$\begin{aligned} \Sigma_{\mu n} = \Sigma_{-\mu n} & \equiv \sum_{k_n l_n} |q_{k_n l_n}^{(\mu)}|^2 (f_{k_n l_n}^+)^2 (E_{k_n l_n})^{-1} (1 - \phi_{k_n l_n}^+)^{-1}, \\ \sigma_n & \equiv \frac{1}{2} \sum_{k_n} q_{k_n k_n}^{(0)} (f_{k_n k_n}^+)^2 (E_{k_n})^{-1} (1 - \phi_{k_n k_n}^+)^{-1}, \\ s_n & \equiv \frac{1}{2} \sum_{k_n} q_{k_n k_n}^{(0)} f_{k_n k_n}^+ g_{k_n k_n}^- \theta_{k_n} (E_{k_n})^{-1} (1 - \phi_{k_n k_n}^+)^{-1}, \\ a_n & \equiv \frac{1}{4} G_n \sum_{k_n} f_{k_n k_n}^+ g_{k_n k_n}^- \theta_{k_n} (E_{k_n})^{-1} (1 - \phi_{k_n k_n}^+)^{-1}, \\ b_n & \equiv \frac{G_n}{4} \sum_{k_n} (f_{k_n k_n}^+)^2 (E_{k_n})^{-1} (1 - \phi_{k_n k_n}^+)^{-1}, \\ c_n & \equiv \frac{G_n}{4} \sum_{k_n} \zeta_{k_n} (g_{k_n k_n}^-)^2 (E_{k_n})^{-1} (1 - \phi_{k_n k_n}^+)^{-1}, \end{aligned} \quad (61a)$$

$$\begin{aligned} \frac{\partial \mathcal{G}_n}{\partial Q_\mu^*(n)} & \equiv 4\kappa_n \sum_{k_n l_n m_n} \frac{q_{l_n k_n}^{(\mu)} J_{k_n m_n} J_{m_n l_n} f_{k_n l_n}^+ g_{k_n m_n}^+ f_{m_n l_n}^-}{E_{k_n l_n} E_{m_n l_n}} (1 - \phi_{k_n l_n}^+)^{-1} \\ & \quad + 2\kappa_n \sum_{k_n l_n m_n} \frac{q_{l_n k_n}^{(\mu)} J_{k_n m_n} J_{m_n l_n} g_{k_n l_n}^- f_{k_n m_n}^- f_{l_n m_n}^-}{E_{k_n m_n} E_{m_n l_n}} (1 - \phi_{k_n l_n}^+)^{-1}, \\ \frac{\partial \mathcal{G}_n}{\partial \Delta_n} & \equiv 2 \sum_{k_n l_n} \frac{\zeta_{k_n} |J_{k_n l_n}|^2 f_{l_n k_n}^- g_{k_n l_n}^+ g_{k_n k_n}^- \theta_{k_n}}{E_{k_n} E_{k_n l_n}} (1 - \phi_{k_n k_n}^+)^{-1} - 2 \sum_{k_n l_n} \frac{|J_{k_n l_n}|^2 (f_{k_n l_n}^-)^2 f_{k_n k_n}^+ \theta_{k_n}}{(E_{k_n l_n})^2} (1 - \gamma_{k_n k_n}), \\ \frac{\partial \mathcal{G}_n}{\partial \lambda_n} & \equiv 2 \sum_{k_n l_n} \frac{|J_{k_n l_n}|^2 f_{l_n k_n}^- g_{k_n l_n}^+ f_{k_n k_n}^+}{E_{k_n} E_{k_n l_n}} (1 - \phi_{k_n k_n}^+)^{-1} + 2 \sum_{k_n l_n} \frac{|J_{k_n l_n}|^2 (f_{k_n l_n}^-)^2 g_{k_n k_n}^-}{(E_{k_n l_n})^2} (1 - \phi_{k_n k_n}^+)^{-1}. \end{aligned} \quad (61b)$$

The corresponding proton contributions  $\Sigma_{\mu p}, \dots, \partial \mathcal{G}_p / \partial Q_\mu^*(p)$ , etc., are obtained by substituting the labels  $p$  in place of  $n$  in Eq. (61). The quantities, Eq. (61b), are partial derivatives of the moment of inertia, Eq. (58b), which depends on the  $\Delta$ 's,  $\lambda$ 's, and  $Q_\mu$ 's through the single-particle states. The derivative  $\partial \mathcal{G}_n / \partial Q_\mu^*(n)$ , for example, is defined with the other  $Q_\mu$ 's,  $\Delta$ 's, and  $\lambda$ 's being held constant, and the same is true for the other derivatives. The derivatives are evaluated at the equilibrium values  $Q_\mu^{(0)}$ ,  $\Delta^{(0)}$ , and  $\lambda^{(0)}$ . Since the equilibrium shape is axial  $Q_{\pm 2}^{(0)}(n) = Q_{\pm 2}^{(0)}(p) = 0$ .

The recognition that the right-hand sides of Eqs. (61b) correspond to the derivatives comes easily by differentiating the general moment of inertia formula given by Eq. (44) and from the known dependence of the density matrix on the  $Q_\mu$ ,  $\Delta$ , and  $\lambda$ .

The linear equations for the second order changes in the quadrupole moments, gap parameters, and Lagrange multipliers break up into subsets corresponding to  $\mu=0, \pm 1, \pm 2$ , when the Wigner-Eckhardt theorem is applied to the  $K$  quantum number.

For  $\mu=0$ , the equations are

$$\begin{array}{llllll}
 Q_0^{(2)}(n)(1-\kappa_n \Sigma_{0n}) & -Q_0^{(2)}(p)\kappa_{np} \Sigma_{0n} & -\Delta_n^{(2)} s_n & & -\lambda_n^{(2)} \sigma_n & = \Omega^2(1/2\kappa_n)[\partial \mathcal{G}_n / \partial Q_0(n)] \\
 -Q_0^{(2)}(n)\kappa_{np} \Sigma_{0p} & +Q_0^{(2)}(p)(1-\kappa_p \Sigma_{0p}) & & -\Delta_p^{(2)} s_p & & = \Omega^2(1/2\kappa_p)[\partial \mathcal{G}_p / \partial Q_0(p)] \\
 -Q_0^{(2)}(n)\frac{1}{2}\kappa_n G_n s_n & -Q_0^{(2)}(p)\frac{1}{2}\kappa_p G_n s_n & +\Delta_n^{(2)}(1-c_n) & & -\lambda_n^{(2)} a_n & = \Omega^2(G_n/4)(\partial \mathcal{G}_n / \partial \Delta_n) \\
 -Q_0^{(2)}(n)\frac{1}{2}\kappa_{np} G_p s_p & -Q_0^{(2)}(p)\frac{1}{2}\kappa_p G_p s_p & & +\Delta_p^{(2)}(1-c_p) & & = \Omega^2(G_p/4)(\partial \mathcal{G}_p / \partial \Delta_p) \\
 -Q_0^{(2)}(n)\kappa_n \sigma_n & -Q_0^{(2)}(p)\kappa_{np} \sigma_n & -\Delta_n^{(2)} 2a_n / G_n & & -\lambda_n^{(2)} 2b_n / G_n & = \frac{1}{2}\Omega^2(\partial \mathcal{G}_n / \partial \lambda_n) \\
 -Q_0^{(2)}(n)\kappa_{np} \sigma_p & -Q_0^{(2)}(p)\kappa_p \sigma_p & & -\Delta_p^{(2)} 2a_p / G_p & & -\lambda_p^{(2)} 2b_p / G_p = \frac{1}{2}\Omega^2(\partial \mathcal{G}_p / \partial \lambda_p),
 \end{array} \quad (62a)$$

where  $Q_0^{(2)}$  has been taken to be real.

The solutions for  $\Delta_n^{(2)}$  and  $\lambda_n^{(2)}$  will be given in terms of the changes in the quadrupole moments

$$\Delta_n^{(2)} = \frac{1}{4}\Omega^2 G_n \frac{b_n d\mathcal{G}_n / d\Delta_n - 2(a_n \sigma_n - b_n s_n)(\kappa_n Q_0^{(2)}(n) + \kappa_{np} Q_0^{(2)}(p))\Omega^{-2}}{a_n^2 + b_n(1-c_n)}, \quad (63a)$$

$$\lambda_n^{(2)} = -\frac{1}{4}\Omega^2 G_n \frac{a_n \partial \mathcal{G}_n / \partial \Delta_n + (1-c_n) \partial \mathcal{G}_n / \partial \lambda_n + 2[a_n s_n + (1-c_n)\sigma_n](\kappa_n Q_0^{(2)}(n) + \kappa_{np} Q_0^{(2)}(p))\Omega^{-2}}{a_n^2 + b_n(1-c_n)}, \quad (63b)$$

where

$$\frac{d\mathcal{G}_n}{d\Delta_n} = \frac{\partial \mathcal{G}_n}{\partial \Delta_n} + \frac{\partial \lambda_n}{\partial \Delta_n} \frac{\partial \mathcal{G}_n}{\partial \lambda_n}, \quad \frac{\partial \lambda_n}{\partial \Delta_n} = -\frac{a_n}{b_n}. \quad (64)$$

The quantity  $\partial \lambda_n / \partial \Delta_n$  is obtained from the next-to-last of Eqs. (62a), with the  $Q_0$  (and the number of particles) held constant, and the right-hand side set equal to zero. The quantities  $\Delta_p^{(2)}$  and  $\lambda_p^{(2)}$  are obtained from the above by interchange of neutron and proton labels. The quadrupole moments are given by

$$Q_0^{(2)}(n) = \frac{1}{2}\Omega^2 \left[ C_{0p} \frac{d\mathcal{G}_n}{dQ_0(n)} + \kappa_{np} \left(1 - \frac{C_{0n}}{\kappa_n}\right) \frac{d\mathcal{G}_p}{dQ_0(p)} \right] / \left[ C_{0n} C_{0p} - \kappa_{np}^2 \left(1 - \frac{C_{0n}}{\kappa_n}\right) \left(1 - \frac{C_{0p}}{\kappa_p}\right) \right], \quad (65a)$$

where the derivatives are defined by

$$\frac{d\mathcal{G}_n}{dQ_0(n)} = \frac{\partial \mathcal{G}_n}{\partial Q_0(n)} + \frac{\partial \mathcal{G}_n}{\partial \Delta_n} \frac{\partial \Delta_n}{\partial Q_0(n)} + \frac{\partial \mathcal{G}_n}{\partial \lambda_n} \frac{\partial \lambda_n}{\partial Q_0(n)}. \quad (66)$$

That is, when taking the derivatives only the other  $Q_\mu$  are held constant, but  $\Delta_n$  and  $\lambda_n$  are allowed to vary. From Eqs. (63) with the right-hand side set equal to zero,

$$\frac{\partial \Delta_n}{\partial Q_0(n)} = -\frac{1}{2} \frac{G_n \kappa_n (a_n \sigma_n - b_n s_n)}{a_n^2 + b_n(1-c_n)}, \quad \frac{\partial \lambda_n}{\partial Q_0(n)} = -\frac{1}{2} \frac{G_n \kappa_n [a_n s_n + (1-c_n)\sigma_n]}{a_n^2 + b_n(1-c_n)}. \quad (67)$$

The quantity  $C_{0n}$  is defined by

$$C_{0n} \equiv \kappa_n - \kappa_n^2 \Sigma_{0n} + \kappa_n^2 \frac{G_n s_n (a_n \sigma_n - b_n s_n) + \sigma_n [a_n s_n + (1-c_n)\sigma_n]}{2(a_n^2 + b_n(1-c_n))}. \quad (68a)$$

The proton moment  $Q_0^{(2)}(p)$  is obtained by interchanging  $n$  and  $p$  labels in Eqs. (65)–(68).

For  $\mu=\pm 1, \pm 2$ , the linear equations are

$$\begin{array}{l}
 Q_\mu^{(2)}(n)(1-\kappa_n \Sigma_{\mu n}) - Q_\mu^{(2)}(p)\kappa_{np} \Sigma_{\mu n} = \Omega^2(1/2\kappa_n)[\partial \mathcal{G}_n / \partial Q_\mu(n)^*], \\
 -Q_\mu^{(2)}(n)\kappa_{np} \Sigma_{\mu p} + Q_\mu^{(2)}(p)(1-\kappa_p \Sigma_{\mu p}) = \Omega^2(1/2\kappa_p)[\partial \mathcal{G}_p / \partial Q_\mu(p)^*].
 \end{array} \quad (62b)$$

From (61b) and the time-reversal properties of the matrix element (8) and (54), it is easy to show that

$$\partial \mathcal{G}_n / \partial Q_{\pm 1}(n)^* = \partial \mathcal{G}_p / \partial Q_{\pm 1}(p)^* = 0, \quad (69)$$

so that for  $\mu = \pm 1$ , (62b) become homogeneous with the trivial solutions

$$Q_{\pm 1}^{(2)}(n) = Q_{\pm 1}^{(2)}(p) = 0. \quad (70a)$$

Equation (70a) is necessary if the rotating reference frame is to coincide with the principal axes of the density distribution.<sup>10</sup>

For  $\mu = 2$ , Eq. (62b) yields, analogously to (65a),

$$Q_2^{(2)}(n) = \frac{1}{2}\Omega^2 \left[ C_{2p} \frac{\partial g_n}{\partial Q_2(n)^*} + \kappa_{np} \left( 1 - \frac{C_{2n}}{\kappa_n} \right) \frac{\partial g_p}{\partial Q_2(p)^*} \right] / \left[ C_{2n} C_{2p} - \kappa_{np}^2 \left( 1 - \frac{C_{2n}}{\kappa_n} \right) \left( 1 - \frac{C_{2p}}{\kappa_p} \right) \right], \quad (65b)$$

where

$$C_{2n} = C_{-2n} = \kappa_n - \kappa_n^2 \Sigma_{2n}. \quad (68b)$$

The equation for  $Q_2^{(2)}(p)$  is obtained by interchange of  $n$  and  $p$  labels.

In this order of perturbation theory, the change in the moments  $Q_2(n)$  and  $Q_2(p)$  are independent of changes in the  $\Delta$ 's and the  $\lambda$ 's, which are coupled only to  $Q_0(n)$  and  $Q_0(p)$ . Thus  $\partial g_n / \partial Q_2(n)^*$  is the derivative holding only the  $Q_{-2}$ 's and  $Q_0$ 's constant.

For  $\mu = -2$ , Eq. (62b) just yields

$$\begin{aligned} Q_{-2}^{(2)}(n) &= Q_2^{(2)}(n)^*, \\ Q_{-2}^{(2)}(p) &= Q_2^{(2)}(p)^*. \end{aligned} \quad (65c)$$

One can choose a representation with real matrix ele-

ments so that

$$\begin{aligned} Q_{-2}^{(2)}(n) &= Q_2^{(2)}(n), \\ Q_{-2}^{(2)}(p) &= Q_2^{(2)}(p), \end{aligned} \quad (70b)$$

which, together with (70a) guarantees that the rotating reference frame coincides with the principal axes of the density distribution.<sup>10</sup>

Assuming that (70b) holds, the derivatives of the moments of inertia with respect to the  $Q_2$ 's are real, and it is best to introduce the derivative  $d\mathcal{G}/dQ_2$  by

$$\frac{1}{2}(d\mathcal{G}/dQ_2) \equiv (\partial\mathcal{G}/\partial Q_2)_{Q_{-2}, Q_0} = (\partial\mathcal{G}/\partial Q_{-2})_{Q_2, Q_0}. \quad (71)$$

In the derivatives  $\partial\mathcal{G}/\partial Q_2$ ,  $Q_{-2}$  and  $Q_0$  are held constant, while in  $d\mathcal{G}/dQ_2$ , it is assumed that  $Q_{-2} = Q_2$ , and only  $Q_0$  is held constant, so that (65b) may be written

$$Q_2^{(2)}(n) = \frac{1}{4}\Omega^2 \left[ C_{2p} \frac{d g_n}{d Q_2(n)} + \kappa_{np} \left( 1 - \frac{C_{2n}}{\kappa_n} \right) \frac{d g_p}{d Q_2(p)^*} \right] / \left[ C_{2n} C_{2p} - \kappa_{np}^2 \left( 1 - \frac{C_{2n}}{\kappa_n} \right) \left( 1 - \frac{C_{2p}}{\kappa_p} \right) \right]. \quad (65b')$$

Let us now discuss the physical significance of the results given by Eqs. (63) and (65). The quantities  $C_{\mu n}$  and  $C_{\mu p}$  are adiabatic vibrational force constants defined in the following way. Collective vibrational states may be described by means of the rigorously quantal random phase approximation (RPA)<sup>50</sup> or else by means of the ostensibly semiclassical time-dependent HFB equations.<sup>52</sup> Both methods give exactly the same dispersion equations for the frequencies of collective excitations. The energy in the time-dependent method for a given normal mode of vibration has the schematic form (for a multipole-multipole interaction) in terms of normal coordinates,  $Q_\mu$ :

$$E_\mu = \frac{1}{2}B(\omega) |dQ_\mu(t)/dt|^2 + \frac{1}{2}C(\omega) |Q_\mu(t)|^2,$$

where  $Q_\mu(t)$  is a linear combination of oscillating multipole moments;  $B(\omega)$  is a mass parameter and  $C(\omega)$  is a force constant, and both, in general, depend upon the frequency of oscillation,  $\omega$ .<sup>19</sup>

The energy in the time-dependent method can be regarded as a collective-model Hamiltonian, which, when (second-) quantized gives the RPA Hamiltonian. If the frequency  $\omega$  is small compared to quasiparticle excita-

tion energies, one may use the adiabatic approximation and set  $\omega = 0$  in  $B(\omega)$  and  $C(\omega)$ .

For the case of  $\gamma$  vibrations of deformed nuclei, for example, the collective potential energy when  $\kappa_{np} = 0$  is then given by

$$V = \frac{1}{2}C_{2n} (|\delta Q_2(n)|^2 + |\delta Q_{-2}(n)|^2) + \frac{1}{2}C_{2p} (|\delta Q_2(p)|^2 + |\delta Q_{-2}(p)|^2), \quad (72a)$$

where  $\delta Q_2(n)$  is a small displacement from the equilibrium quadrupole moment.

In the limit when all the interactions have the same strength  $\kappa_n = \kappa_p = \kappa_{np} \equiv \kappa$ , the potential energy takes the form

$$V = \frac{1}{2}(C_{2n} + C_{2p} - \kappa) (|\delta Q_2(n) + \delta Q_2(p)|^2 + |\delta Q_{-2}(n) + \delta Q_{-2}(p)|^2). \quad (72b)$$

For the problem considered here, one has an effective potential energy given by

$$V = \frac{1}{2} \sum_\mu \mathcal{C}_{\mu n} |\delta Q_\mu(n)|^2 + \frac{1}{2} \sum_\mu \mathcal{C}_{\mu p} |\delta Q_\mu(p)|^2 + \sum_\mu \mathcal{C}_{\mu n p} \delta Q_\mu(n) \delta Q_\mu(p), \quad (72c)$$

where

$$\begin{aligned} \mathcal{C}_{\mu n} &= C_{\mu n} - \kappa_{np}^2 \kappa_p^{-1} (1 - \kappa_p^{-1} C_{\mu p}), \\ \mathcal{C}_{\mu n p} &= -\kappa_{np} (1 - \kappa_n^{-1} C_{\mu n} - \kappa_p^{-1} C_{\mu p}). \end{aligned} \quad (72d)$$

<sup>52</sup> The time-dependent equations are just an average of the Heisenberg equations of motion of the RPA theory taken with respect to a time-dependent state vector.

Equation (72c) reduces to Eq. (72a) or Eq. (72b) in the appropriate limits.

The centrifugal stretching given by Eqs. (65) corresponds exactly to the "classical" result, well known in the theory of molecules,<sup>53</sup> obtained by adding the rotational kinetic energy (with a quadrupole moment-dependent moment of inertia) to (72c) and minimizing the result with respect to the quadrupole moments. The results (63) for the changes in the gap parameters are obtained analogously, although perhaps these quantities are not genuine vibrational coordinates. It is quite plausible that the classical centrifugal stretching should have been obtained, since the HFB procedure for the case of the quadrupole force is equivalent to minimizing the expectation value of the Hamiltonian (7), which includes the angular momentum constraint with respect to the quadrupole moments and gap parameters, which closely resembles the classical procedure.

In a previous semiphenomenological attempt to calculate vibration-rotation coefficients, somewhat different force constants were arbitrarily used.<sup>37</sup> The elasticity constants used in Ref. 37 were first defined by Kisslinger and Sorensen<sup>38</sup> as the response of the nucleus to an external deforming force. Within the framework of the HFB method, the external deforming force can correspond to the constraint that the mass quadrupole moments have prescribed values. One can then treat by the methods previously described the perturbation

$$-\sum_{\mu} \xi_n^{(\mu)} \hat{Q}_{\mu}(n) - \sum_{\mu} \xi_p^{(\mu)} \hat{Q}_{\mu}(p),$$

where

$$\hat{Q}_{\mu}(n) = \sum_{k_n l_n} q_{k_n l_n}^{(\mu)} a_{k_n}^{\dagger} a_{l_n}.$$

The perturbation increment in energy in lowest order has the form (72c), but  $\mathcal{C}_{\mu n}$ ,  $\mathcal{C}_{\mu p}$ , and  $\mathcal{C}_{\mu n p}$  have a different dependence on  $C_{\mu n}$ ,  $C_{\mu p}$  than given by (72d). In the case when  $\kappa_{np} = 0$ , for example, the neutron elasticity constant as defined by Kisslinger and Sorensen is

$$\mathcal{C}_{\mu n}(\text{K.S.}) = \frac{C_{\mu n}}{1 - C_{\mu n}/\kappa_n},$$

which is greater than the value given by (72), unless  $C_{0n} = 0$ , but this can only happen if the RPA dispersion equations have the solution  $\omega = 0$ , which means that the vibrational mode is on the bound of instability.<sup>54</sup>

In fact, as the strength parameters  $\kappa_n$ ,  $\kappa_p$ ,  $\kappa_{np}$  are increased, the denominators of Eqs. (65) tend to zero, corresponding to instability of the RPA solution, and the whole treatment breaks down. Thus, there is a paradox here. Although, as previously noted, our treatment of the Coriolis perturbation is expected to be valid when

the collective vibrations are adiabatic, the perturbation theory breaks down if they are too adiabatic. The intimate connection between the RPA and the present HFB treatment is due to the fact that the determinant of Eqs. (62) is essentially the adiabatic limit of the determinant of the homogeneous equations of the RPA theory.<sup>55,56</sup>

It is of interest to consider the sign of  $\Delta_n^{(2)}$  [Eq. (63a)], which consists of positive and negative contributions. According to (61a),  $a_n$  and  $s_n$  are sums of positive and negative contributions which largely cancel out, except for  $b_n$  and  $c_n$  which are sums of positive terms. Thus  $\Delta_n^{(2)}$  is roughly given by

$$\Delta_n^{(2)} \approx -\frac{\Omega^2}{4} \frac{d g_n / d \Delta_n}{1 - c_n}.$$

With the aid of the gap equation (12), it is easy to establish the inequality  $(1 - c_n) > 0$ , so that the gap parameters  $\Delta_n$  and  $\Delta_p$  are expected to decrease as a consequence of the Coriolis perturbation, since  $d g_n / d \Delta_n < 0$ , in analogy with the pair-destroying effect of a magnetic field on a superconductor.

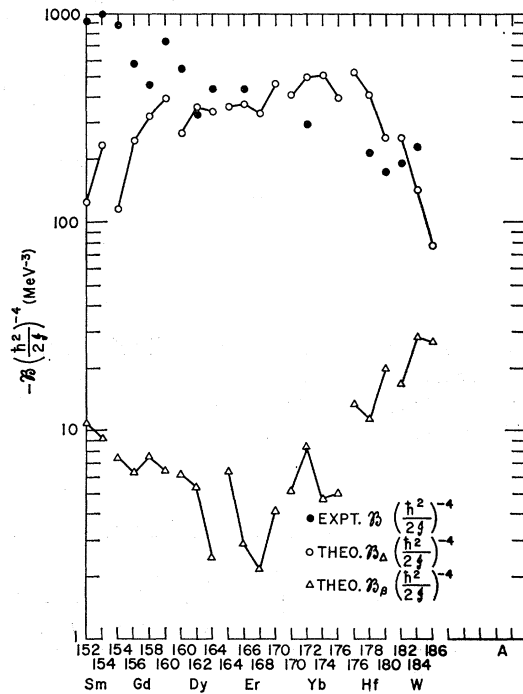


FIG. 1. Theoretical values of  $-\mathcal{B}_{\Delta}/(\hbar^2/2g)^4$  and  $-\mathcal{B}_{\beta}/(\hbar^2/2g)^4$  in the rare-earth region. The experimental points refer to the total  $\mathcal{B}$  as obtained from the ground-state rotational band, using at least the first three members. The vertical scale is semilog because of the great differences in magnitude of the points plotted.

<sup>55</sup> D. R. Bés, Nucl. Phys. **49**, 544 (1963).

<sup>56</sup> In Ref. 55, the change in the expectation value of the particle number due to deviation of the wave function from the BCS form was not kept at zero as was done in the present work. In fact there is no need for such a correction in the lowest RPA, where rotation-vibration coupling is neglected. Thus Eq. (62a) has two additional rows and columns arising from the neutron and proton number corrections, for which there is no counterpart in Ref. 55.

<sup>53</sup> G. Herzberg, *Spectra of Diatomic Molecules* (D. van Nostrand Inc., New York, 1959), p.103.

<sup>54</sup> Another difference in the treatment of Ref. 37 is that it is based on the work of Ref. 39 in which the Kisslinger-Sorensen approach was applied to the case of interacting neutrons and protons, but with the potential energy corresponding to Eq. (72) differing slightly from the present work.

From Eqs. (A3c) and (21), 3rd-order corrections to the density matrix are given by

$$\begin{aligned}
(1+\phi_{kl}^-)\rho_{kl}^{(3)} = & -\Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}f_{kn}^-f_{mn}^-f_{ml}^-f_{kl}^-}{E_{kn}E_{ml}E_{kl}} - \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}f_{kn}^-f_{mn}^-f_{ml}^-f_{kl}^-}{E_{kn}E_{nm}E_{ml}} \\
& + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}g_{kn}^+f_{nm}^-f_{lm}^-g_{kl}^+}{E_{km}E_{nm}E_{ml}} + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}f_{kn}^-f_{mn}^-g_{ml}^+g_{kl}^+}{E_{kn}E_{nm}E_{nl}} \\
& + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}g_{kn}^+g_{nm}^+f_{ml}^-f_{kl}^-}{E_{kl}E_{nl}E_{ml}} + \Omega^3 \sum_{nm} \frac{J_{kn}J_{nm}J_{ml}f_{nk}^-g_{nm}^+g_{ml}^+f_{lk}^-}{E_{kn}E_{km}E_{kl}} \\
& + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}f_{kn}^-g_{nm}^+f_{ml}^-g_{kl}^+\theta_n\theta_l}{E_{kn}E_{km}E_{ml}} + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}f_{kn}^-g_{nm}^+f_{ml}^-g_{kl}^+\theta_n\theta_l}{E_{kn}E_{nl}E_{ml}} \\
& + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}g_{kn}^+f_{nm}^-g_{ml}^+f_{lk}^- \theta_m\theta_k}{E_{kl}E_{nm}E_{nl}} + \Omega^3 \sum_{mn} \frac{J_{kn}J_{nm}J_{ml}g_{kn}^+f_{nm}^-g_{ml}^+f_{lk}^- \theta_m\theta_k}{E_{kl}E_{nm}E_{km}} \\
& - \Omega \sum_m \frac{[(\epsilon_{km}^{(2)} - \lambda^{(2)}\delta_{km})f_{km}^+ + \Delta_{k-m}^{(2)}\delta_{mk}g_{km}^-]J_{ml}f_{lm}^-g_{kl}^+}{E_{km}E_{ml}} \\
& - \Omega \sum_m \frac{J_{km}[(\epsilon_{ml}^{(2)} - \lambda^{(2)}\delta_{ml})f_{lm}^+ + \Delta_{l-m}^{(2)}\delta_{ml}g_{lm}^-]f_{km}^-g_{kl}^+}{E_{km}E_{ml}} \\
& - \Omega \sum_m \frac{[(\epsilon_{km}^{(2)} - \lambda^{(2)}\delta_{km})g_{km}^- - \Delta_{k-m}^{(2)}\delta_{mk}f_{km}^+]J_{ml}f_{ml}^-f_{kl}^-}{E_{kl}E_{ml}} \\
& - \Omega \sum_m \frac{J_{km}[(\epsilon_{ml}^{(2)} - \lambda^{(2)}\delta_{ml})g_{ml}^- - \Delta_{m-l}^{(2)}\delta_{ml}f_{ml}^+]f_{mk}^-f_{lk}^-}{E_{km}E_{kl}} \\
& - \Omega \sum_m \frac{[(\epsilon_{km}^{(2)} - \lambda^{(2)}\delta_{km})f_{mk}^+ + \Delta_{m-k}^{(2)}\delta_{mk}g_{km}^-]J_{ml}g_{ml}^+f_{lk}^-}{E_{km}E_{kl}} \\
& - \Omega \sum_m \frac{J_{km}[(\epsilon_{ml}^{(2)} - \lambda^{(2)}\delta_{ml})f_{ml}^+ + \Delta_{m-l}^{(2)}\delta_{ml}g_{ml}^-]g_{km}^+f_{kl}^-}{E_{kl}E_{ml}}, \tag{73}
\end{aligned}$$

where the summation indices either all refer to neutron or all to proton single-particle states, and correspondingly  $\lambda$  is either  $\lambda_n$  or  $\lambda_p$ , depending on whether  $\rho_{kl}^{(3)}$  is a neutron or proton density matrix element.

Since  $\epsilon_{kl}^{(2)}$  and  $\Delta_{k-k}^{(2)}$  are given completely by Eqs. (53a), (55a), (63), and (65), the  $\mathfrak{B}$  coefficient can be evaluated from the definition (45). After permuting indices and doing a little algebra, one obtains

$$\mathfrak{B} = \mathfrak{B}_\beta + \mathfrak{B}_\gamma + \mathfrak{B}_\Delta + \mathfrak{B}_\lambda + \mathfrak{B}_{\text{Coriolis}}. \tag{74a}$$

The contribution  $\mathfrak{B}_\beta$  arises from the centrifugal stretching of the  $Q_0(n)$  and  $Q_0(p)$  moments and is given by

$$\mathfrak{B}_\beta = -\frac{\hbar^4}{8g^4} \frac{\left(\frac{d\mathcal{G}_n}{dQ_0(n)}\right)^2 \left[ C_{0p} \left(1 - \frac{\kappa_n p^2}{\kappa_n \kappa_p}\right) + \frac{\kappa_n p^2}{\kappa_n} \right] + \left(\frac{d\mathcal{G}_p}{dQ_0(p)}\right)^2 \left[ C_{0n} \left(1 - \frac{\kappa_n p^2}{\kappa_n \kappa_p}\right) + \frac{\kappa_n p^2}{\kappa_p} \right] + 2\kappa_{np} \frac{d\mathcal{G}_n}{dQ_0(n)} \frac{d\mathcal{G}_p}{dQ_0(p)}}{C_{0n}C_{0p} - \kappa_{np}^2 \left(1 - \frac{C_{0n}}{\kappa_n}\right) \left(1 - \frac{C_{0p}}{\kappa_p}\right)}. \tag{74b}$$

The contribution  $\mathfrak{B}_\gamma$  arises from the centrifugal stretching of the  $Q_2(n) = Q_{-2}(n)$  and  $Q_2(p) = Q_{-2}(p)$  moments and is given by

$$\mathfrak{B}_\gamma = -\frac{\hbar^4}{16g^4} \frac{\left(\frac{d\mathcal{G}_n}{dQ_2(n)}\right)^2 \left[ C_{2p} \left(1 - \frac{\kappa_n p^2}{\kappa_n \kappa_p}\right) + \frac{\kappa_n p^2}{\kappa_n} \right] + \left(\frac{d\mathcal{G}_p}{dQ_2(p)}\right)^2 \left[ C_{2n} \left(1 - \frac{\kappa_n p^2}{\kappa_n \kappa_p}\right) + \frac{\kappa_n p^2}{\kappa_p} \right] + 2\kappa_{np} \frac{d\mathcal{G}_n}{dQ_2(n)} \frac{d\mathcal{G}_p}{dQ_2(p)}}{C_{2n}C_{2p} - \kappa_{np}^2 \left(1 - \frac{C_{2n}}{\kappa_n}\right) \left(1 - \frac{C_{2p}}{\kappa_p}\right)}. \tag{74c}$$

The contribution  $\mathfrak{B}_\Delta$  arises from the decrease in  $\Delta$  and the corresponding change in  $\lambda$  for fixed nuclear deformation and particle number. The term  $\mathfrak{B}_\lambda$  arises from the change in the  $\lambda$ , for fixed particle number and fixed  $\Delta$ , due to the effect of the Coriolis perturbation on the individual quasiparticle structure:

$$\mathfrak{B}_\Delta = -\frac{\hbar^4 G_n}{g^4 16} \frac{b_n (d\mathcal{G}_n/d\Delta_n)^2}{a_n^2 + b_n(1-c_n)} + \text{corresponding proton term}, \quad (74d)$$

$$\mathfrak{B}_\lambda = +\frac{\hbar^4 G_n}{g^4 16} \frac{(\partial\mathcal{G}_n/\partial\lambda_n)^2}{b_n} + \text{corresponding proton term}. \quad (74e)$$

The contribution  $\mathfrak{B}_{\text{Coriolis}}$  arises from the effect of the Coriolis perturbation on the individual quasiparticle structure, independent of changes in the quadrupole field, pairing potentials, and Lagrange multipliers:

$$\begin{aligned} \mathfrak{B}_{\text{Coriolis}} = & -\frac{\hbar^4}{g^4} \sum_{klmn}^{(n)} \frac{J_{kn} J_{nm} J_{ml} J_{lk} g_{kn}^+ f_{nm}^- f_{lm}^- g_{lk}^+}{E_{km} E_{mn} E_{ml}} (1-\phi_{km}^+)^{-1} + \frac{\hbar^4}{g^4} \sum_{lkmn}^{(n)} \frac{J_{kn} J_{nm} J_{ml} J_{lk} f_{kn}^- g_{nm}^+ f_{lm}^- g_{lk}^+ \theta_m \theta_n}{E_{km} E_{kn} E_{ml}} \\ & \times (1-\phi_{km}^+)^{-1} + \frac{\hbar^4}{2g^4} \sum_{klmn}^{(n)} \frac{J_{kn} J_{nm} J_{ml} J_{lk} f_{kn}^- f_{mn}^- f_{ml}^- f_{kl}^-}{E_{kn} E_{mn} E_{ml}} (1-\mu_{klm}) + \text{corresponding proton contributions}, \end{aligned} \quad (74f)$$

where

$$\mu_{klm} \equiv G_n \frac{(g_{km}^-)^2 E_{kl}^{-1} - 4f_{mk}^+ g_{km}^- g_{lk}^+ (f_{lk}^-)^{-1} E_{km}^{-1}}{1 - G_n (f_{km}^+)^2 E_{km}^{-1}} \cdot \zeta_k \zeta_m. \quad (75)$$

The symbol  $\sum^{(n)}$  means that all the summation indices refer to neutron single-particle states. For each neutron term in (74f), there is a corresponding proton term. Equation (74f) includes contributions due to changes in the self-consistent field associated with the pairing force because of the use of the matrix elements  $J_{kl}$  instead of  $j_{kl}^\pi$  and because of the terms  $\phi_{km}^+$  and  $\mu_{klm}$ . These are corrections proportional to  $\frac{1}{2}G\Delta^{-1}$ , but it is clear that these corrections accumulate in higher order.

Further discussion of Eq. (74) will be deferred until the last section.

#### IV. APPROXIMATE CALCULATIONS

The quantities  $\mathfrak{B}_\beta$  and  $\mathfrak{B}_\gamma$  [Eqs. (74b) and (74c)] have the form of a vibration-rotation interaction, with  $\mathfrak{B}_\beta$  corresponding to the mixing of the ground-state band with the  $\beta$ -vibrational band, and  $\mathfrak{B}_\gamma$  corresponding to the mixing with the  $\gamma$ -vibrational band. For the case  $\kappa_{np} = \kappa_n = \kappa_p = \kappa$ , and  $Q_\mu \equiv Q_\mu(n) + Q_\mu(p)$ , one obtains

$$\mathfrak{B}_\beta = -\frac{\hbar^4}{8g^4} \frac{(d\mathcal{G}/dQ_0)^2}{C_{0n} + C_{0p} - \kappa}, \quad (76a)$$

$$\mathfrak{B}_\gamma = -\frac{\hbar^4}{16g^4} \frac{(d\mathcal{G}/dQ_2)^2}{C_{2n} + C_{2p} - \kappa}, \quad (76b)$$

which agrees with the collective-model result (2), if one defines new variables  $\beta$  and  $\gamma$  by  $Q_0 \propto \beta \cos\gamma$ , and  $Q_2 \propto (2)^{-1/2} \beta \sin\gamma$ , so that  $C_\beta \propto C_{0n} + C_{0p} - \kappa$ , and  $C_\gamma \propto \beta_0^2 (C_{2n} + C_{2p} - \kappa)$ . For the case when the spatial dependence of the spherical part of the self-consistent field is given by the harmonic oscillator  $V = \frac{1}{2}m\omega_0^2 r^2$ , and the  $Q_\mu$  are mass quadrupole moments, one has

$Q_0 = m\omega_0^2 \kappa^{-1} \beta \cos\gamma$ , etc. If one further argues that the strength of the quadrupole force should be chosen so that the shape of the ellipsoidal self-consistent field coincides with the shape of the average density distribution, one obtains<sup>57</sup>

$$\kappa = (4\pi/5)(m\omega_0^2 / \langle \sum r^2 \rangle). \quad (77)$$

Furthermore, if the quadrupole-quadrupole force acts between all pairs of nucleons, the mean-square radius per nucleon is given by  $\langle \sum r^2 \rangle / A = \frac{3}{5} R_0^2$ , with  $R_0 \sim 1.2 A^{1/3} \times 10^{-13}$  cm. Then the mass quadrupole moments are given by  $Q_0 = (3/4\pi) A R_0^2 \beta \cos\gamma$ ,  $Q_2 = (2)^{-1/2} (3/4\pi) A R_0^2 \beta \times \sin\gamma$  as for a uniform charge distribution. The force constants for  $\beta$  and  $\gamma$  vibration are then given by

$$C_\beta = \left( \frac{3}{4\pi} A R_0^2 \right)^2 \left( C_{0n} + C_{0p} - \frac{4\pi m\omega_0^2}{3 A R_0^2} \right), \quad (78a)$$

$$C_\gamma = \left( \frac{3}{4\pi} A R_0^2 \right)^2 \left( C_{2n} + C_{2p} - \frac{4\pi m\omega_0^2}{3 A R_0^2} \right). \quad (78b)$$

It is easy to obtain approximate estimates of  $\mathfrak{B}_\beta$  corresponding to (78a) based on already available calculations. Nilsson and Prior had calculated the moment of inertia using Eqs. (58) (with  $\phi_{kl} = 0$ ) for three values of  $\beta$  for each nucleus in the rare-earth region,<sup>24</sup> from which data it is possible to estimate the derivative  $d\mathcal{G}/d\beta$ . It is interesting to note that if one fits their calculated data with the expansion

$$\mathcal{G} = A\beta^2 + B\beta^3 + C\beta^4, \quad (79)$$

<sup>57</sup> B. Mottelson, in *Proceedings of the International School of Physics, "Enrico Fermi," XV Course*, edited by G. Racah (Academic Press Inc., New York, 1962), p. 51.



one finds that the successive terms are all of about the same order of magnitude, suggesting that such an expansion converges poorly, if at all, for typical equilibrium values of  $\beta$  in the rare-earth region. This result conflicts with a common assumption used in many exploitations of the phenomenological collective model, that (79) or its leading term is valid for strongly deformed nuclei.<sup>14,58</sup> Of course, one may define a new collective coordinate so that  $\mathcal{J}$  depends on it quadratically, but this is not what is usually done. In the present calculations, an expansion about the equilibrium value  $\beta_0$ ,

$$\mathcal{J} = \mathcal{J}_0 + \frac{d\mathcal{J}}{d\beta}(\beta - \beta_0) + \frac{1}{2} \frac{d^2\mathcal{J}}{d\beta^2}(\beta - \beta_0)^2,$$

was used instead, which, of course, is not valid in the neighborhood of  $\beta=0$ , when  $\mathcal{J}=0$ .

Calculations of  $C_\beta$ , previously made by the author, based on a cranking model method, can be used to estimate  $\mathcal{B}_\beta$ .<sup>19</sup> These values of  $C_\beta$  differed from (78a) in two ways. First, there were some additional terms arising from the somewhat *ad hoc* incompressibility constraint imposed on the deformed single-particle potential as postulated by Nilsson.<sup>41</sup> These terms tend to inflate  $C_\beta$  by an increment of the order of  $\beta_0$ , or about 30%. Second, the calculations of Ref. 19 neglected the last term in (68a), which is needed to make the spurious state arising from particle number nonconservation orthogonal to the physical states. The work of Bés suggests that this omission has the (strong) effect of decreasing  $C_\beta$  and thus to some extent cancelling the first deviation.<sup>55</sup> Thus the values of  $C_\beta$  calculated in Ref. 19 should serve at least to give an order-of-magnitude estimate for  $\mathcal{B}_\beta$ .

For comparison with experiment, it is probably most meaningful to compute  $\mathcal{B}/(\hbar^2/2\mathcal{J})^4$ , since the theoretical expression for  $\mathcal{B}$  is obviously very sensitive to small errors in  $\mathcal{J}$ , and therefore to the ( $\sim 20\%$ ) uncertainties in the parameters such as  $\Delta_n$ ,  $\Delta_p$ , and  $\beta_0$  which go into the theoretical calculation of  $\mathcal{J}$ .

The results for  $\mathcal{B}_\beta/(\hbar^2/2\mathcal{J})^4$  are shown in Fig. 1. The theoretical values generally account for only 1–2% of the total experimental value except at the end of the rare-earth region where it is 12%. This result strongly conflicts with the viewpoint of Ref. 5 and Ref. 58, where high-spin rotational energies were fitted by means of the phenomenological model using the beta vibration-rotation interaction exclusively. Actually, the values of  $C_\beta$  at the beginning of the rare-earth region are probably too large, and  $\mathcal{B}_\beta$ , therefore, too small, since the calculations of Ref. 19 could not reproduce the low-lying beta vibrational level in  $\text{Sm}^{152}$ . This might be due to the incompressibility constraint, or the estimate of  $\kappa$  given by Eq. (77) may be too small. However, in the middle of the rare-earth region, the second  $0^+$  states lie near the

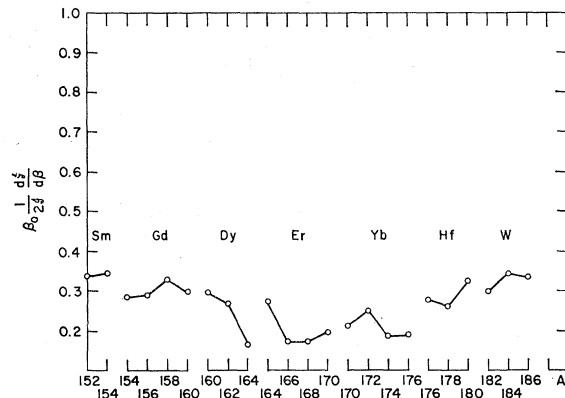


FIG. 2. Theoretical values of  $(\beta_0/2\mathcal{J})d\mathcal{J}/d\beta$ . The quantity  $\beta_0$  is the equilibrium deformation, and  $d\mathcal{J}/d\beta$  is evaluated at  $\beta=\beta_0$ . If it were the case that  $\mathcal{J} \propto \beta^2$ , then  $(\beta_0/2\mathcal{J})d\mathcal{J}/d\beta=1$ .

energy gap and can best be described as two-quasiparticle excitations. It is then not surprising that  $\mathcal{B}_\beta$  should be small. According to recent Coulomb excitation data the beta vibration-rotation interaction accounts for about 13% of the observed  $\mathcal{B}$  in  $\text{Sm}^{152}$  and 18% in  $\text{Sm}^{154}$ , which is much greater than the present theoretical estimates but still much smaller than had generally been believed.<sup>21</sup> One of the chief reasons that the importance of the beta vibration-rotation mixing has been exaggerated is due to the assumption that  $\mathcal{J} \propto \beta^2$ . It is shown in Fig. 2 that the present calculated values of  $d\mathcal{J}/d\beta$  are generally only about 25% of the value obtained from the  $\mathcal{J} \propto \beta^2$  assumption.

Similar estimates of  $\mathcal{B}_\gamma$  were not made since no calculations of  $\mathcal{J}$  as a function  $\gamma$  are available. However, estimates of  $\mathcal{B}_\gamma$  using a formula similar to (76b) were performed for a few cases in Ref. 37. The calculated  $\mathcal{B}_\gamma$  were of the order of magnitude of the experimental  $\mathcal{B}_\gamma$ , which amount to only 5–15% of the total experimental  $\mathcal{B}$ .<sup>20</sup>

The term  $\mathcal{B}_\lambda$  [Eq. (74e)], in contrast to  $\mathcal{B}_\beta$  and  $\mathcal{B}_\gamma$ , has a positive sign. It was evaluated for a typical rare-earth nucleus, using Nilsson single-particle states and found to be rather negligible, amounting in magnitude to about 0.5% of  $\mathcal{B}_\Delta$ . The difference between  $\mathcal{B}_\lambda$  and  $\mathcal{B}_\Delta$  is due to the fact that  $\partial\mathcal{J}/\partial\lambda \ll d\mathcal{J}/d\Delta$ . At any rate,  $\mathcal{B}_\lambda$  is difficult to interpret physically and may very well be a spurious result of number nonconservation.

The negative contribution  $\mathcal{B}_\Delta$  could easily be evaluated as follows. Nilsson and Prior calculated the change in  $\mathcal{J}_n$  and  $\mathcal{J}_p$  due to a 20% change in  $\Delta_n$  and  $\Delta_p$ , respectively.<sup>24</sup> Thus the derivatives  $d\mathcal{J}_n/d\Delta_n$  and  $d\mathcal{J}_p/d\Delta_p$  could be approximated by the ratio of the finite differences. It would have been more accurate if  $\mathcal{J}$  had been calculated for three values of  $\Delta$ , but a check in one case indicated that  $\mathcal{J}$  is a reasonably linear function of  $\Delta$  in the neighborhood of interest. The sums  $a_n$ ,  $b_n$ ,  $c_n$  [Eq. (61a)] and the corresponding proton quantities were easily evaluated (with  $\varphi_{kk^+}=0$ ) using values of  $\Delta$ ,  $\lambda$

<sup>58</sup> R. M. Diamond, F. S. Stephens, and W. J. Swiatecki, Phys. Letters 11, 315 (1964).

already available to the author and corresponding very closely to those employed by Nilsson and Prior. In fact, with  $\varphi_{kk^+}=0$ , we have the identity  $1-c_n=b_n$ , and  $a_n \ll b_n$  (and similarly for protons). From (64), this implies  $d\mathcal{G}/d\Delta \approx \partial\mathcal{G}/\partial\Delta$ .

The calculated values of  $\mathcal{B}_\Delta/(\hbar^2/2\mathcal{G})^4$  are shown in Fig. 1 and vary from about 14% of the experimental  $\mathcal{B}/(\hbar^2/2\mathcal{G})^4$  at the beginning of the rare-earth region to almost a factor 2 larger in Hf<sup>178</sup>. The qualitative prediction of Fig. 1 is that  $\mathcal{B}_\Delta/\mathcal{B}_\beta \approx 15-60$ . With a more precise calculation and small adjustment of  $\Delta_n$  and  $\Delta_p$ , one probably could make  $\mathcal{B}_\Delta$  agree with the total experimental  $\mathcal{B}$ , at least in the middle of the region. But the validity of such a procedure depends on  $\mathcal{B}_{\text{Coriolis}}$  [Eq. (74f)].

The contribution  $\mathcal{B}_{\text{Coriolis}}$  has not yet been evaluated, since this involves a great deal of tedious computation. It is the only term in  $\mathcal{B}$  whose sign cannot be determined in advance. If it turns out to be positive in certain cases, it might cancel some of the excess of  $\mathcal{B}_\Delta$ . On the other hand, if it is large and negative at the beginning of the rare-earth region, it might explain the large values of  $\mathcal{B}$  in Sm<sup>152</sup>, which the other terms apparently cannot. Thus  $\mathcal{B}_{\text{Coriolis}}$  plays a crucial role in testing the model.

A computer program is now being drafted to calculate all of the terms in  $\mathcal{B}$  given by Eq. (74), and more exactly than the present estimates. The results will be reported in a later paper.

## V. CONCLUSIONS

The contributions  $\mathcal{B}_\beta$  and  $\mathcal{B}_\gamma$  have been interpreted as arising from band mixing, and it seems likely that  $\mathcal{B}_{\text{Coriolis}}$  and  $\mathcal{B}_\Delta$  are the "intrinsic" contributions discussed in the Introduction. However, strictly within the framework of the HFB theory, one cannot say which contributions arise from band mixing and which are intrinsic, since the angular momentum has been treated as a  $c$  number, and all one gets is the total energy with both kinds of contributions treated on the same footing. It may even be the case that  $\mathcal{B}_\Delta$ , as well as  $\mathcal{B}_\beta$ , correspond to mixing with the  $0^+$  excitations, since in the time-dependent self-consistent field description of vibrations,  $\Delta$  becomes formally a dynamic variable on a par with the quadrupole moments, but coupled to them. Both  $\Delta$  and  $Q$  oscillations are needed to give rise to  $\beta$  oscillations. Unfortunately, the HFB wave functions, which are not eigenfunctions of the angular momentum, are not suitable for calculating branching ratios. One can project out eigenfunctions of the angular momentum from these, but this requires considerable labor.<sup>59</sup> What one really desires is a microscopic method for deriving a collective-model Hamiltonian in terms of angular momentum operators. Some progress in this direction has recently been made.<sup>60</sup>

Finally, it should be pointed out how the theory presented here can be extended to describe rotational bands in odd- $A$  nuclei and bands based on excited states of even-even nuclei. The expansion corresponding to Eq. (1) for odd- $A$  nuclei can be obtained from the expansion of the generalized quasiparticle energy  $\mathcal{E}_\sigma$  given by Eq. (9a') in powers of  $\Omega$ . In fact,  $\mathcal{E}_\sigma(\Omega)$  and the rotational energy for even-even nuclei could have been obtained simultaneously by perturbing the matrix equations for the HFB theory, but this turns out to be somewhat cumbersome. Alternatively, the perturbation of the one-quasiparticle eigenstates of the Hamiltonian (9a) could be considered to obtain  $\mathcal{E}_\sigma(\Omega)$ , which is straightforward since the self-consistency problem has already been solved for the vacuum state. Since the Hamiltonian (9a) corresponds to a set of independent generalized quasiparticles given by Eq. (9a'), the expansion (1) for rotational bands based on 2, 4, etc., quasiparticle states can be obtained by expanding in powers of  $\Omega$  the combinations  $\mathcal{E}_\sigma(\Omega) + \mathcal{E}_{\sigma'}(\Omega)$ ,  $\mathcal{E}_\sigma(\Omega) + \mathcal{E}_{\sigma'}(\Omega) + \mathcal{E}_{\sigma''}(\Omega) + \mathcal{E}_{\sigma'''}(\Omega)$ , etc. Since the quasiparticle energies are excitation energies, one gets in this manner the differences in moments of inertia between the ground-state and excited-state bands.

A complication is that some of the two-quasiparticle states are strongly admixed into  $\beta$  and  $\gamma$  vibrations. In order to get the  $\mathcal{G}$  and  $\mathcal{B}$  parameters for rotational bands based on collective states, one could use the fully time-dependent HFB theory as previously discussed, and thus the adiabatic approximation would be avoided. Alternatively, the Hamiltonian (7) could be treated by the RPA method.<sup>55</sup> This would not only give excited-state parameters but should provide corrections to the ground-state value of  $\mathcal{G}$  and  $\mathcal{B}$  parameters obtained here. Some of the semiclassical aspects of the HFB theory can then be avoided by using the constraint of a fixed value of the angular momentum operators  $\hat{J}^2$  and  $\hat{J}^4$  instead of  $\hat{J}$ . At any rate, the HFB solutions obtained here can serve as a useful basis for the RPA treatment, and work is now in progress by the author to obtain the parameters for  $\beta$  and  $\gamma$  bands.<sup>61</sup> Of particular interest is the  $\mathcal{B}$  coefficient for the excited bands which often differs considerably from that of the ground-state band, which cannot be explained by a phenomenological approach.

The perturbation treatment described in this paper could be continued to high order to obtain a full expansion of the form of Eq. (1). However, this would be very tedious. The higher order terms beginning with  $I^3(I+1)^3$  include effects of anharmonicity in the collective potential energy, but the static treatment given in this paper is expected to neglect anharmonic kinetic energy effects. However, such effects could, in principle, be included by employing the fully time-dependent (RPA) method.

<sup>59</sup> R. E. Peierls and D. J. Thouless, Nucl. Phys. **38**, 154 (1962).

<sup>60</sup> A. K. Kerman and A. Klein, Phys. Rev. **132**, 1326 (1963).

<sup>61</sup> Some work along these lines has also been done recently by I. M. Pavlichenkov, Nucl. Phys. **55**, 225 (1964).

It is questionable whether it is worthwhile to consider such higher-order corrections at all. Empirically, the expansion (1) does not seem to converge beyond  $I \sim 10, 12$ . In that case, exact diagonalizations of the HFB equations in the rotating reference frame would be needed to avoid the Taylor series expansion for very high angular-momentum states, and that is indeed a formidable task. Assuming that such diagonalizations could be performed, would it be meaningful? The answer might very well be negative for two reasons. The first reason is that the time-dependent HFB theory, while providing some of the previously mentioned anharmonic effects, neglects certain other, possibly equally important anharmonicities, namely those provided by the "higher RPA."<sup>62</sup> To include all the anharmonic terms would necessitate highly complex corrections to the Hartree-Fock theory.<sup>62</sup>

The second difficulty is connected with the sharp rotational phase transition from a superfluid to a normal state at high angular momenta predicted by Mottelson and Valatin.<sup>44</sup> Recent work suggests that this effect, if it really is a mathematical property of the HFB equations (and this has not rigorously been shown), is a spurious result of the particle number nonconservation, at least in atomic nuclei where the number of particles is not very large.<sup>63</sup> In that case, the HFB equations could not be trusted for high angular-momentum states when  $\Delta \approx 0$ .

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**APPENDIX A**

The  $\chi_{k-l}^{(n)}$  are not listed. These can be obtained from the corresponding  $\rho_{k-l}^{(n)}$  by replacing  $f_{ki}^{\pm}$  by  $g_{ki}^{\mp}$  and

$g_{ki}^{\mp}$  by  $-f_{ki}^{\pm}$  where these factors explicitly appear in the following formulas.

First order:

$$b_0^{(1)} = 0, \tag{A1a}$$

$$b^{(1)}(k-l) = -B_{kl}^{(1)}/E_{kl}, \tag{A1b}$$

$$\rho_{kl}^{(1)} = -B_{kl}^{(1)}f_{ki}^{\pm}/E_{kl}, \tag{A1c}$$

$$\lambda^{(1)} = \left[ \sum_k (f_{kk}^+)^2/E_k \right]^{-1} \times \sum_k (B_{kk}^{(1)} + \lambda^{(1)}f_{kk}^{\pm})f_{kk}^{\pm}/E_k. \tag{A1d}$$

Note that the right-hand side of (A1d) is independent of  $\lambda^{(1)}$  according to Eq. (21b).

Second order:

$$b_0^{(2)} = -\frac{1}{4} \sum_{kl} |B_{kl}^{(1)}|^2/(E_{kl})^2, \tag{A2a}$$

$$E_{kl}b^{(2)}(k-l) = \sum_m B_{km}^{(1)}A_{-l-m}^{(1)}/E_{km} + \sum_m A_{km}^{(1)}B_{ml}^{(1)}/E_{ml} - B_{kl}^{(2)}. \tag{A2b}$$

In this order, four-quasiparticle states are also admixed but do not contribute to  $\rho^{(2)}$  or  $\chi^{(2)}$ . The amplitudes are

$$b^{(2)}(k-lm-n) = \frac{B_{kl}^{(1)}B_{mn}^{(1)}}{E_{kl}E_{mn}} - \frac{B_{ml}^{(1)}B_{kn}^{(1)}}{E_{ml}E_{kn}} + \frac{B_{k-m}^{(1)}B_{-nl}^{(1)}}{E_{km}E_{nl}}. \tag{A2c}$$

The appearance of two-quasiparticle rather than four-quasiparticle energy denominators in (A2c) is a consequence of the identity

$$(E_{kl}E_{mn})^{-1} = (E_{klmn})^{-1}(E_{mn}^{-1} + E_{kl}^{-1}),$$

$$\rho_{kl}^{(2)} = \sum_m \frac{A_{km}^{(1)}B_{ml}^{(1)}f_{kl}^+}{E_{kl}E_{ml}} + \sum_m \frac{B_{km}^{(1)}A_{-l-m}^{(1)}f_{kl}^+}{E_{km}E_{kl}} + \sum_m \frac{B_{km}^{(1)}B_{lm}^{(1)*}g_{kl}^-}{E_{km}E_{ml}} - \frac{B_{kl}^{(2)}f_{kl}^+}{E_{kl}}, \tag{A2d}$$

$$\lambda^{(2)} = \left[ \sum_k (f_{kk}^+)^2/E_k \right]^{-1} \left\{ -2 \sum_{kl} |B_{kl}^{(1)}|^2 g_{kk}^- / (E_{kl})^2 - 2 \sum_{kl} A_{kl}^{(1)} B_{lk}^{(1)} f_{kk}^+ / (E_k E_{kl}) + \sum_k (B_{kk}^{(2)} + \lambda^{(2)} f_{kk}^+) f_{kk}^+ / E_k \right\}. \tag{A2e}$$

<sup>62</sup> J. Da. Providencia, Nucl. Phys. **61**, 87 (1965).  
<sup>63</sup> M. Rho and J. O. Rasmussen, Phys. Rev. **135**, B1295 (1964).

Third order:

$$b_0^{(3)} = \sum_{klm} \frac{A_{km}^{(1)} B_{ml}^{(1)} B_{kl}^{(1)*}}{(E_{kl})^2 E_{ml}} - \frac{1}{2} \sum_{kl} \frac{B_{kl}^{(1)*} B_{kl}^{(2)}}{(E_{kl})^2}, \quad (\text{A3a})$$

$$\begin{aligned} E_{kl} b^{(3)}(k-l) = & \frac{1}{4} \sum_{mn} \frac{B_{kl}^{(1)} |B_{mn}^{(1)}|^2}{(E_{mn})^2} + \sum_{mn} \frac{B_{km}^{(1)} B_{nm}^{(1)*} B_{nl}^{(1)}}{E_{km} E_{nl}} - \sum_{mn} \frac{A_{km}^{(1)} A_{mn}^{(1)} B_{nl}^{(1)}}{E_{ml} E_{nl}} - \sum_{mn} \frac{A_{km}^{(1)} B_{mn}^{(1)} A_{-l-n}^{(1)}}{E_{mn} E_{ml}} \\ & - \sum_{mn} \frac{A_{km}^{(1)} B_{mn}^{(1)} A_{-l-n}^{(1)}}{E_{kn} E_{nm}} - \sum_{mn} \frac{B_{km}^{(1)} A_{-n-m}^{(1)} A_{-l-n}^{(1)}}{E_{kn} E_{km}} + \sum_m \frac{A_{km}^{(2)} B_{ml}^{(1)}}{E_{ml}} \\ & + \sum_m \frac{B_{km}^{(1)} A_{-l-m}^{(2)}}{E_{km}} + \sum_m \frac{A_{km}^{(1)} B_{ml}^{(2)}}{E_{ml}} + \sum_m \frac{B_{km}^{(2)} A_{-l-m}^{(1)}}{E_{km}} - B_{kl}^{(3)}. \quad (\text{A3b}) \end{aligned}$$

The third-order corrections to the four- and six-quasiparticle amplitudes do not contribute to  $\varrho^{(3)}$  and  $\varkappa^{(3)}$  and will not be given here.

$$\begin{aligned} \rho_{kl}^{(3)} = & + \sum_{mn} \frac{B_{km}^{(1)} B_{nm}^{(1)*} B_{nl}^{(1)} f_{kl}^{\pm}}{E_{km} E_{mn} E_{nl}} + \sum_{mn} \frac{B_{km}^{(1)} B_{nm}^{(1)*} B_{nl}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{km} E_{nl}} - \sum_{mn} \frac{A_{km}^{(1)} B_{mn}^{(1)} B_{ln}^{(1)*} g_{kl}^{\mp}}{E_{kn} E_{mn} E_{nl}} \\ & - \sum_{mn} \frac{B_{km}^{(1)} B_{nm}^{(1)*} A_{nl}^{(1)} g_{kl}^{\mp}}{E_{km} E_{mn} E_{ml}} - \sum_{mn} \frac{B_{km}^{(1)} A_{-n-m}^{(1)} B_{ln}^{(1)*} g_{kl}^{\mp}}{E_{km} E_{kn} E_{nl}} - \sum_{mn} \frac{B_{km}^{(1)} A_{-n-m}^{(1)} B_{ln}^{(1)*} g_{kl}^{\mp}}{E_{km} E_{nl} E_{ml}} \\ & - \sum_{mn} \frac{A_{km}^{(1)} A_{mn}^{(1)} B_{nl}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{nl} E_{ml}} - \sum_{mn} \frac{B_{km}^{(1)} A_{-n-m}^{(1)} A_{-l-n}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{km} E_{kn}} - \sum_{mn} \frac{A_{km}^{(1)} B_{mn}^{(1)} A_{-l-n}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{mn} E_{ml}} \\ & - \sum_{mn} \frac{A_{km}^{(1)} B_{mn}^{(1)} A_{-l-n}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{mn} E_{kn}} + \sum_m \frac{B_{km}^{(2)} B_{lm}^{(1)*} g_{kl}^{\mp}}{E_{km} E_{ml}} + \sum_m \frac{B_{km}^{(1)} B_{lm}^{(2)*} g_{kl}^{\mp}}{E_{km} E_{ml}} + \sum_m \frac{A_{km}^{(2)} B_{ml}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{ml}} \\ & + \sum_m \frac{B_{km}^{(1)} A_{-l-m}^{(2)} f_{kl}^{\pm}}{E_{kl} E_{km}} + \sum_m \frac{A_{km}^{(1)} B_{ml}^{(2)} f_{kl}^{\pm}}{E_{kl} E_{ml}} + \sum_m \frac{B_{km}^{(2)} A_{-l-m}^{(1)} f_{kl}^{\pm}}{E_{kl} E_{km}} - \frac{B_{kl}^{(3)} f_{kl}^{\pm}}{E_{kl}}, \quad (\text{A3c}) \end{aligned}$$

$$\begin{aligned} \lambda^{(3)} = & \left[ \sum_k \frac{(f_{kk}^+)^2}{E_k} \right]^{-1} \left[ -2 \sum_{klm} \frac{B_{kl}^{(1)} B_{ml}^{(1)*} B_{mk}^{(1)} f_{kk}^{\pm}}{E_{kl} E_{lm} E_{mk}} - \sum_{klm} \frac{B_{kl}^{(1)} B_{ml}^{(1)*} B_{mk}^{(1)} f_{kk}^{\pm}}{E_k E_{kl} E_{km}} \right. \\ & + 2 \sum_{klm} \frac{A_{kl}^{(1)} B_{lm}^{(1)} B_{km}^{(1)*} (g_{kk}^{\mp} \pm g_{mm}^{\mp})}{(E_{km})^2 E_{lm}} + \text{c.c.} + 2 \sum_{klm} \frac{A_{kl}^{(1)} A_{lm}^{(1)} B_{mk}^{(1)} f_{kk}^{\pm}}{E_k E_{kl} E_{km}} + 2 \sum_{klm} \frac{A_{kl}^{(1)} B_{lm}^{(1)} A_{-k-m}^{(1)} f_{kk}^{\pm}}{E_k E_{lm} E_{kl}} \\ & - 2 \sum_{kl} \frac{B_{kl}^{(2)} B_{kl}^{(1)*} (g_{kk}^{\mp} \pm g_{ll}^{\mp})}{E_{kl}^2} - 2 \sum_{kl} \frac{A_{kl}^{(2)} B_{lk}^{(1)} f_{kk}^{\pm}}{E_k E_{kl}} - 2 \sum_{kl} \frac{A_{kl}^{(1)} B_{lk}^{(2)} f_{kk}^{\pm}}{E_k E_{kl}} \\ & \left. + \sum_k \frac{(B_{kk}^{(3)} + \lambda^{(3)} f_{kk}^{\pm}) f_{kk}^{\pm}}{E_k} \right]. \quad (\text{A3d}) \end{aligned}$$