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Nuclear Rotation and Boson Expansions. I*

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The Beliaev-Zelevinsky method, which represents fermion-pair operators by infinite expansions in exact bosons, is applied to the problem of nuclear rotation. In the harmonic order, which is essentially the random-phase approximation (RPA), the rotation, viewed as infinitesimal, is decoupled from the collective vibrations. The higher orders, however, give rise to various band-mixing terms, which may be interpreted as rotation-vibration and higher-order Coriolis interactions, as well as to vibrational anharmonicities and renormalization of the moment of inertia. A systematic approach is given for extracting these higher-order corrections for the idealized case of a two-dimensional system of interacting particles. Both the Hamiltonian and transition operators are treated. The self-consistent-field approximation is then formulated in the boson picture and applied to the cranking model. The advantage of this formulation is that it allows one to establish the correctness of the higher-order cranking model, which is shown to provide the ground-state-band rotational energies with an error of the order of the small boson-expansion parameter (or the square of this parameter, depending on its definition). The usefulness of the cranking model for obtaining the angular momentum dependence of transition operators is also demonstrated. The Appendix illustrates some of the ideas by way of application to a system of particles interacting through a two-dimensional analog of the quadrupole-quadrupole force.

I. INTRODUCTION

A recent paper by the authors was concerned with the solution of some problems which had remained in the random-phase approximation (RPA) theory of nuclear rotation.[1] The context of the discussion was provided by the interpretation of the RPA as the harmonic order in a boson expansion of fermion-pair operators. In particular, it was shown that although nuclear rotations are not small oscillations, expansion of all the degrees of freedom, vibrations and rotations inclusive, on an equal footing can still be a very useful technique, not only for obtaining the rotational energy, but also for calculating transition matrix elements. It was also shown that the lowest-order self-consistent cranking prescription, which identifies the moment of inertia, can be directly derived from the RPA Hamiltonian. The present paper is a direct extension of this work to include higher orders of the boson expansion for deformed systems with an even number of particles. The notation and background are provided by Ref. 1, while the notion of boson expansions as applied to spherical nuclei has been discussed in several papers,[2-5] beginning with the work of Beliaev and Zelevinsky (BZ).[2] For didactic simplicity, the discussion will be limited to the rotation of a two-dimensional system of particles, as was done in Ref. 1.

We begin in Sec. II, not with a specific boson expansion, but with the construction of the most general form of the Hamiltonian through quartic boson terms, subject to the usual invariance laws, in particular, rotational invariance. The bosons used are assumed to correspond to particle-hole or quasiparticle pairs of a deformed potential well and are conveniently expressed as linear combinations of the normal-mode bosons. It is then shown how the large conglomeration of higher-order terms can be grouped together into meaningful combinations which may be interpreted as rotation-vibration and other types of band interactions, as well as vibrational anharmonicities. Transition operators are also treated similarly. The deviations from the perfect rotational spectrum, and the effects of band mixing on transition probabilities are then easily calculated.

In Sec. III, the BZ-type expansion for nonsuperconducting systems is introduced. This is an expansion about a Hartree rather than Hartree-Fock minimum. A simple formulation of the Hartree ground-state problem is found in the boson representation and then applied to the cranking model. The ground-state rotational-energy spacings are given by the expansion

$$E(M) = (2\mathcal{I})^{-1}M^2 + \mathcal{B}M^4 + \mathcal{C}M^6 + \cdots , \qquad (I.1)$$

in powers of the angular momentum quantum num-

ber M, for not-too-large values. With the aid of the boson picture, it is shown in detail that the cranking-model values of the coefficients $\mathcal{I}$ and $\mathcal{C}$ agree with those obtained directly from the boson expansion in Sec. II up to an error of the order of the small expansion parameter squared. In other words, the rotational coefficients are each expansions in powers of this parameter, and the cranking model picks up the leading term in each coefficient. An argument is sketched to show that this property of the cranking model holds to all orders. In this way, support is provided for the higher-order cranking model,[6,7] which is the only available microscopic model readily applicable to high angular momentum states, although $E(M)$ must then be obtained exactly as a function of M, not as an expansion. Additional support is provided by the fact that the cranking model to all orders has also been derived as a first approximation to four other methods: the generalized Hartree-Fock method (GHFA),[8] a modified GHFA,[9] the generator-coordinate method,[10] and a Green's function theory.[11] However, the starting points of at least three of the methods are approximate and the corrections to the cranking model are not as visible as in the present approach.

In Sec. III it is seen that the cranking-model expression for the $\mathcal{C}$ coefficient is a sum of many contributions from the interactions of the ground-state band with excited bands. It is then shown how the cranked wave function may be used to extract the coupling with individual bands. A similar technique is also applied to transition operators in order to find their angular momentum dependence.

We conclude the paper with an Appendix in which definite expressions are derived for rotational parameters of a system of particles interacting via the two-dimensional analog of the quadrupole-quadrupole force. The expressions should be of interest as a basis for comparison with other methods and are similar to those of axially symmetric three-dimensional systems.

II. BOSON HAMILTONIAN AND TRANSITION OPERATORS

A. Form of the Hamiltonian

In order to identify J^4 terms, where J is the angular momentum, the Hamiltonian must be expanded through quartic boson terms:

$$H = H_B + H_{\mathrm{III}} + H_{\mathrm{IV}} + \cdots , \tag{II.1}$$

where H_B (in the notation of Ref. 1) is quadratic, H_{III} is cubic, and H_{IV} is quartic in bosons. Each successive term represents a higher order of the expansion. Throughout the paper, we shall use Roman-numeral subscripts to indicate the order in the expansion.

It is very important to note that in the method of BZ, the spirit of which we essentially follow, the successive terms H_{III}, H_{IV}, etc., in the expansion of H, and other operators as well, are not in normal order when written as homogeneous functions of boson operators.[2] This is in contrast to the procedure of several other investigators who employ normal-ordered expansions.[3-5] Let us therefore briefly review the idea of BZ. In this method, fermion-pair operators are represented by Taylor series expansions in exact bosons in such a way that the correct commutation rules for fermion pairs are fulfilled in each order of the expansion. The expansions for fermion pairs are so chosen that the corresponding expansions of physically interesting operators, especially those associated with collective modes, become expansions in a small parameter. The basic expansion parameter, which we denote generally by ϵ, depends on the nature of the system. It is usually a geometric parameter like Ω in the two-dimensional case (or $\Omega^{-1/2}$ in the three-dimensional case), where Ω is the number of levels available to the active particles and is of the order of the number of active particles. More generally, one can introduce dynamic small parameters such as the roots of the zero-point amplitudes of the harmonic approximation. As discussed in Sec. III, the expansions of fermion pairs can be arranged such as to maintain a correlation between the order in ϵ and the number of boson operators in each term. Of course, the successive terms are then not in normal order. The terms H_B, H_{III}, H_{IV}, etc., in Eq. (II.1) are obtained by simply inserting the boson expansions for the fermion pairs and then collecting together all terms of the same order without contracting any bosons. It is in this way that the correlation between the number of boson operators and the order of the term in the expansion is maintained. Thus, if H_B is taken to be of zero order, then H_{III} is of relative order ϵ and H_{IV} of relative order ϵ^2. Now, for example, H_{IV} may contain terms schematically of the form $B^\dagger BB^\dagger B$, where $B^\dagger$ is an elementary boson corresponding to the creation of a pair of quasiparticles. Normal ordering of such a term would create a quadratic boson term, which, however, is not included in the definition of H_B. In other words, all terms of the same order are kept together in Eq. (II.1). This makes it easy to separate orders in the expansion of various commutators in the ensuing discussion.

Instead of writing everything in terms of the elementary bosons, it is convenient to use the set of normal-mode bosons ($\mathcal{O}_\mu$, $\mathcal{O}_\mu^\dagger$, J_B, Φ_B), related to the former by a canonical transformation, in terms of which H_B takes the diagonal form

$$H_B = \text{constant} + \sum_\mu E_\mu \mathcal{O}_\mu^\dagger \mathcal{O}_\mu + \frac{J_B^2}{2\mathcal{I}_0} \tag{II.2}$$

The set $(\mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$ consists of the vibrational phonons, J_B is the leading-order approximation to the angular momentum J, and Φ_B is an angle variable canonically conjugate to J_B. The dependence on other zero-frequency modes, such as the total momentum and c.m. coordinates, will not be explicitly shown.

It should be noted that J_B is odd under time reversal, Φ_B is even, and the $\mathcal{O}_\mu$, $\mathcal{O}_\mu^\dagger$ can also be taken to be even with a proper choice of phases (recall, we are dealing with two-dimensional phonons). Then, the most general Hermitian, time-reversal symmetric form for $H_{\rm III}$ may be written as

$$\begin{aligned} H_{\rm III} = {} & J_B^2 \sum_\mu [h_\mu^{(3)}(21)\mathcal{O}_\mu^\dagger + \text{H.c.}] + \tfrac{1}{4}h^{(3)}(20)\{\{\Phi_B, J_B\}, J_B\} + ih^{(3)}(10)[J_B, \Phi_B^2] \\ & + \tfrac{1}{2}i\{\Phi_B, J_B\}\sum_\mu [h_\mu^{(3)}(11)\mathcal{O}_\mu^\dagger - \text{H.c.}] + iJ_B \sum_{\mu\nu} \{h_{\mu\nu}^{(3)}(12)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu + \tfrac{1}{2}[h_{\mu\nu}'^{(3)}(12)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu^\dagger - \text{H.c.}]\} \\ & + h^{(3)}(00)\Phi_B^3 + \tfrac{1}{2}\Phi_B^2 \sum_\mu [h_\mu^{(3)}(01)\mathcal{O}_\mu^\dagger + \text{H.c.}] + \Phi_B \sum_{\mu\nu}\{h_{\mu\nu}^{(3)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu + \tfrac{1}{2}[h_{\mu\nu}'^{(3)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu^\dagger + \text{H.c.}]\} \\ & + \text{cubic phonons}. \end{aligned} \tag{II.3}$$

Phonon terms which are not explicitly written out, such as the cubic phonon terms above, are generally not in normal order. The coefficients $h^{(k)}(nm)$ correspond to a term containing J_B to the nth power and a product of m phonons, while the superscript k denotes the total number of bosons in the term. The coefficients may be taken to be real for our two-dimensional problem. It should also be noted that the coefficients of terms depending on Φ_B may be of significantly larger magnitude than the other coefficients. In the final analysis, however, the Hamiltonian will contain no dependence on an angular degree of freedom.

The form of $H_{\rm IV}$ is given by

$$\begin{aligned} H_{\rm IV} = {} & h^{(4)}(40)J_B^4 + iJ_B^3 \sum_\mu [h_\mu^{(4)}(31)\mathcal{O}_\mu^\dagger - \text{H.c.}] + h^{(4)}(20)\{J_B^2, \Phi_B^2\} + \{J_B, \{J_B, \Phi_B\}\}\sum_\mu [h_\mu^{(4)}(21)\mathcal{O}_\mu^\dagger + \text{H.c.}] \\ & + J_B^2 \times \text{quadratic phonons} + i\{\Phi_B, \{\Phi_B, J_B\}\}\sum_\mu [h_\mu^{(4)}(11)\mathcal{O}_\mu^\dagger - \text{H.c.}] + \{\Phi_B, J_B\} \times \text{quadratic phonons} \\ & + J_B \times \text{cubic phonons} + h^{(4)}(00)\Phi_B^4 + \Phi_B^3 \sum_\mu [h_\mu^{(4)}(01)\mathcal{O}_\mu^\dagger + \text{H.c.}] + \Phi_B^2 \times \text{quadratic phonons} \\ & + \Phi_B \times \text{cubic phonons} + \text{quartic phonons}. \end{aligned} \tag{II.4}$$

Again, phonon terms which are not explicitly written out are not in normal order. It may be noted that certain terms like $h^{(4)}(31)[J_B^3, \Phi_B] \propto J_B^2$ have not been explicitly written down. However, the term of the form $J_B^2 \times$(quadratic phonons) also gives rise to a J_B^2 term when the phonons are written out in normal order. Therefore, the $J_B^2 \times$(quadratic phonon) term is intended to include J_B^2 terms from all sources. Other similar simplifications have also been made. Actually, only the J_B^4 term will be used in the later discussion.

In addition to Hermiticity and time reversal, rotational invariance places an essential restriction on H. In order to take this into account, the expansion of the angular momentum J is needed:

$$J = J_B + J_{\rm II} + J_{\rm III} + \cdots, \tag{II.5}$$

where J_B is a linear boson operator, and the Roman numerals indicate the number of bosons in the other terms. Taking into account that J is odd under time reversal, we obtain for $J_{\rm II}$ the expression

$$\begin{aligned} J_{\rm II} = {} & J_B \sum_\mu [j_\mu^{(2)}(11)\mathcal{O}_\mu^\dagger + \text{H.c.}] + \tfrac{1}{2}j^{(2)}(10)\{J_B, \Phi_B\} + \Phi_B i \sum_\mu [j_\mu^{(2)}(01)\mathcal{O}_\mu^\dagger - \text{H.c.}] \\ & + i\sum_{\mu\nu}\{j_{\mu\nu}^{(2)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu + \tfrac{1}{2}[j_{\mu\nu}'^{(2)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu^\dagger - \text{H.c.}]\}, \end{aligned} \tag{II.6}$$

and for $J_{\rm III}$ the expression

$$\begin{aligned} J_{\rm III} = {} & j^{(3)}(30)J_B^3 + J_B^2 i\sum_\mu [j_\mu^{(3)}(21)\mathcal{O}_\mu^\dagger - \text{H.c.}] + J_B \times \text{quadratic phonons} + \tfrac{1}{2}\{\Phi_B, J_B\}\sum_\mu [j_\mu^{(3)}(11)\mathcal{O}_\mu^\dagger + \text{H.c.}] \\ & + \tfrac{1}{2}j^{(3)}(10)\{\Phi_B, \{\Phi_B, J_B\}\} + i\Phi_B^2 \sum_\mu [j_\mu^{(3)}(01)\mathcal{O}_\mu^\dagger - \text{H.c.}] + i\Phi_B \sum_{\mu\nu}\{j_{\mu\nu}^{(3)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu + \tfrac{1}{2}[j_{\mu\nu}'^{(3)}(02)\mathcal{O}_\mu^\dagger \mathcal{O}_\nu^\dagger - \text{H.c.}]\} \\ & + \text{cubic phonons}. \end{aligned} \tag{II.7}$$

The coefficients $j^{(k)}(nm)$ may be taken to be real for our problem.

The condition of rotational invariance, $[H, J]=0$, then implies, upon separating orders in the boson expansion parameter, that

$$[H_B, J_{II}]+[H_{III}, J_B]=0, \tag{II.8a}$$

and

$$[H_B, J_{III}]+[H_{III}, J_{II}]+[H_{IV}, J_B]=0. \tag{II.8b}$$

The condition (II.8b), which restricts H_{IV}, will not be needed. Equation (II.8a) implies that

$$h^{(3)}(00)=0, \tag{II.9a}$$

$$h^{(3)}(10)=0, \tag{II.9b}$$

$$h^{(3)}(20)=g_0^{-1}j^{(2)}(10), \tag{II.9c}$$

$$h_\mu^{(3)}(11)=E_\mu j_\mu^{(2)}(11)+g_0^{-1}j_\mu^{(2)}(01), \tag{II.9d}$$

$$h_\mu^{(3)}(01)=-E_\mu j_\mu^{(2)}(01), \tag{II.9e}$$

$$h_{\mu\nu}^{(3)}(02)=-(E_\mu-E_\nu)j_{\mu\nu}^{(2)}(02), \tag{II.9f}$$

$$h_{\mu\nu}'^{(3)}(02)=-(E_\mu+E_\nu)j_{\mu\nu}'^{(2)}(02). \tag{II.9g}$$

B. Angular Momentum Decomposition of the Hamiltonian

Now that the general form of the boson expansion of H has been obtained to the order of interest, we are confronted with the problem of making sense out of the plethora of terms obtained. This can be done by relating the boson expansion to the angular momentum decomposition of H given by

$$H=\sum_{n=0}^{\infty}\frac{\mathcal{H}_n J^n}{n!}, \tag{II.10}$$

where the $\mathcal{H}_n$ are intrinsic operators, i.e., operators which commute with both J and an angle variable Φ:

$$[\mathcal{H}_n, J]=[\mathcal{H}_n, \Phi]=0. \tag{II.11}$$

As pointed out by Villars, any rotationally invariant Hamiltonian can be written in the form (II.10), with the $\mathcal{H}_n$ formally expressed in terms of multiple commutators of H with Φ.[12] Therefore, given a boson expansion of Φ, one can always obtain the boson expansions of the intrinsic operators $\mathcal{H}_n$. Since the expansion of J is assumed known, the many terms in H_{III} and H_{IV} could then be classified as arising from the boson expansion of the form (II.10). In addition, the expansion of the $\mathcal{H}_n$ in terms of all degrees of freedom, say the set $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$, could be rewritten as an expansion in a new set of intrinsic degrees of freedom alone.

However, as is well known, the condition of canonical conjugation with J is insufficient by itself to define Φ uniquely. An ostensible difficulty, consequently, which has deterred progress through the years, has been the fact that a suitable definition of Φ is not known *a priori*. By a "suitable" definition of Φ, we mean one which makes the angular momentum expansion (II.10) also an expansion in a small parameter so that coupling terms can be treated by perturbation theory; and the most ideal definition is one which eliminates all coupling terms. The purpose of this section is to show that we need not sit and wait for such a Φ to make its propitious appearance. Instead, we turn the matter around: We begin with an expansion of J and H in the parameter ϵ – this is a boson expansion of all degrees of freedom, rotational and intrinsic, on an equal footing – and then we apply in each order the criterion for a suitable Φ in terms of ϵ as the small parameter. In this way, we generate a *concomitant* expansion of Φ. The first crucial step, described in Ref. 1, is the lowest-order choice $\Phi\approx\Phi_B$, which diagonalizes H_B and thus eliminates the Coriolis-type coupling term of the form $J_B\times$phonon. In fact, as we shall see, any expansion for Φ beginning with Φ_B essentially meets the "suitability" criterion and all such possibilities are related by unitary transformations. As a consequence, the corresponding angular momentum expansions (II.10) are also related by unitary transformations. This additional arbitrariness in the expansion of Φ will be exploited to diagonalize various J-dependent band-mixing terms.

We begin by considering the form of the boson expansion of Φ, which starts with Φ_B:

$$\Phi=\Phi_B+\Phi_{II}+\Phi_{III}+\cdots, \tag{II.12}$$

and we shall solve for Φ_{II}, Φ_{III}, etc., as we go along. Using the known boson expansion of J given by Eq. (II.5), and the condition of canonical conjugation

$$[\Phi, J]=i, \tag{II.13a}$$

one obtains upon separating orders the set of equations

$$\begin{aligned}&[\Phi_{II}, J_B]+[\Phi_B, J_{II}]=0,\\ &\qquad\cdots\\ &[\Phi_n, J_B]+[\Phi_{n-1}, J_{II}]+\cdots+[\Phi_B, J_n]=0.\end{aligned} \tag{II.13b}$$

Obviously, Eqs. (II.13) cannot determine the parts of Φ which are independent of Φ_B. Therein lies the arbitrariness in the choice of Φ. For example, taking into account the first of Eqs. (II.13b), and requiring in addition that Φ be Hermitian and time-reversal symmetric, one obtains the following sufficiently general form for Φ_{II}:

$$\Phi_{II} = -\tfrac{1}{2} j^{(2)}(10)\Phi_B{}^2 - \Phi_B \sum_\mu [j_\mu^{(2)}(11)\mathcal{O}_\mu{}^\dagger + \text{H.c.}] + iJ_B \sum_\mu [f_\mu^{(2)}(11)\mathcal{O}_\mu{}^\dagger - \text{H.c.}] + \sum_{\mu\nu}\{f_{\mu\nu}^{(2)}(02)\mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu + \tfrac{1}{2}[f_{\mu\nu}'^{(2)}(02)\mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu{}^\dagger + \text{H.c.}]\}\,, \tag{II.14}$$

where the f coefficients are undetermined by Eq. (II.13b).[13] An arbitrary term proportional to $J_B{}^2$ has been omitted, since it can play no role in the analysis to follow. This is related to the fact that one can always add to Φ an arbitrary function of J to obtain a new angle variable satisfying Eq. (II.13a). Such a redefinition of Φ cannot alter the intrinsic operators $\mathcal{K}_n$, which are expressible in terms of multiple commutators of the rotationally invariant operator H with Φ. Therefore, terms in Φ interpretable as arising from powers of J may as well be dropped. Actually, odd powers are already eliminated by the requirement that Φ be time-reversal symmetric and Hermitian. The $J_B{}^2$ term is such a term interpretable as arising from a J^2 dependence. The other undetermined terms in Eq. (II.14) do influence the definition of intrinsic operators and will thus be retained.

In order to utilize the angular momentum expansion (II.10), it is very convenient to express the intrinsic operators $\mathcal{K}_n$ as functions of new phonons $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ which commute with the full angular momentum J and the angle variable Φ:

$$[\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\nu] = 0\,, \quad [\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\nu{}^\dagger] = \delta_{\mu\nu}\,; \tag{II.15a}$$

$$[J, \tilde{\mathcal{O}}_\mu] = 0\,, \quad [\Phi, \tilde{\mathcal{O}}_\mu] = 0\,. \tag{II.15b}$$

The phonons $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ are not uniquely determined by Eqs. (II.15) once Φ is chosen, since any such set can be transformed, $\tilde{\mathcal{O}}_\mu \to e^{iS}\tilde{\mathcal{O}}_\mu e^{-iS}$, with S a function of the $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ alone, to give another set of phonons satisfying Eq. (II.15). Conversely, however, specification of the intrinsic operators $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ is sufficient to define Φ. The additional arbitrariness can be used to diagonalize anharmonic vibrational terms. We define the new phonons to have a boson expansion beginning with the normal-mode phonons:

$$\tilde{\mathcal{O}}_\mu = \mathcal{O}_\mu + (\tilde{\mathcal{O}}_\mu)_{II} + (\tilde{\mathcal{O}}_\mu)_{III} + \cdots\,. \tag{II.16}$$

The restrictions on $(\tilde{\mathcal{O}}_\mu)_{II}$, which will be of primary interest, are given by

$$[J_B, (\tilde{\mathcal{O}}_\mu)_{II}] + [J_{II}, \mathcal{O}_\mu] = 0\,, \quad [\Phi_B, (\tilde{\mathcal{O}}_\mu)_{II}] + [\Phi_{II}, \mathcal{O}_\mu] = 0\,. \tag{II.17}$$

Requiring, in addition, time-reversal symmetry, one may write $(\tilde{\mathcal{O}}_\mu)_{II}$ in the form

$$(\tilde{\mathcal{O}}_\mu)_{II} = \tfrac{1}{2} i j_\mu^{(2)}(11)\{J_B, \Phi_B\} - \tfrac{1}{2} j_\mu^{(2)}(01)\Phi_B{}^2 - \Phi_B \sum_\nu [j_{\mu\nu}^{(2)}(02)\mathcal{O}_\nu + j_{\mu\nu}'^{(2)}(02)\mathcal{O}_\nu{}^\dagger] + \tfrac{1}{2} f_\mu^{(2)}(11) J_B{}^2 - iJ_B \sum_\nu [f_{\mu\nu}^{(2)}(02)\mathcal{O}_\nu + f_{\mu\nu}'^{(2)}(02)\mathcal{O}_\nu{}^\dagger] + \text{quadratic phonons}\,, \tag{II.18}$$

where the quadratic phonon terms are essentially arbitrary, except for the canonicity restriction imposed by Eq. (II.15a).

Our next objective is to rewrite the Hamiltonian H as an expansion in the set $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$. Since H is rotationally invariant, it must be independent of Φ, and we shall thus obtain the form (II.10), with the intrinsic operators $\mathcal{K}_n$ expressed as functions of the new phonons $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$. A convenient way to achieve this aim is to relate the two sets of dynamic variables $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu{}^\dagger)$ and $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ by a unitary transformation. This is always possible, since the mutual commutation relations within each set are the same. The advantage of introducing the unitary transformation is the ease of inverting the expansions given by Eqs. (II.5), (II.12), and (II.16).

It will be convenient to write the unitary transformation as a product of two unitary transformations, the first, e^{iG}, introducing those terms required by the commutation rules, and the second, e^{iF}, introducing the additional arbitrary terms. We therefore define the "kinematic" choice of Φ, $\Phi = \Phi^{(k)}$, as that Φ obtained by setting all arbitrary terms equal to zero. The phonons obtained in the corresponding way are denoted by $\tilde{\mathcal{O}}_\mu = \tilde{\mathcal{O}}_\mu^{(k)}$. Thus, we have from Eqs. (II.14) and (II.18),

$$\Phi = \Phi^{(k)} = \Phi_B[1 - \tfrac{1}{2} j^{(2)}(10)\Phi_B - \sum_\mu [j_\mu^{(2)}(11)\mathcal{O}_\mu{}^\dagger + \text{H.c.}]] + \text{quadratic and higher orders}\,, \tag{II.19}$$

and

$$\tilde{\mathcal{O}}_\mu = \tilde{\mathcal{O}}_\mu^{(k)} = \mathcal{O}_\mu + \tfrac{1}{2} i j_\mu^{(2)}(11)\{J_B, \Phi_B\} - \tfrac{1}{2} j_\mu^{(2)}(01)\Phi_B{}^2 - \Phi_B \sum_\nu [j_{\mu\nu}^{(2)}(02)\mathcal{O}_\nu + j_{\mu\nu}'^{(2)}(02)\mathcal{O}_\nu{}^\dagger] + \text{cubic and higher orders}. \tag{II.20}$$

The first unitary transformation is defined by

$$J = e^{iG} J_B e^{-iG}, \tag{II.21a}$$

$$\Phi^{(k)} = e^{iG} \Phi_B e^{-iG}, \tag{II.21b}$$

$$\tilde{\mathcal{O}}_\mu^{(k)} = e^{iG} \mathcal{O}_\mu e^{-iG}. \tag{II.21c}$$

In order to leave J invariant, the second unitary transformation must be generated by a scalar F such that

$$\begin{aligned} \Phi &= e^{iF} \Phi^{(k)} e^{-iF}, \\ \tilde{\mathcal{O}}_\mu &= e^{iF} \tilde{\mathcal{O}}_\mu^{(k)} e^{-iF}, \end{aligned} \tag{II.22}$$

for a general Φ and $\tilde{\mathcal{O}}_\mu$. The desired inverse transformation is then given by

$$J_B = e^{-iF} e^{-iG} J e^{iG} e^{iF}, \tag{II.23a}$$

$$\Phi_B = e^{-iF} e^{-iG} \Phi e^{iG} e^{iF}, \tag{II.23b}$$

$$\mathcal{O}_\mu = e^{-iF} e^{-iG} \tilde{\mathcal{O}}_\mu e^{iG} e^{iF}. \tag{II.23c}$$

The generator G has a boson expansion beginning with cubic terms:

$$G = G_{\mathrm{III}} + G_{\mathrm{IV}} + \cdots. \tag{II.24}$$

The Eq. (II.21a) leads to the following equations upon separation of orders:

$$i[J_B, G_{\mathrm{III}}] = -J_{\mathrm{II}}, \tag{II.25a}$$

$$i[J_B, G_{\mathrm{IV}}] = -J_{\mathrm{III}} + \tfrac{1}{2} i[G_{\mathrm{III}}, J_{\mathrm{II}}], \text{ etc.}, \tag{II.25b}$$

where G is Hermitian and required to be odd under time reversal in order to preserve the time-reversal symmetry of transformed quantities. Actually, we shall only need G_{III} explicitly in what follows. Of course, Eqs. (II.25) leave undetermined terms of G which do not depend on Φ_B, but Eqs. (II.21a) and (II.21b) require that these vanish. The solution X of the equation

$$i[J_B, X] = A \tag{II.26}$$

can be developed in a series proceeding as follows:

$$X = \tfrac{1}{2}\{\Phi_B, A\} + \tfrac{1}{8} i\{\Phi_B, \{\Phi_B, [A, J_B]\}\} - \tfrac{1}{48}\{\Phi_B, \{\Phi_B, \{\Phi_B, [[A, J_B], J_B]\}\}\} + \cdots. \tag{II.27}$$

The series terminates when a multiple commutator of A with J_B vanishes, and this will always occur as long as A contains finite powers of Φ_B. In this way, one obtains the explicit expression

$$\begin{aligned} G_{\mathrm{III}} = &-\tfrac{1}{2}\{\Phi_B, J_B\} \sum_\mu [j_\mu^{(2)}(11) \mathcal{O}_\mu{}^\dagger + \text{H.c.}] - \tfrac{1}{8} j^{(2)}(10)\{\{J_B, \Phi_B\}, \Phi_B\} - \tfrac{1}{2} \Phi_B{}^2 i \sum_\mu [j_\mu^{(2)}(01) \mathcal{O}_\mu{}^\dagger - \text{H.c.}] \\ &- i \Phi_B \sum_{\mu\nu} \{ j_{\mu\nu}^{(2)}(02) \mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu + \tfrac{1}{2} [j_{\mu\nu}'^{(2)}(02) \mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu{}^\dagger - \text{H.c.}] \}. \end{aligned} \tag{II.28}$$

The boson expansion of F likewise begins with cubic boson terms:

$$F = F_{\mathrm{III}} + F_{\mathrm{IV}} + \cdots, \tag{II.29}$$

where F_{III} is found to be

$$F_{\mathrm{III}} = \tfrac{1}{2} i J_B{}^2 \sum_\mu [f_\mu^{(2)}(11) \mathcal{O}_\mu{}^\dagger - \text{H.c.}] + J_B \sum_{\mu\nu} \{ f_{\mu\nu}^{(2)}(02) \mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu + \tfrac{1}{2} [f_{\mu\nu}'^{(2)}(02) \mathcal{O}_\mu{}^\dagger \mathcal{O}_\nu{}^\dagger + \text{H.c.}] \} + \text{cubic phonons}. \tag{II.30}$$

The cubic phonon terms in Eq. (II.30) produce the arbitrary quadratic phonon terms in Eq. (II.18).

We can now write out the inverse transformations (II.23). Of the higher-order terms, we shall be primarily concerned with those which provide the main contribution to the $\mathcal{B}$ coefficient in the rotational energy (I.1). The only quartic term providing such a contribution is proportional to J^4. For this reason, the only cubic term in the expansion of J_B in the set $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$ explicitly needed is that proportional to J^3. The expansions of Φ_B and $\mathcal{O}_\mu$ are only needed through quadratic terms. In the following equations, we use the notation $\tilde{A} = e^{iF} e^{iG} A e^{-iG} e^{-iF}$ for the transform of an operator A. From Eqs. (II.25), we have that

$$\begin{aligned} i[J, \tilde{G}_{\mathrm{III}}] &= -\tilde{J}_{\mathrm{II}}, \\ i[J, \tilde{G}_{\mathrm{IV}}] &= -\tilde{J}_{\mathrm{III}} + \tfrac{1}{2} i[\tilde{G}_{\mathrm{III}}, \tilde{J}_{\mathrm{II}}]. \end{aligned} \tag{II.31}$$

Using Eq. (II.31) and the fact that $[J, F]=0$, we can evaluate the transformation (II.23a) as follows:

$$\begin{aligned}J_B &= J + i[J, \tilde{G}_{III}] + \{i[J, \tilde{G}_{IV}] - \tfrac{1}{2}[[J, \tilde{G}_{III}], \tilde{G}_{III}] - [[J, \tilde{G}_{III}], \tilde{F}_{III}]\} + \cdots \\ &= J - \tilde{J}_{II} - (\tilde{J}_{III} + i[\tilde{J}_{II}, \tilde{G}_{III} + \tilde{F}_{III}]) + \cdots \\ &= J - J\sum_\mu [j_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger + \text{H.c.}] - \tfrac{1}{2}j^{(2)}(10)\{J, \Phi\} - i\Phi\sum_\mu [j_\mu^{(2)}(01)\tilde{\mathcal{O}}_\mu{}^\dagger - \text{H.c.}] - i\sum_{\mu\nu}\{j_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu \\ &\quad + \tfrac{1}{2}[j_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu{}^\dagger - \text{H.c.}]\} + [\sum_\mu f_\mu^{(2)}(11)j_\mu^{(2)}(11) - j^{(3)}(30)]J^3 + \text{other cubic terms + higher orders.}\end{aligned} \tag{II.32}$$

The remaining Eqs. (II.23) are

$$\begin{aligned}\mathcal{O}_\mu &= \tilde{\mathcal{O}}_\mu - i[\tilde{F}_{III} + \tilde{G}_{III}, \tilde{\mathcal{O}}_\mu] + \cdots \\ &= \tilde{\mathcal{O}}_\mu - \tfrac{1}{2}ij_\mu^{(2)}(11)\{\Phi, J\} + \tfrac{1}{2}j_\mu^{(2)}(01)\Phi^2 + \Phi\sum_\nu [j_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\nu + j_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\nu{}^\dagger] - \tfrac{1}{2}f_\mu^{(2)}(11)J^2 \\ &\quad + iJ\sum_\nu [f_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\nu + f_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\nu{}^\dagger] + \text{quadratic phonons + cubic and higher orders,}\end{aligned} \tag{II.33}$$

and

$$\begin{aligned}\Phi_B &= \Phi - i[\tilde{F}_{III} + \tilde{G}_{III}, \Phi] + \cdots \\ &= \Phi\{1 + \sum_\mu [j_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger + \text{H.c.}] + \tfrac{1}{2}j^{(2)}(10)\Phi\} - iJ\sum_\mu [f_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger - \text{H.c.}] - \sum_{\mu\nu}\{f_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu \\ &\quad + \tfrac{1}{2}[f_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu{}^\dagger + \text{H.c.}]\} + \text{cubic and higher orders.}\end{aligned} \tag{II.34}$$

The expansions (II.32)–(II.34) may now be inserted into the Hamiltonian defined by Eqs. (II.1)–(II.4) to obtain H as a function of J, $\tilde{\mathcal{O}}_\mu$, and $\tilde{\mathcal{O}}_\mu{}^\dagger$. We shall explicitly exhibit the cancellation of Φ-dependent cubic terms. Of the quartic terms, only the coefficient of the J^4 term will be obtained explicitly. First, consider the transformation of the terms in H_B. The rotational term transforms as follows:

$$\begin{aligned}\frac{J_B{}^2}{2\mathcal{I}_0} = \frac{J^2}{2\mathcal{I}_0} - \mathcal{I}_0{}^{-1}\Big(&J^2\sum_\mu [j_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger + \text{H.c.}] + \tfrac{1}{4}j^{(2)}(10)\{\{\Phi, J\}, J\} + \tfrac{1}{2}i\{\Phi, J\}\sum_\mu [j_\mu^{(2)}(01)\tilde{\mathcal{O}}_\mu{}^\dagger - \text{H.c.}] \\ &+ iJ\sum_{\mu\nu}\{j_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu + \tfrac{1}{2}[j_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu{}^\dagger - \text{H.c.}]\}\Big) + \mathcal{I}_0{}^{-1}[\sum_\mu f_\mu^{(2)}(11)j_\mu^{(2)}(11) - j^{(3)}(30)]J^4 \\ &+ \text{other quartic terms + higher orders.}\end{aligned} \tag{II.35}$$

The vibrational term is transformed as follows:

$$\begin{aligned}\sum_\mu E_\mu \mathcal{O}_\mu{}^\dagger\mathcal{O}_\mu &= \sum_\mu E_\mu\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\mu + \tfrac{1}{2}\Phi^2\sum_\mu E_\mu[j_\mu^{(2)}(01)\tilde{\mathcal{O}}_\mu{}^\dagger + \text{H.c.}] - \tfrac{1}{2}i\{\Phi, J\}\sum_\mu E_\mu[j_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger - \text{H.c.}] \\ &\quad + \Phi\sum_{\mu\nu}\{(E_\mu - E_\nu)j_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu + \tfrac{1}{2}(E_\mu + E_\nu)[j_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu{}^\dagger + \text{H.c.}]\} - \tfrac{1}{2}J^2\sum_\mu E_\mu[f_\mu^{(2)}(11)\tilde{\mathcal{O}}_\mu{}^\dagger + \text{H.c.}] \\ &\quad + iJ\sum_{\mu\nu}\{(E_\mu - E_\nu)f_{\mu\nu}^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu + \tfrac{1}{2}(E_\mu + E_\nu)[f_{\mu\nu}'^{(2)}(02)\tilde{\mathcal{O}}_\mu{}^\dagger\tilde{\mathcal{O}}_\nu{}^\dagger - \text{H.c.}]\} + \text{cubic phonons} \\ &\quad + \tfrac{1}{4}J^4\sum_\mu E_\mu|f_\mu^{(2)}(11)|^2 + \text{other quartic terms + higher orders.}\end{aligned} \tag{II.36}$$

In transforming H_{III} and H_{IV}, we need only to note that

$$H_{III} = \tilde{H}_{III} - \sum_\mu h_\mu^{(3)}(21)f_\mu^{(2)}(11)J^4 + \text{other quartic terms + higher orders,} \tag{II.37}$$

and

$$H_{IV} = h^{(4)}(40)J^4 + \text{other quartic terms + higher orders.} \tag{II.38}$$

Of course, $\tilde{H}_{III}$ is obtained from H_{III} [Eqs. (II.3) and (II.9)] by the replacement $J_B \to J$, $\Phi_B \to \Phi$, $\mathcal{O}_\mu \to \tilde{\mathcal{O}}_\mu$, $\mathcal{O}_\mu{}^\dagger \to \tilde{\mathcal{O}}_\mu{}^\dagger$.

Adding together Eqs. (II.35)–(II.38), and taking into account the rotational invariance restrictions, Eqs. (II.9), one explicitly sees the cancellation of all Φ-dependent terms of $\tilde{H}_{III}$ against those arising from the transformation of H_B. Of course, the Φ-dependent terms of $\tilde{H}_{IV}$ must be cancelled by those arising from

the transformation of H_B and $\tilde{H}_{III}$. It therefore follows that H may be rewritten as the following expansion in $(J, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu^\dagger)$:

$$H = H'_B + H'_{III} + H'_{IV} + \cdots , \tag{II.39a}$$

where

$$H'_B = \text{constant} + \sum_\mu E_\mu \tilde{\mathcal{O}}_\mu^\dagger \tilde{\mathcal{O}}_\mu + \frac{J^2}{2\mathcal{I}_0} , \tag{II.39b}$$

$$H'_{III} = J^2 \sum_\mu (\Gamma^{(3)}_\mu \tilde{\mathcal{O}}_\mu^\dagger + \text{H.c.}) + iJ \sum_{\mu\nu} [\Gamma^{(3)}_{\mu\nu} \tilde{\mathcal{O}}_\mu^\dagger \tilde{\mathcal{O}}_\nu + \tfrac{1}{2}(\Gamma'^{(3)}_{\mu\nu} \tilde{\mathcal{O}}_\mu^\dagger \tilde{\mathcal{O}}_\nu^\dagger - \text{H.c.})] + \text{cubic phonons} , \tag{II.39c}$$

$$H'_{IV} = \Gamma^{(4)} J^4 + J^3 \times \text{linear phonons} + J^2 \times \text{quadratic phonons} + J \times \text{cubic phonons} + \text{quartic phonons} . \tag{II.39d}$$

The phonon terms not fully specified are not in normal order. The coefficients of the terms in Eq. (II.39) are:

$$\Gamma^{(3)}_\mu = h^{(3)}_\mu(21) - \mathcal{I}_0^{-1} j^{(2)}_\mu(11) - \tfrac{1}{2} E_\mu f^{(2)}_\mu(11) , \tag{II.40a}$$

$$\Gamma^{(3)}_{\mu\nu} = h^{(3)}_{\mu\nu}(12) - \mathcal{I}_0^{-1} j^{(2)}_{\mu\nu}(02) + (E_\mu - E_\nu) f^{(2)}_{\mu\nu}(02) , \tag{II.40b}$$

$$\Gamma'^{(3)}_{\mu\nu} = h'^{(3)}_{\mu\nu}(12) - \mathcal{I}_0^{-1} j'^{(2)}_{\mu\nu}(02) + (E_\mu + E_\nu) f'^{(2)}_{\mu\nu}(02) , \tag{II.40c}$$

$$\Gamma^{(4)} = h^{(4)}(40) - \mathcal{I}_0^{-1} j^{(3)}(30) + \tfrac{1}{4} \sum_\mu E_\mu |f^{(2)}_\mu(11)|^2 - \sum_\mu f^{(2)}_\mu(11)[h^{(3)}_\mu(21) - \mathcal{I}_0^{-1} j^{(2)}_\mu(11)] . \tag{II.40d}$$

It is understood that the Hamiltonian (II.39) is nothing more than a regrouping of the terms of the original boson expansion (II.1), which can be retrieved with the insertion of the definitions of J, $\tilde{\mathcal{O}}_\mu$, and $\tilde{\mathcal{O}}_\mu^\dagger$ in terms of the set $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$. We have thus accomplished our aim of writing H in the form of the angular momentum decomposition (II.10), with the intrinsic operators $\mathcal{H}_n$ expansions in the phonons $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu^\dagger)$. We have therefore shown that boson expansions of all degrees of freedom may be utilized in a straightforward manner to identify coefficients of band-mixing and anharmonic vibrational terms. Of course, in order to obtain numerical values for the coefficients, a definite boson expansion must be invoked. A specific example is treated in the Appendix.

The angular momentum expansion of H given by Eq. (II.39) holds for any Φ of the form (II.12) and corresponding phonons $(\tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu^\dagger)$, as shown by the dependence of the coefficients (II.40) on the f coefficients, which define the generator F, Eq. (II.29). If a particular choice of F is replaced by another, F', so that Φ is replaced correspondingly by Φ', the angular momentum expansion of H is modified by the unitary transformation $H \to e^{-i(F'-F)} H e^{i(F'-F)}$. Other operators are also modified by this transformation. Therefore, we just have an automorphism of the whole space, so that the energy and all matrix elements must be independent of the f coefficients, the choice of which is dictated by convenience.

Suppose, first of all, that all the f coefficients are taken to be zero, corresponding to the kinematic choice $\Phi = \Phi^{(k)}$, $\tilde{\mathcal{O}}_\mu = \tilde{\mathcal{O}}_\mu^{(k)}$ [Eqs. (II.19) and (II.20)]. Then we have

$$\Gamma^{(3)}_\mu = h^{(3)}_\mu(21) - \mathcal{I}_0^{-1} j^{(2)}_\mu(11) , \tag{II.41a}$$

$$\Gamma^{(3)}_{\mu\nu} = h^{(3)}_{\mu\nu}(12) - \mathcal{I}_0^{-1} j^{(2)}_{\mu\nu}(02) , \tag{II.41b}$$

$$\Gamma'^{(3)}_{\mu\nu} = h'^{(3)}_{\mu\nu}(12) - \mathcal{I}_0^{-1} j'^{(2)}_{\mu\nu}(02) , \tag{II.41c}$$

$$\Gamma^{(4)} = h^{(4)}(40) - \mathcal{I}_0^{-1} j^{(3)}(30) . \tag{II.41d}$$

The expansion (II.39a) is then governed by the same parameter as the original expansion (II.1). If this parameter is indeed small, as one expects it to be for large systems, then one can hope for convergence, barring unforeseen coherences in higher orders. The kinematic choice is at least a very reasonable one. It has the obvious disadvantage of providing many off-diagonal terms which must be treated by perturbation theory.

However, one can eliminate off-diagonal terms by a suitable choice of the f coefficients. In particular, we shall be concerned with eliminating all couplings of the ground-state rotational band with excited bands. The angle variable corresponding to the option of diagonalization is denoted by $\Phi = \Phi^{(d)}$, the phonons by $\tilde{\mathcal{O}}_\mu = \tilde{\mathcal{O}}_\mu^{(d)}$, and F by $F = F^{(d)}$. The diagonalization of the kinematic expansion is thus effected by the transformation $H \to e^{-iF^{(d)}} \times H e^{iF^{(d)}}$. As an example, to eliminate the cubic terms, H'_{III}, we must take

$$f^{(2)}_\mu(11) = 2[h^{(3)}_\mu(21) - \mathcal{I}_0^{-1} j^{(2)}_\mu(11)] / E_\mu , \tag{II.42a}$$

$$f^{(2)}_{\mu\nu}(02) = -[h^{(3)}_{\mu\nu}(12) - \mathcal{I}_0^{-1} j^{(2)}_{\mu\nu}(02)] / (E_\mu - E_\nu) , \tag{II.42b}$$

$$f'^{(2)}_{\mu\nu}(02) = -[h'^{(3)}_{\mu\nu}(12) - g_0^{-1} j'^{(2)}_{\mu\nu}(02)]/(E_\mu + E_\nu) . \tag{II.42c}$$

We shall not explicitly consider the elimination of cubic phonon terms. The generator $F = F^{(d)}$ to the given order may be found from Eqs. (II.42) and (II.30).

Since the choice $F = F^{(d)}$ corresponds to the perturbative diagonalization of the kinematic expansion, the convergence must be as good. Suppose, however, that one were to choose the f coefficients to be of very large magnitude. Then the boson expansion (II.39) would no longer be characterized by a small parameter. Nevertheless, all physical quantities are independent of the f coefficients, which must therefore cancel out, and the cancellation must occur order by order. As an example of how this happens, let us consider the $\mathfrak{B}$ coefficient in the ground-state-band rotational energy. The leading-order contributions to this coefficient come from two sources: the vibration-rotation-interaction-type term $J^2 \times$ (phonon), which couples the ground-state band to one-phonon bands, and thus contributes in second-order perturbation theory, and the diagonal J^4 term. Together, the two terms give

$$\mathfrak{B} = \mathfrak{B}_0 = -\sum_\mu \frac{|\Gamma^{(3)}_\mu|^2}{E_\mu} + \Gamma^{(4)} . \tag{II.43a}$$

Using the general expressions (II.40a) for $\Gamma^{(3)}_\mu$, and (II.40d) for $\Gamma^{(4)}$, one sees that the f dependences of the two terms of Eq. (II.43a) exactly cancel, leaving

$$\mathfrak{B}_0 = -\sum_\mu \frac{|h^{(3)}_\mu(21) - g_0^{-1} j^{(2)}_\mu(11)|^2}{E_\mu} + h^{(4)}(40) - g_0^{-1} j^{(3)}(30) . \tag{II.43b}$$

Elimination of the vibration-rotation coupling term of H'_{III} with the choice (II.42a) of $f^{(2)}_\mu(11)$ then shoves the full burden of the correction on the diagonal J^4 term, which becomes $\mathfrak{B}_0 J^4$, as can be seen by substituting Eq. (II.42a) into (II.40d). In general, no matter what the choice of the f coefficients, one can still treat the expansion (II.39a) by perturbation theory. The point is, however, that one must formally label the successive terms H'_{III}, H'_{IV}, etc., by an order parameter and keep together all terms of the same order. Then the dependence on the f coefficients will cancel in each order of perturbation theory, and the expansions of physical quantities will still be governed by the kinematic expansion parameter. This fortunate state of affairs can be traced back to the fact that the expansions of Φ and $\tilde{\mathcal{O}}_\mu$ were assumed to begin with Φ_B and $\mathcal{O}_\mu$, respectively. More general definitions of Φ and $\tilde{\mathcal{O}}_\mu$ can, of course, be introduced; some of them may improve the convergence, certainly others can make matters worse.

Let us go on to discuss briefly the qualitative effects of the remaining terms in H'_{III}. First of all, there are anharmonic phonon terms, which, in lowest-order perturbation theory, cannot contribute to the ground-state-band rotational energy, but do affect intrinsic energy spacings. In higher-order perturbation theory, these can interfere with J-dependent terms to contribute to the ground-state-band rotational energy. Then there is a term of the form $J \times$(quadratic phonons), a sort of generalized Coriolis term. The $J\tilde{\mathcal{O}}^\dagger\tilde{\mathcal{O}}$ terms do not contribute to the ground-state-band rotational energy in lowest order, but do renormalize the effective moment of inertia of excited-state bands. The $J\tilde{\mathcal{O}}^\dagger\tilde{\mathcal{O}}^\dagger$ term, which couples the ground-state band to two-phonon bands, renormalizes the moment of inertia of the ground-state band in lowest order. However, a possible $J^2\tilde{\mathcal{O}}\tilde{\mathcal{O}}^\dagger$ term in H'_{IV} provides a diagonal contribution of the same order of magnitude, and must thus be taken into account at the same time. The dependence of the two types of terms on the $f'^{(2)}_{\mu\nu}(02)$ coefficients must be such as to guarantee independence for the moment of inertia. The choice (II.42c) for $f'^{(2)}_{\mu\nu}(02)$ eliminates the cubic term and shifts the full renormalization of $(2g)^{-1}$ to the $J^2\tilde{\mathcal{O}}\tilde{\mathcal{O}}^\dagger$ term. This renormalization, of course, is down by a factor of ϵ^2 compared with the leading-order coefficient $(2g_0)^{-1}$. In general, the coefficients in the rotational energy (I.1) are each expansions in the small parameter ϵ^2.

C. Treatment of Transition Operators and Matrix Elements

The above treatment of the Hamiltonian is readily extended to transition operators $Q^{(M)}$, which are the two-dimensional analogs of spherical tensor operators, obeying the commutation rules

$$[J, Q^{(M)}] = MQ^{(M)} , \quad M = \text{integer} . \tag{II.44}$$

The Hermitian adjoint then satisfies

$$[J, Q^{(M)\dagger}] = -MQ^{(M)\dagger} . \tag{II.45}$$

We shall discuss operators with phases chosen to satisfy the following time-reversal behavior:

$$\mathcal{T}Q^{(M)}\mathcal{T}^{-1} = Q^{(M)\dagger} \quad \text{(even operators)} \tag{II.46a}$$

or

$$\mathcal{T}Q^{(M)}\mathcal{T}^{-1} = -Q^{(M)\dagger} \quad \text{(odd operators)} . \tag{II.46b}$$

The procedure is to expand the operators $Q^{(M)}$ in the set $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu{}^\dagger)$, the coefficients of the expansion being limited by Eqs. (II.44) and (II.46). The terms of the expansion may then be organized by noting that $Q^{(M)}$ may be written in the form

$$Q^{(M)} = \tfrac{1}{2}\{e^{iM\Phi}, \mathcal{Q}^{(M)}\} , \tag{II.47}$$

where $\mathcal{Q}^{(M)}$ is a scalar, i.e.,[24a]

$$[J, \mathcal{Q}^{(M)}] = 0 . \tag{II.48}$$

It therefore follows that $\mathcal{Q}^{(M)}$ has an angular momentum expansion analogous to Eq. (II.10):

$$\mathcal{Q}^{(M)} = \mathcal{Q}_0^{(M)} + \mathcal{Q}_1^{(M)} J + \tfrac{1}{2}\mathcal{Q}_2^{(M)} J^2 + \cdots , \tag{II.49}$$

where the $\mathcal{Q}_n^{(M)}$ are intrinsic operators, i.e., commute with J and Φ, and may thus be written as functions of the phonons $\tilde{\mathcal{O}}_\mu$ and $\tilde{\mathcal{O}}_\mu{}^\dagger$.

The boson expansions of the transition operators are given by

$$Q^{(M)} = Q_B^{(M)} + Q_{II}^{(M)} + \cdots , \tag{II.50}$$

where the linear boson part for even operators has the form

$$Q_B^{(M)} = (1 + iM\Phi_B)\langle 0|Q^{(M)}|0\rangle + \sum_\mu q_\mu^{(M)(1)}(0)(\mathcal{O}_\mu{}^\dagger + \mathcal{O}_\mu) \quad \text{(even operators)}, \tag{II.51}$$

and for odd operators the form

$$Q_B^{(M)} = q^{(M)(1)}(1) J_B + \sum_\mu q_\mu^{(M)(1)}(0)(\mathcal{O}_\mu{}^\dagger - \mathcal{O}_\mu) \quad \text{(odd operators)}. \tag{II.52}$$

As noted in Ref. 1, the coefficient of Φ_B in Eq. (II.51) follows from the relation $[J_B, Q_B^{(M)}] = M\langle 0|Q^{(M)}|0\rangle$, where $\langle 0|Q^{(M)}|0\rangle$ is the average taken with respect to the self-consistent-field ground state.

The quadratic boson part for even operators has the form

$$Q_{II}^{(M)} = \tfrac{1}{2}q^{(M)(2)}(20) J_B{}^2 + J_B \sum_\mu q_\mu^{(M)(2)}(11)(\mathcal{O}_\mu{}^\dagger - \mathcal{O}_\mu) + \tfrac{1}{2}q^{(M)(2)}(00)\Phi_B{}^2 + \Phi_B \sum_\mu q_\mu^{(M)(2)}(01)(\mathcal{O}_\mu{}^\dagger + \mathcal{O}_\mu)$$
$$+ \text{quadratic phonons} \quad \text{(even operators)} . \tag{II.53}$$

Upon separating orders, Eq. (II.44) implies that

$$[J_B, Q_{II}^{(M)}] + [J_{II}, Q_B^{(M)}] = M(Q_B^{(M)} - \langle 0|Q^{(M)}|0\rangle) , \tag{II.54}$$

giving the following limitations on the coefficients:

$$q^{(M)(2)}(00) = -M[ij^{(2)}(10) + M]\langle 0|Q^{(M)}|0\rangle - 2\sum_\mu q_\mu^{(M)(1)}(0) j_\mu^{(2)}(01) ,$$

$$q_\mu^{(M)(2)}(01) = iM[q_\mu^{(M)(1)}(0) - \langle 0|Q^{(M)}|0\rangle j_\mu^{(2)}(11)] + \sum_\nu q_\nu^{(M)(1)}(0)[j_{\mu\nu}^{(2)}(02) - j_{\mu\nu}'^{(2)}(02)] \quad \text{(even operators)} . \tag{II.55}$$

For odd operators we have the form

$$Q_{II}^{(M)} = J_B \sum_\mu q_\mu^{(M)(2)}(11)(\mathcal{O}_\mu{}^\dagger + \mathcal{O}_\mu) + \tfrac{1}{2}q^{(M)(2)}(10)\{\Phi_B, J_B\} + \Phi_B \sum_\mu q_\mu^{(M)(2)}(01)(\mathcal{O}_\mu{}^\dagger - \mathcal{O}_\mu) + \text{quadratic phonons}$$
$$\text{(odd operators)}, \tag{II.56}$$

with the additional restrictions

$$q^{(M)(2)}(10) = q^{(M)(1)}(1)[j^{(2)}(10) + iM] - i2\sum_\mu q_\mu^{(M)(1)}(0) j_\mu^{(2)}(11) ,$$

$$q_\mu^{(M)(2)}(01) = iMq_\mu^{(M)(1)}(0) + iq^{(M)(1)}(1) j_\mu^{(2)}(01) + \sum_\nu q_\nu^{(M)(1)}(0)[j_{\mu\nu}^{(2)}(02) + j_{\mu\nu}'^{(2)}(02)] \quad \text{(odd operators)} . \tag{II.57}$$

We shall not analyze the cubic term $Q_{III}^{(M)}$ here, although it is worthwhile to mention that odd operators may contain a term proportional to $J_B{}^3$, which contributes to a J dependence of the g factor of magnetic operators.

We can now carry out the transformation of Eq. (II.50) from the set $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu{}^\dagger)$ to the set $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$. Substitution of the expressions (II.32)–(II.34) gives for even operators

$$Q^{(M)} = \tilde{Q}_B^{(M)} + \Lambda^{(M)(2)}(20) J^2 + J \sum_\mu \Lambda_\mu^{(M)(2)}(11)(\tilde{\mathcal{O}}_\mu{}^\dagger - \tilde{\mathcal{O}}_\mu) + \text{quadratic phonons} - \tfrac{1}{2}M^2\langle 0|Q^{(M)}|0\rangle \Phi^2$$
$$+ iM\Phi \sum_\mu q_\mu^{(M)(1)}(0)(\tilde{\mathcal{O}}_\mu{}^\dagger + \tilde{\mathcal{O}}_\mu) + \text{cubic and higher orders} \quad \text{(even operators)}, \tag{II.58a}$$

where the coefficients are

$$\Lambda^{(M)(2)}(20) = \tfrac{1}{2}q^{(M)(2)}(20) - \sum_\mu q_\mu^{(M)(1)}(0) f_\mu^{(2)}(11) , \tag{II.58b}$$

$$\Lambda_\mu^{(M)(2)}(11) = q_\mu^{(M)(2)}(11) + M\langle 0|Q^{(M)}|0\rangle f_\mu^{(2)}(11) - i\sum_\nu q_\nu^{(M)(1)}(0)[f_{\mu\nu}^{(2)}(02) - f_{\mu\nu}'^{(2)}(02)] , \tag{II.58b'}$$

and for odd operators,

$$Q^{(M)} = \tilde{Q}_B^{(M)} + J\sum_\mu \Lambda_\mu^{(M)(2)}(\tilde{\mathcal{O}}_\mu{}^\dagger + \tilde{\mathcal{O}}_\mu) + \text{quadratic phonons} + \tfrac{1}{2}iMq^{(M)(1)}(1)\{\Phi, J\} + iM\Phi\sum_\mu q_\mu^{(M)(1)}(0)(\tilde{\mathcal{O}}_\mu{}^\dagger - \tilde{\mathcal{O}}_\mu)$$
$$+ \text{cubic and higher orders} \quad \text{(odd operators)}, \tag{II.59a}$$

where

$$\Lambda_\mu^{(M)(2)}(11) = q_\mu^{(M)(2)}(11) - q^{(M)(1)}(1)j_\mu^{(2)}(11) - i\sum_\nu [f_{\mu\nu}^{(2)}(02) + f_{\mu\nu}'^{(2)}(02)]q_\nu^{(M)(1)}(0)\,. \tag{II.59b}$$

Since the operators can be written in the form (II.47), where $\mathcal{Q}^{(M)}$ is a scalar and thus independent of Φ, the Φ dependence in Eqs. (II.58a) and (II.59a) must arise from the expansion of $e^{iM\Phi}$. This fact allows us to identify $\mathcal{Q}^{(M)}$. For even operators, we obtain through quadratic boson terms

$$\mathcal{Q}^{(M)} = \langle 0|Q^{(M)}|0\rangle + \sum_\mu q_\mu^{(M)(1)}(0)(\tilde{\mathcal{O}}_\mu{}^\dagger + \tilde{\mathcal{O}}_\mu) + \Lambda^{(M)(2)}(20)J^2 + J\sum_\mu \Lambda_\mu^{(M)(2)}(11)(\tilde{\mathcal{O}}_\mu{}^\dagger - \tilde{\mathcal{O}}_\mu) + \text{quadratic phonons}$$
$$+ \text{cubic and higher orders} \quad \text{(even operators)}, \tag{II.60}$$

where the coefficients $\Lambda^{(M)(2)}(20)$ and $\Lambda_\mu^{(M)(2)}(11)$ are given by Eqs. (II.58b). For odd operators,

$$\mathcal{Q}^{(M)} = q^{(M)(1)}(1)J + \sum_\mu q_\mu^{(M)(1)}(0)(\tilde{\mathcal{O}}_\mu{}^\dagger - \tilde{\mathcal{O}}_\mu) + J\sum_\mu \Lambda_\mu^{(M)(2)}(11)(\tilde{\mathcal{O}}_\mu{}^\dagger + \tilde{\mathcal{O}}_\mu) + \text{quadratic phonons}$$
$$+ \text{cubic and higher orders} \quad \text{(odd operators)}, \tag{II.61}$$

where $\Lambda_\mu^{(M)(2)}(11)$ is given by Eq. (II.59b).

As an example, we calculate transition matrix elements of even operators within the ground-state band and between the ground-state band and one-phonon bands. Since the matrix elements must be independent of the choice of f coefficients, we may as well choose the coefficients given by Eqs. (II.42), corresponding to the diagonalization of H through cubic boson terms. This is highly convenient, since the unperturbed wave functions may then be used. These are, of course, given by

$$|M, 0\rangle = (2\pi)^{-1/2}e^{iM\Phi}|\text{vac}\rangle \tag{II.62a}$$

for the ground-state band, and

$$|M, \mu\rangle = (2\pi)^{-1/2}e^{iM\Phi}\tilde{\mathcal{O}}_\mu{}^\dagger|\text{vac}\rangle \tag{II.62b}$$

for the one-phonon bands, where $\Phi = \Phi^{(d)}$, $\tilde{\mathcal{O}}_\mu{}^\dagger = \tilde{\mathcal{O}}_\mu{}^{(d)\dagger}$, and the state $|\text{vac}\rangle$ is the vacuum of the phonon operators.

It should be noted that all the f coefficients appearing in Eq. (II.58b′) are of the same order. But the coefficients $q_\nu^{(M)(1)}(0)$ are one order higher than $\langle 0|Q^{(M)}|0\rangle$, so that the last term in Eq. (II.58b′) should be considered as being of higher order than the others and considered along with some cubic terms of the same order for consistency. Indeed, among the cubic terms not shown, there are some, for example, which are schematically of the form $q_\nu^{(M)(1)}(0)[f_{\mu\nu}^{(2)}(02) - f_{\mu\nu}'^{(2)}(02)]\,\tilde{\mathcal{O}}\,\tilde{\mathcal{O}}^\dagger\tilde{\mathcal{O}}^\dagger$ and thus contribute a comparable amount to matrix elements between states differing by one phonon. Since we shall be interested only in the lowest-order corrections to the matrix elements, all of these higher-order terms which take into account the effect of the Coriolis-type term $J\times$(quadratic phonons) in $H'_{\rm III}$ on the transitions will be dropped. Using the expression (II.42a) for $f_\mu^{(2)}(11)$, which takes into account the diagonalization of the vibration-rotation term $J^2\times$(phonon) in $H'_{\rm III}$, one obtains

$$\Lambda^{(M)(2)}(20) = \tfrac{1}{2}q^{(M)(2)}(20) - 2\sum_\mu q_\mu^{(M)(1)}(0)\,\frac{h_\mu^{(3)}(21) - g_0{}^{-1}j_\mu^{(2)}(11)}{E_\mu}\,, \tag{II.63a}$$

$$\Lambda_\mu^{(M)(2)}(11) = q_\mu^{(M)(2)}(11) + 2M\langle 0|Q^{(M)}|0\rangle\,\frac{h_\mu^{(3)}(21) - g_0{}^{-1}j_\mu^{(2)}(11)}{E_\mu}\,, \tag{II.63b}$$

where $\Lambda^{(-M)(2)}(20) = \Lambda^{(M)(2)*}(20)$, $\Lambda_\mu^{(-M)(2)}(11) = -\Lambda_\mu^{(M)(2)*}(11)$.

In calculating matrix elements within the ground-state band, it should be noted that the quadratic phonon terms in Eq. (II.60) are not generally in normal order. Putting these in normal order gives a small higher-order renormalization of the moment $\langle 0|Q^{(M)}|0\rangle$, which we neglect. The intraband matrix elements are then[14]

$$\langle M_2 0|Q^{(M)}|M_1 0\rangle = \delta_{M_2-M_1,M}\langle 0|Q^{(M)}|0\rangle\left[1 + \frac{1}{2}\frac{\Lambda^{(M)(2)}(20)}{\langle 0|Q^{(M)}|0\rangle}(M_1{}^2 + M_2{}^2)\right], \tag{II.64}$$

while the interband matrix elements are

$$\langle M_2\mu|Q^{(M)}|M_1 0\rangle = \delta_{M_2-M_1,M}\, q_\mu^{(M)(1)}(0)\left[1+\frac{1}{2}\frac{\Lambda_\mu^{(M)(2)}(11)}{q_\mu^{(M)(1)}(0)}(M_1+M_2)\right]. \tag{II.65}$$

Since the coefficients $\Lambda^{(M)(2)}(20)$ and $\Lambda_\mu^{(M)(2)}(11)$ are of the same order, while $q_\mu^{(M)(1)}(0)$ is of higher order than $\langle 0|Q^{(M)}|0\rangle$, the corrections are much more important for the interband transitions than for the intraband transitions, a result well known in the three-dimensional case. It is important to note that the corrections are not entirely dependent on the vibration-rotation band mixing, but also depend on the additional parameters $q^{(M)(2)}(20)$ and $q_\mu^{(M)(2)}(11)$ in the transition operators. Thus, knowledge of the transition matrix elements does not generally determine the contribution of the band mixing to the $\mathcal{B}$ coefficient, as is often assumed in phenomenological models.

III. CRANKING MODEL AND THE BELIAEV-ZELEVINSKY EXPANSION

A. Beliaev-Zelevinsky Expansions

Thus far, our analysis has been essentially phenomenological, based only on the assumption that a boson expansion in a small parameter is given and on the exploitation of elementary symmetries. In order to obtained definite expressions for the coefficients, one must, of course, choose a definite boson expansion. The interest in this section, however, will not be focused on these expressions, some of which are given in the Appendix, but rather on the link with the cranking model, which also requires closer specification of the type of boson expansion as a preliminary step. Once this link has been established, the cranking model may be used in lieu of the boson expansion for calculating some of the coefficients. And the type of boson expansion which must be used is that of Beliaev and Zelevinsky (BZ).

We must, first of all, clarify a slight modification in our definition of the self-consistent field from that used in Ref. 1. The BZ expansion was originally designed to be used with schematic separable forces, such as the quadrupole-quadrupole or pairing force, or some combination thereof. When working with such forces, it is expedient not to begin with the Hartree-Fock approximation (or the Hartree-Fock-Bogoliubov approximation when pairing is included), which includes direct and exchange factorization of the two-body force, but rather with the approximation based only on direct factorization, which we shall call the Hartree or simply self-consistent-field approximation (or the Hartree-Bogoliubov approximation when pairing is included).[15] It is this latter definition which turns out to be natural as the zeroth order of the BZ expansion. When dealing with more realistic forces, one would prefer to begin with the Hartree-Fock approximation, and, indeed, in Ref. 1 the RPA was interpreted as the harmonic order in a boson expansion about a Hartree-Fock minimum. We still believe this point of view is viable, but there are some well-known problems with the RPA correlation energy which are more awkward than serious,[16,17] and further problems arise when the residual interaction is treated by the higher orders of the BZ expansion.[18] These problems occur because the exchange effects included at the outset really belong to the higher orders of the boson expansion. The recent paper of da Providencia and Weneser[18] shows how to deal with these difficulties and points the way to development of boson expansions about Hartree-Fock solutions. In this paper, the difficulties will be avoided by starting with a Hartree-like approximation, even when dealing with nonseparable forces. The treatment of the harmonic boson Hamiltonian given in Ref. 1 still applies to this situation, and the exchange terms are properly included in the higher orders of the BZ expansion. As in Ref. 1, pairing correlations will not be taken into account, the generalizations being straightforward.

We begin by rewriting the Hamiltonian so that the interaction more closely resembles the quadrupole-quadrupole force:

$$H = \sum_{ab} T_{ab}\eta_a^\dagger\eta_b + \tfrac{1}{2}\sum_{abcd} V_{ab,cd}\eta_a^\dagger\eta_b^\dagger\eta_d\eta_c$$

$$= \sum_{ab}\epsilon_{ab}\eta_a^\dagger\eta_b + \tfrac{1}{2}\sum_{abcd} V_{ab,cd}\eta_a^\dagger\eta_c\eta_b^\dagger\eta_d\ , \tag{III.1a}$$

where

$$\epsilon_{ab} = T_{ab} - \tfrac{1}{2}\sum_c V_{ac,cb}\ . \tag{III.1b}$$

The indices a, b, c, d run through a complete set of single-particle states, and the two-body matrix element is not antisymmetrized.

The main idea of the BZ method for systems of even numbers of particles is to replace fermion-pair operators $\eta_b^\dagger \eta_a$ by functions of a set of exact boson operators $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$,

$$\eta_b^\dagger \eta_a = \hat{\rho}_{ab}(\tilde{B}_\mu, \tilde{B}_\mu^\dagger), \tag{III.2}$$

chosen in such a way that the fermion-pair algebra given by

$$[\eta_a^\dagger \eta_b, \eta_c^\dagger \eta_d] = \delta_{cb}\eta_a^\dagger \eta_d - \delta_{da}\eta_c^\dagger \eta_b \tag{III.3a}$$

is preserved.[19] [Instead of boson operators one may, of course, use a set of canonical pairs (P_μ, Q_μ).] The BZ procedure thus guarantees that the equations of motion will be preserved.

The boson mapping of pair operators can also be used to define a corresponding mapping of state vectors. It can then be shown that as a consequence of the commutation rules all matrix elements are correctly transcribed into the physical boson subspace (image of the fermion space). The boson images of fermion operators also have nonvanishing matrix elements in the spurious subspace (complement of the physical subspace), but there is no coupling between physical and spurious states when the boson expansions are carried to infinite order. Hence, in this limit, there is no trouble with the Pauli principle; the physical energies and eigenvectors are correctly given, and they are orthogonal to the spurious states. In practice, truncation must lead to some mixing of physical and spurious states. But one can still correctly generate perturbation expansions in the small boson-expansion parameter, which is all we do.

In order to give a concrete example of a BZ expansion for nonsuperconducting systems, it is convenient to introduce particle-hole notation. If the occupied Hartree-Fock orbitals are denoted by the index α, where $\alpha = 1, \cdots, N$, and the empty orbitals by the index i, where $i = N+1, \ldots$, the transcription to particle and hole operators is defined by

$$b_\alpha = \eta_\alpha^\dagger, \quad b_\alpha^\dagger = \eta_\alpha,$$
$$a_i^\dagger = \eta_i^\dagger, \quad a_i = \eta_i .$$

Throughout the paper we adhere to the convention of denoting occupied single-particle states by the indices α, β, γ, δ and empty single-particle states by the indices i, j, k, l. Then, the algebra (III.3a) may be rewritten as follows:

$$[a_i^\dagger a_j, a_k^\dagger a_l] = \delta_{jk}a_i^\dagger a_l - \delta_{li}a_k^\dagger a_j ,$$
$$[b_\alpha^\dagger b_\beta, b_\gamma^\dagger b_\delta] = \delta_{\gamma\beta}b_\alpha^\dagger b_\delta - \delta_{\delta\alpha}b_\gamma^\dagger b_\beta , \tag{III.3b}$$
$$[a_i^\dagger a_j, b_\alpha^\dagger b_\beta] = 0 ;$$
$$[b_\alpha a_i, a_k^\dagger a_j] = \delta_{ki}b_\alpha a_j, \quad [b_\alpha a_i, b_\gamma^\dagger b_\beta] = \delta_{\gamma\alpha}b_\beta a_i , \tag{III.3c}$$

and Hermitian conjugate equations;

$$[a_i^\dagger b_\alpha^\dagger, a_j^\dagger b_\beta^\dagger] = [b_\alpha a_i, b_\beta a_j] = 0 ; \tag{III.3d}$$
$$[b_\alpha a_i, a_j^\dagger b_\beta^\dagger] = \delta_{ij}\delta_{\beta\alpha} - \delta_{ij}b_\beta^\dagger b_\alpha - \delta_{\beta\alpha}a_j^\dagger a_i . \tag{III.3e}$$

Any boson expansion obeying the algebra of Eqs. (III.3) will be referred to as a BZ expansion.

The most familiar example of this type is given in terms of the particle-hole bosons $(B_{i\alpha}, B_{i\alpha}^\dagger)$, where

$$[B_{i\alpha}, B_{j\beta}] = 0, \quad [B_{i\alpha}, B_{j\beta}^\dagger] = \delta_{ij}\delta_{\beta\alpha} .$$

This particular expansion is obtained by requiring that in addition to fulfillment of the algebra, the particle-hole vacuum be mapped into the boson vacuum, both of which will be denoted by the symbol $|0\rangle$; that particle-hole states be mapped into one-boson states, $a_i^\dagger b_\alpha^\dagger|0\rangle = B_{i\alpha}^\dagger|0\rangle$, where $B_{i\alpha}|0\rangle = 0$; and that the values of all one-particle density-matrix elements $\langle 0|\eta_a^\dagger \eta_b|0\rangle$ be preserved, which determines the remaining constants in the expansion. We call this the "special BZ expansion." Defining the operators A_{ji} and $A_{\beta\alpha}$,

$$A_{ji} = \sum_\alpha B_{i\alpha}^\dagger B_{j\alpha}, \quad A_{\beta\alpha} = \sum_i B_{i\alpha}^\dagger B_{i\beta} , \tag{III.4}$$

which commute,

$$[A_{ji}, A_{\beta\alpha}] = 0 , \tag{III.5}$$

we can write the special BZ expansion as follows:

$$a_i^\dagger a_j = \hat{\rho}_{ji} \equiv A_{ji}\ , \quad b_\alpha^\dagger b_\beta = \delta_{\beta\alpha} - \hat{\rho}_{\alpha\beta} \equiv A_{\beta\alpha}; \tag{III.6a}$$

$$\begin{aligned} b_\alpha a_i = \hat{\rho}_{i\alpha} \equiv B_{i\alpha} &- \tfrac{1}{2}\sum_\beta A_{\alpha\beta}B_{i\beta} - \tfrac{1}{8}\sum_{\beta\gamma} A_{\alpha\beta}A_{\beta\gamma}B_{i\gamma} - \tfrac{1}{16}\sum_{\beta\gamma\delta} A_{\alpha\beta}A_{\beta\gamma}A_{\gamma\delta}B_{i\delta} \\ &+ \cdots + C_n \sum_{\alpha_1\cdots\alpha_n} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}A_{\alpha_{n-1}\alpha_n}B_{i\alpha_n} + \cdots \\ = B_{i\alpha} &- \tfrac{1}{2}\sum_j A_{ij}B_{j\alpha} - \tfrac{1}{8}\sum_{jk} A_{ij}A_{jk}B_{k\alpha} - \tfrac{1}{16}\sum_{jkl} A_{ij}A_{jk}A_{kl}B_{l\alpha} \\ &+ \cdots + C_n \sum_{i_1\cdots i_n} A_{ii_1}A_{i_1i_2}\cdots A_{i_{n-2}i_{n-1}}A_{i_{n-1}i_n}B_{i_n\alpha} + \cdots, \end{aligned}$$

$$a_i^\dagger b_\alpha^\dagger = \hat{\rho}_{i\alpha}^\dagger\ .^{24b} \tag{III.6b}$$

We see that each term in the expansion of the particle-hole operators is arranged in two ways:

$$\sum_{\alpha_1\cdots\alpha_n} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}A_{\alpha_{n-1}\alpha_n}B_{i\alpha_n} = \sum_{i_1\cdots i_n} A_{ii_1}A_{i_1i_2}\cdots A_{i_{n-2}i_{n-1}}A_{i_{n-1}i_n}B_{i_n\alpha}\ . \tag{III.7}$$

Since this identity turns out to be quite useful, we provide its straightforward derivation. Denoting the left-hand side of Eq. (III.7), for example, by $P_{i\alpha}^{(n)}$, we carry out the following manipulations, making use of Eq. (III.5):

$$\begin{aligned} P_{i\alpha}^{(n)} &= \sum_{\alpha_1\cdots\alpha_n} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}A_{\alpha_{n-1}\alpha_n}B_{i\alpha_n} \\ &= \sum_{j\alpha_1\cdots\alpha_n} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}B_{j\alpha_n}^\dagger B_{j\alpha_{n-1}}B_{i\alpha_n} \\ &= \sum_{j\alpha_1\cdots\alpha_{n-1}} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}\sum_{\alpha_n} B_{j\alpha_n}^\dagger B_{i\alpha_n}B_{j\alpha_{n-1}} \\ &= \sum_{j\alpha_1\cdots\alpha_{n-1}} A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-2}\alpha_{n-1}}A_{ij}B_{j\alpha_{n-1}} \\ &= \sum_{j\alpha_1\cdots\alpha_{n-1}} A_{ij}A_{\alpha\alpha_1}A_{\alpha_1\alpha_2}\cdots A_{\alpha_{n-3}\alpha_{n-2}}A_{\alpha_{n-2}\alpha_{n-1}}B_{j\alpha_{n-1}} \\ &= \sum_j A_{ij}P_{j\alpha}^{(n-1)}\ . \end{aligned} \tag{III.8}$$

We therefore have

$$P_{i\alpha}^{(n)} = \sum_j A_{ij}P_{j\alpha}^{(n-1)}\ , \quad n \geq 1, \tag{III.9}$$

where $P_{i\alpha}^{(0)} = B_{i\alpha}$. Iterated application of Eq. (III.9) establishes Eq. (III.7). For later application, we note that manipulations analogous to those of Eq. (III.8) can be applied to the right-hand side of Eq. (III.7) to give

$$P_{i\alpha}^{(n)} = \sum_j A_{ij}P_{j\alpha}^{(n-1)} = \sum_\beta A_{\alpha\beta}P_{i\beta}^{(n-1)}, \quad n \geq 1\ . \tag{III.10}$$

Since $\hat{\rho}_{i\alpha} = \sum_n C_n P_{i\alpha}^{(n)}$, $A_{ij} = \hat{\rho}_{ij}$, and $A_{\alpha\beta} = \delta_{\beta\alpha} - \hat{\rho}_{\beta\alpha}$, Eq. (III.10) leads to the identity

$$\sum_j \hat{\rho}_{ij}\hat{\rho}_{j\alpha} - \sum_\beta (\delta_{\beta\alpha} - \hat{\rho}_{\beta\alpha})\hat{\rho}_{i\beta} = 0\ , \tag{III.11}$$

which holds independently of the values of the coefficients C_n in Eq. (III.6b). An important application of Eq. (III.11) will be made later.

Let us now check that the series (III.6) satisfies the commutation rules (III.3). It is readily verified that the density matrix elements are preserved. First of all, as noted in a recent paper, the finite expressions (III.6a) clearly satisfy the commutation rules (III.3b).[18] The form of the expansion (III.6b) for particle-hole operators allows the commutation rules (III.3c) to be fulfilled for any values of the coefficients C_n. This is easily seen by choosing the appropriate form of (III.6b). Thus, when calculating $[b_\alpha a_i, a_k^\dagger a_j] = [\hat{\rho}_{i\alpha}, A_{jk}]$, the first form should be chosen, and because of Eq. (III.5), the calculation then becomes trivial. Likewise, use of Eq. (III.5) and the two forms of writing the particle-hole expansion enables one to prove that the commutation rules (III.3d) are satisfied. Finally, it is not hard to see that the expansion (III.6b) must be infinite to satisfy Eq. (III.3e), from which the coefficients C_n are finally obtained.

It is very important to note that the boson expansion (III.6) satisfies the commutator algebra (III.3) term by term, each successive term corresponding to a higher order in the Taylor series. To

make this point more definite, let us write the expansion (III.6) in our previous notation:

$$\eta_a^\dagger \eta_b = (\eta_a^\dagger \eta_b)_0 + (\eta_a^\dagger \eta_b)_I + (\eta_a^\dagger \eta_b)_{II} + \cdots , \tag{III.12}$$

where the first term on the right is a constant, the second is linear in bosons, etc. Then, it is readily checked that

$$\begin{aligned}
&[(\eta_a^\dagger \eta_b)_I, (\eta_c^\dagger \eta_d)_I] = \delta_{cb}(\eta_a^\dagger \eta_d)_0 - \delta_{da}(\eta_c^\dagger \eta_b)_0 , \\
&[(\eta_a^\dagger \eta_b)_I, (\eta_c^\dagger \eta_d)_{II}] + [(\eta_a^\dagger \eta_b)_{II}, (\eta_c^\dagger \eta_d)_I] = \delta_{cb}(\eta_a^\dagger \eta_d)_I - \delta_{da}(\eta_c^\dagger \eta_b)_I , \qquad \text{(III.13)} \\
&[(\eta_a^\dagger \eta_b)_I, (\eta_c^\dagger \eta_d)_{III}] + [(\eta_a^\dagger \eta_b)_{II}, (\eta_c^\dagger \eta_d)_{II}] + [(\eta_a^\dagger \eta_b)_{III}, (\eta_c^\dagger \eta_d)_I] = \delta_{cb}(\eta_a^\dagger \eta_d)_{II} - \delta_{da}(\eta_c^\dagger \eta_b)_{II} , \quad \text{etc.}
\end{aligned}$$

It is thus seen that by not writing the expansion in normal order, we have obtained a convenient correlation between the order of a term in the expansion and the number of boson operators in the term. As a consequence of this arrangement, the indices in each term are completely linked. It is expected that this linked structure greatly enhances the tendency of the expansion toward convergence. If, on the other hand, the series is rewritten in normal order, the contractions give rise to terms with unlinked indices. Thus, for example, the quintic term in Eq. (III.6b) written in normal order is

$$-\tfrac{1}{8}\sum_{\beta\gamma} A_{\alpha\beta}A_{\beta\gamma}B_{i\gamma} = -\tfrac{1}{8}\Big(\sum_{j\beta} B_{j\beta}^\dagger B_{j\beta}\Big)B_{i\alpha} - \tfrac{1}{8}\sum_{j\beta k\gamma} B_{j\beta}^\dagger B_{k\gamma}^\dagger B_{j\alpha}B_{k\beta}B_{i\gamma} .$$

(Cubic terms will arise from normal ordering of all other higher-order terms as well.) The appearance of this coherent cubic term would seem to bode ill for the convergence of the series if it is mistaken as belonging to the same order as the incoherent cubic term. In fact, however, it should be considered together with the normal-ordered quintic term, and then cancellation of coherences becomes possible.

An expansion parameter ϵ clearly labeling the order may be defined by passing from the purely kinematic bosons to more physically interesting combinations, for example, the RPA normal modes or the angular momentum coupled bosons used for spherical nuclei, which establish the parameter $\Omega^{-1/2}$.

Of the more general BZ-type expansions, we shall be interested mainly in those which can be obtained from the special one (III.6) by a canonical transformation in the boson space. We shall also require for later applications that in the more general expansions, the successive terms $(\eta_a^\dagger \eta_b)_{II}$, $(\eta_a^\dagger \eta_b)_{III}$, etc., satisfying Eq. (III.13), be so arranged that the number of boson operators in each term correspond to the order of the term. In other words, the kth term is a homogeneous function of the boson operators of degree k. A boson expansion arranged to satisfy this requirement shall be called a "c-ordered expansion."[20] Obviously, a c-ordered expansion cannot, in general, be a normal-ordered expansion. It is not hard to show that expansions written in c order have the property that if all boson operators $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$ are replaced by c numbers $(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*)$, with $\tilde{\sigma}_\mu$ and $i\tilde{\sigma}_\mu^*$ interpreted as classical complex canonical variables, then all commutator relations are replaced by the corresponding classical Poisson-bracket relations. We shall call this the classical correspondence property, and it plays an important role in the discussion in Sec. (III B). If the c-number replacement is made on the expansions written in normal order, different functions are obtained which do not obey all the required Poisson-bracket relations as is easily shown by examples.

That the classical correspondence holds for the expansion (III.6) can be independently seen from the fact that the expansion can be obtained by quantizing a classical expansion satisfying Poisson-bracket relations corresponding to Eq. (III.13). The c-ordered quantized expansion is obtained by replacing the classical variables by boson operators frozen in a permutation which allows the quantal commutator algebra to be fulfilled. There is more than one such permutation, the proper choice depending on additional considerations. Specifically, the ordering of operators in Eq. (III.6a) is determined by the requirement that $\langle 0|a_i^\dagger a_j|0\rangle = \langle 0|b_\alpha^\dagger b_\beta|0\rangle = 0$. The ordering of the operators in the successive terms of the infinite expansion (III.6b) is then fixed by the commutators (III.3e). There are still two arrangements left, but the identity (III.7) shows that the expansions are identical. As long as no contractions are carried out afterward, one can retrieve the classical expansion with the c-number replacement. More general BZ expansions may be obtained in a similar way with greater ease than would be the case when working with quantized expressions from the outset.

In practice, the general BZ expansions will be obtained from the special one by defining a canonical transformation from the particle-hole bosons

$(B_{i\alpha}, B_{i\alpha}^\dagger)$ to general bosons $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$. The general bosons can be expressed as a c-ordered series in the particle-hole bosons, which may be inverted to give the particle-hole bosons as a c-ordered series in the general bosons. If the inverse expansion is then substituted into the special expansion (III.6) and terms of the same order are collected together *without contracting any operators*, the result will be a c-ordered expansion for fermion pairs in the set $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$ having the classical correspondence property. As an example, consider the expansion of the fermion pairs in terms of the normal-mode operators $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$ which are related to the particle-hole bosons by the equations[1]

$$B_{i\alpha} = \sum_\mu [-Y_{i\alpha}(\mu)^* \mathcal{O}_\mu^\dagger + X_{i\alpha}(\mu)\mathcal{O}_\mu] + g_0^{-1} C_{i\alpha} J_B - i J_{i\alpha} \Phi_B ,$$

$$B_{i\alpha}^\dagger = \sum_\mu [X_{i\alpha}(\mu)^* \mathcal{O}_\mu^\dagger - Y_{i\alpha}(\mu)\mathcal{O}_\mu] + g_0^{-1} C_{i\alpha}^* J_B + i J_{i\alpha}^* \Phi_B .$$

One need only substitute these directly into Eqs. (III.6) and not contract any terms to obtain a c-ordered expansion in the new set. One may perform a second transformation from the normal modes to the set $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu^\dagger)$. This is provided by Eqs. (II.32)–(II.34) and is c ordered to the order shown. The expansion of the operators $a_i^\dagger a_j$ and $b_\alpha^\dagger b_\beta$ then becomes infinite, and that for the particle-hole operators acquires even as well as odd boson terms.

Why do we introduce expansions written in c order rather than the more orthodox normal order? One reason, already provided, is the ease of keeping track of the order of a term. But a more important reason, as will be seen, is that it then becomes possible to state a simple prescription for carrying out the Hartree approximation in the boson picture.

B. Hartree Approximation in the Boson Picture

Let us insert the special BZ expansion (III.6) into the Hamiltonian (III.1) and collect terms of the same order *without contraction* to give the c-ordered expansion

$$H = H_{\rm I} + H_B + H_{\rm III} + \cdots , \tag{III.14}$$

in which the linear boson term is

$$H_{\rm I} = \sum_{i\alpha} (\varepsilon_{i\alpha} + \sum_\beta V_{i\beta,\alpha\beta}) B_{i\alpha}^\dagger + \text{H.c.} , \tag{III.15}$$

and the quadratic boson term is

$$H_B = E_{\rm SCF} + \sum_{ij\alpha} (\varepsilon_{ij} + \sum_\beta V_{i\beta,j\beta}) B_{i\alpha}^\dagger B_{j\alpha} - \sum_{i\alpha\beta} (\varepsilon_{\alpha\beta} + \sum_\gamma V_{\alpha\gamma,\beta\gamma}) B_{i\beta}^\dagger B_{i\alpha} + \sum_{ij\alpha\beta} V_{i\beta,\alpha j} \tfrac{1}{2} (B_{i\alpha}^\dagger B_{j\beta} + B_{j\beta} B_{i\alpha}^\dagger) + \tfrac{1}{2} \sum_{ij\alpha\beta} V_{ij,\alpha\beta} (B_{i\alpha}^\dagger B_{j\beta}^\dagger + \text{H.c.}) , \tag{III.16}$$

where $E_{\rm SCF}$ is the constant

$$E_{\rm SCF} = \sum_\alpha (\varepsilon_{\alpha\alpha} + \tfrac{1}{2} \sum_\beta V_{\alpha\beta,\alpha\beta}) = \sum_{ab} \varepsilon_{ab} \langle 0|\eta_a^\dagger \eta_b|0\rangle + \tfrac{1}{2} \sum_{abcd} V_{ab,cd} \langle 0|\eta_a^\dagger \eta_c|0\rangle \langle 0|\eta_b^\dagger \eta_d|0\rangle . \tag{III.17}$$

If the single-particle basis is chosen to consist of the eigenstates of the Hartree or directly factorized Hamiltonian $H_{\rm SCF}$, given by

$$H_{\rm SCF} = E_{\rm SCF} + \sum_{ab} (\varepsilon_{ab} + \sum_{cd} V_{ac,bd} \langle 0|\eta_c^\dagger \eta_d|0\rangle) \eta_a^\dagger \eta_b , \tag{III.18}$$

then the following conditions hold:

$$\varepsilon_{i\alpha} + \sum_\beta V_{i\beta,\alpha\beta} = 0 ,$$

$$\varepsilon_{ij} + \sum_\beta V_{i\beta,j\beta} = \epsilon_i \delta_{ji} ,$$

$$\varepsilon_{\alpha\beta} + \sum_\gamma V_{\alpha\gamma,\beta\gamma} = \epsilon_\alpha \delta_{\beta\alpha} . \tag{III.19}$$

Consequently, the linear boson term $H_{\rm I}$ vanishes,

$$H_{\rm I} = 0 , \tag{III.20}$$

the constant $E_{\rm SCF}$ becomes the Hartree ground-state energy, and H_B takes the form

$$H_B = E_{\rm SCF} + \sum_{i\alpha} (\epsilon_i - \epsilon_\alpha) B_{i\alpha}^\dagger B_{i\alpha} + \sum_{ij\alpha\beta} V_{i\beta,\alpha j} \tfrac{1}{2} (B_{i\alpha}^\dagger B_{j\beta} + B_{j\beta} B_{i\alpha}^\dagger) + \tfrac{1}{2} \sum_{ij\alpha\beta} V_{ij,\alpha\beta} (B_{i\alpha}^\dagger B_{j\beta}^\dagger + \text{H.c.}) . \tag{III.21}$$

Apart from the modification (III.1b) in the definition of the quantities ε_{ab}, Eq. (III.21) differs from the RPA Hamiltonian, also denoted by H_B in Ref. 1,

through the replacement of antisymmetrized two-body matrix elements by unantisymmetrized ones; this includes Eq. (III.19) and the constant E_{SCF} (which corresponds to E_{HF} in Ref. 1). However, all of the desirable features of H_B found in Ref. 1 still hold – conservation laws are preserved and the quadratic form is positive if the self-consistent field is stable. We note that $E_{\mathrm{SCF}} \neq \langle 0|H|0\rangle$; in fact, the following condition holds:

$$\langle 0|H|0\rangle = \langle 0|H_B|0\rangle = E_{\mathrm{SCF}} + \tfrac{1}{2}\sum_{i\alpha} V_{i\alpha,\alpha i} \ . \qquad \text{(III.22)}$$

This guarantees that cubic and higher-order terms will not contribute to $\langle 0|H|0\rangle$.

We have thus seen that if the Hamiltonian is first written down in the Hartree single-particle basis and then the special BZ expansion is inserted to produce the c-ordered expansion of H, linear boson terms will be absent. We emphasize that these linear boson terms are defined *relative to the c order*. Additional linear boson terms can still arise if one puts higher-order terms into normal order, as, for example, the term H_{III} given by Eq. (A17). Now, in this procedure, one must first solve the Hartree problem in the fermion picture before introducing the bosons. If, on the other hand, an arbitrary single-particle basis is used together with the special BZ expansion, or some more general expansion is used, even with a Hartree basis, linear boson terms (relative to c order) will in general be present. However, these terms can be removed by an additional unitary transformation in the boson space. This is obviously equivalent to introducing from the outset a new boson expansion related to the special one by a canonical transformation. In this way, it is possible to solve the Hartree problem working entirely within the boson picture, and it is just such a technique which is needed to establish the link between the boson-expansion method and the cranking model.

Now, there are many unitary transformations $H \to e^{-iS}He^{iS}$ capable of removing linear boson terms in H. Which correspond to the Hartree approximation? One obvious answer is a direct transcription of the Hartree problem from the fermion to the boson picture. It is well known that in the fermion picture S can be chosen as a one-body operator, $S=\sum_{i\alpha}(S_{i\alpha}a_i^{\dagger}b_\alpha^{\dagger}+\mathrm{H.c.})$, such that the transform of H_{SCF} contains no $a_i^{\dagger}b_\alpha^{\dagger}$ and $b_\alpha a_i$ terms. Let H_{SCF} and S be transcribed into the boson picture by means of the special BZ expansion. It is then clear that S must have an infinite expansion containing only terms with odd numbers of bosons chosen to make the transform of H_{SCF} a finite quadratic form:

$$e^{-iS}H_{\mathrm{SCF}}e^{iS} = \mathrm{const} + \sum_{i\alpha,j\beta} h_{i\alpha,j\beta}B_{i\alpha}^{\dagger}B_{j\beta} \ .$$

In order to relate the cranking model to the boson expansion of H, it is necessary to transform H as well as H_{SCF}, and the infinite form of S makes this task very cumbersome. But in the cranking model, only the ground-state energy E_{SCF} and expectation values of one-body operators with respect to the Hartree ground state are all that is required. In that case, fortunately, another much simpler form is available for S yielding exactly the same results for these quantities, as we now proceed to demonstrate.

We shall prove the following theorem: Let $H(\tilde{B}_\mu, \tilde{B}_\mu^{\dagger})$ be a c-ordered boson expansion of the Hamiltonian and $K(\tilde{B}_\mu, \tilde{B}_\mu^{\dagger})$ the corresponding c-ordered expansion of any one-body operator, the boson expansion being either the special BZ expansion or any other one obtained from it by a canonical transformation in the boson space.[21] Let S_B be defined as the generator of the pure inhomogeneous transformation

$$\tilde{B}_\mu \to e^{-iS_B}\tilde{B}_\mu e^{iS_B} = \tilde{\sigma}_\mu + \tilde{B}_\mu \ ,$$

$$\tilde{B}_\mu^{\dagger} \to e^{-iS_B}\tilde{B}_\mu^{\dagger} e^{iS_B} = \tilde{\sigma}_\mu^{*} + \tilde{B}_\mu^{\dagger} \ , \qquad \text{(III.23)}$$

where the $(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^{*})$ are constants determined by the condition that the transformed Hamiltonian $e^{-iS_B} \times He^{iS_B}$ (written as a c-ordered expansion) contain no terms linear in the bosons. The transformation (III.23) is just a shift in the origin of each oscillator, and the generator must have the form

$$S_B = -i\sum_{\mu}(\tilde{\sigma}_\mu\tilde{B}_\mu^{\dagger} - \tilde{\sigma}_\mu^{*}\tilde{B}_\mu) \ . \qquad \text{(III.24)}$$

Then (as will be proven), the constant term in the c-ordered expansion $e^{-iS_B}He^{iS_B}$ is just the Hartree energy for the Hamiltonian H, and the constant term in the c-ordered expansion $e^{-iS_B}Ke^{iS_B}$ is the expectation value of K in the Hartree ground state.

Before proceeding with the proof, we emphasize the following obvious point in order to avoid possible misunderstanding: The transform of a c-ordered expansion and that of the same expansion written in normal order are, of course, one and the same operator; but what we mean by "constant" and "linear-boson" terms relative to the two orderings is different. For example, consider a factor $B_{j\beta}^{\dagger}B_{k\beta}B_{i\alpha}^{\dagger}$, which may occur among the terms of H_{III} in the c-ordered expansion of H. The transform of this factor written in c order is

$$e^{-iS_B}B_{j\beta}^{\dagger}B_{k\beta}B_{i\alpha}^{\dagger}e^{iS_B} = \sigma_{i\alpha}^{*}\sigma_{j\beta}^{*}\sigma_{k\beta} + (\sigma_{j\beta}^{*}\sigma_{k\beta}B_{i\alpha}^{\dagger} + \sigma_{j\beta}^{*}\sigma_{i\alpha}^{*}B_{k\beta} + \sigma_{i\alpha}^{*}\sigma_{k\beta}B_{j\beta}^{\dagger})$$
$$+ (\sigma_{j\beta}^{*}B_{k\beta}B_{i\alpha}^{\dagger} + \sigma_{k\beta}B_{j\beta}^{\dagger}B_{i\alpha}^{\dagger} + \sigma_{i\alpha}^{*}B_{j\beta}^{\dagger}B_{k\beta}) + B_{j\beta}^{\dagger}B_{k\beta}B_{i\alpha}^{\dagger} \ .$$

The "constant" term that we shall be talking about relative to c order is the first term on the right-hand side, and the "linear boson" term relative to c order is the second term in parenthesis. Let us write the above expression in normal order, which is the same result one obtains by directly transforming the normal-ordered term $\delta_{ki}\delta_{\beta\alpha}B_{j\beta}^{\dagger}+B_{i\alpha}^{\dagger}B_{j\beta}^{\dagger}B_{k\beta}$:

$$e^{-iS_B}B_{j\beta}^{\dagger}B_{k\beta}B_{i\alpha}^{\dagger}e^{iS_B}=(\delta_{ki}\delta_{\beta\alpha}\sigma_{j\beta}^{*}+\sigma_{i\alpha}^{*}\sigma_{j\beta}^{*}\sigma_{k\beta})+(\delta_{ki}\delta_{\beta\alpha}B_{j\beta}^{\dagger}+\sigma_{j\beta}^{*}\sigma_{k\beta}B_{i\alpha}^{\dagger}+\sigma_{j\beta}^{*}\sigma_{i\alpha}^{*}B_{k\beta}$$
$$+\sigma_{i\alpha}^{*}\sigma_{k\beta}B_{j\beta}^{\dagger})+(\sigma_{j\beta}^{*}B_{i\alpha}^{\dagger}B_{k\beta}+\sigma_{k\beta}B_{j\beta}^{\dagger}B_{i\alpha}^{\dagger}+\sigma_{i\alpha}^{*}B_{j\beta}^{\dagger}B_{k\beta})+B_{j\beta}^{\dagger}B_{i\alpha}^{\dagger}B_{k\beta}\,.$$

The true constant term and the linear boson term obtained after normal ordering are different, and these are *not* the terms that we shall be considering.

Let us first consider the effect of the inhomogeneous transformation on the boson expansion of fermion pairs. We write $\eta_b^{\dagger}\eta_a=\hat{\rho}_{ab}=f_{ab}(\tilde{B}_{\mu},\tilde{B}_{\mu}^{\dagger})$, where f_{ab} defines the functional form of the dependence of the c-ordered expansion on the bosons. Then, define the matrix $\underline{\rho}$ by $\rho_{ab}=f_{ab}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})$; i.e., ρ_{ab} is obtained from $\hat{\rho}_{ab}$ by replacing the boson operators $(\tilde{B}_{\mu},\tilde{B}_{\mu}^{\dagger})$ with the c numbers $(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})$. The transformation of fermion pairs is then given by

$$e^{-iS_B}\hat{\rho}_{ab}e^{iS_B}=f_{ab}(\tilde{B}_{\mu}+\tilde{\sigma}_{\mu},\tilde{B}_{\mu}^{\dagger}+\tilde{\sigma}_{\mu}^{*})=\rho_{ab}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})+\sum_{\mu}\left(\frac{\partial\rho_{ab}}{\partial\tilde{\sigma}_{\mu}}\tilde{B}_{\mu}+\frac{\partial\rho_{ab}}{\partial\tilde{\sigma}_{\mu}^{*}}\tilde{B}_{\mu}^{\dagger}\right)+\text{quadratic and higher orders}\,. \tag{III.25}$$

This is just a Taylor series and therefore c ordered. The Eq. (III.25) defines the transformation of any one-body operator K,

$$K=\sum_{ab}K_{ba}\eta_b^{\dagger}\eta_a\,,$$

as follows:

$$e^{-iS_B}Ke^{iS_B}=\sum_{ab}K_{ba}\rho_{ab}+\sum_{\mu}\sum_{ab}K_{ba}\left(\frac{\partial\rho_{ab}}{\partial\tilde{\sigma}_{\mu}}\tilde{B}_{\mu}+\frac{\partial\rho_{ab}}{\partial\tilde{\sigma}_{\mu}^{*}}\tilde{B}_{\mu}^{\dagger}\right)+\text{quadratic and higher orders}\,. \tag{III.26}$$

The constant term on the right-hand side, which may be written as $\mathrm{Tr}(\underline{K}\underline{\rho})$, is the quantity which will be identified with the expectation value of K in the Hartree ground state. It should be noted, that since the expansion is not normal ordered, this constant is *not* equal to the expectation value of the expansion taken with respect to the vacuum of the bosons.

The inhomogeneous transformation of the Hamiltonian is readily obtained from Eq. (III.1) and (III.25):

$$e^{-iS_B}He^{iS_B}=E_0(\underline{\rho}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*}))+\sum_{\mu}\left(\frac{\partial E_0}{\partial\tilde{\sigma}_{\mu}}\tilde{B}_{\mu}+\frac{\partial E_0}{\partial\tilde{\sigma}_{\mu}^{*}}\tilde{B}_{\mu}^{\dagger}\right)+\text{quadratic and higher orders}\,, \tag{III.27}$$

where the constant term E_0 is given by

$$E_0=\sum_{ab}\varepsilon_{ab}\rho_{ba}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})+\tfrac{1}{2}\sum_{abcd}V_{ab,cd}\rho_{ca}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})\rho_{db}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})\,. \tag{III.28}$$

Again, because the expansion (III.27) is not normal ordered, E_0 is not the expectation value of the expansion with respect to the vacuum of the bosons. The condition that S be chosen such as to eliminate linear boson terms in Eq. (III.27) is seen to be the variational requirement

$$\frac{\partial E_0(\underline{\rho}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*}))}{\partial\tilde{\sigma}_{\mu}}=\frac{\partial E_0(\underline{\rho}(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*}))}{\partial\tilde{\sigma}_{\mu}^{*}}=0\,. \tag{III.29}$$

The constant E_0, evaluated with the solutions $\tilde{\sigma}_{\mu}=\tilde{\sigma}_{\mu}^{(0)}$ of Eq. (III.29) is to be identified with the Hartree ground-state energy:

$$E_{\mathrm{SCF}}=E_0(\underline{\rho}(\tilde{\sigma}_{\mu}^{(0)},\tilde{\sigma}_{\mu}^{(0)*}))\,. \tag{III.30}$$

From the forms of E_0 and the constant term in Eq. (III.26), it is obvious that in order to prove the theorem we must identify $\underline{\rho}$ with the one-particle reduced density matrix of the Hartree theory, but parametrized by the quantities $(\tilde{\sigma}_{\mu},\tilde{\sigma}_{\mu}^{*})$. Now, it is well known that the Hartree equations can be derived by varying E_0, as given by Eq. (III.28), with respect to the parameters ρ_{ab}, subject to the constraint $\underline{\rho}^2=\underline{\rho}$.[22] It is clear that entirely equivalent results will be obtained if the matrix $\underline{\rho}$ is expressed in terms of a smaller set of essential variational parameters, provided that the parametrization automatically satisfies this con-

straint. Since there is one complex parameter $\tilde{\sigma}_\mu$ for each boson, and there is one boson for each particle-hole excitation, we have one parameter for each particle-hole excitation. As is well known, this is the correct number of essential variational parameters for the Hartree-Fock or Hartree approximations.[23] Therefore, Eq. (III.29) will be equivalent to the Hartree equations, and our theorem will be proven if it can be shown that the conditions

$$\underline{\rho}^2(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*) - \underline{\rho}(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*) = 0 , \tag{III.31}$$

and also

$$\mathrm{Tr}\underline{\rho}(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*) = N , \tag{III.32}$$

where N is the total number of particles, are satisfied for *any values* of $(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*)$. The Eq. (III.32) is required, since it is part of the definition of the reduced one-particle density matrix.

As discussed in Sec. III A, the c-ordered boson expansions have the property that if the boson operators are replaced by c-number variables, all commutator relations are replaced by classical Poisson-bracket relations. Thus, if $\hat{A}$ and $\hat{B}$ are any two such boson expansions, then, upon making the replacements $\tilde{B}_\mu \to \tilde{\sigma}_\mu$, $\tilde{B}_\mu^\dagger \to \tilde{\sigma}_\mu^*$, so that $\hat{A}$ and $\hat{B}$ go over into functions A and B, respectively, of $(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*)$, the commutator $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is replaced by the bracket

$$\{\!\{A, B\}\!\} = \sum_\mu \left(\frac{\partial A}{\partial \tilde{\sigma}_\mu} \frac{\partial B}{\partial \tilde{\sigma}_\mu^*} - \frac{\partial A}{\partial \tilde{\sigma}_\mu^*} \frac{\partial B}{\partial \tilde{\sigma}_\mu} \right) . \tag{III.33}$$

Therefore, the commutation relations for fermion pairs,

$$[\hat{\rho}_{ba}, \hat{\rho}_{dc}] = \delta_{cb}\hat{\rho}_{da} - \delta_{da}\hat{\rho}_{bc} , \tag{III.3'}$$

imply the corresponding "classical" relations

$$\{\!\{\rho_{ba}, \rho_{dc}\}\!\} = \delta_{cb}\rho_{da} - \delta_{da}\rho_{bc} . \tag{III.34}$$

The Eq. (III.34) can also be obtained from Eq. (III.3') by applying the shift transformation (III.23) to both sides of Eq. (III.3a), and then separating orders, making use of Eq. (III.25).

The variational condition (III.29) immediately implies that

$$\{\!\{E_0, \rho_{ab}\}\!\} = 0 \tag{III.35a}$$

for every ρ_{ab}. From Eq. (III.28) it is seen that E_0 depends at most quadratically on the ρ_{ab}, so that the above bracket is readily calculated from Eqs. (III.34) with the aid of the identity $\{\!\{XY, Z\}\!\} = X\{\!\{Y, Z\}\!\} + Y\{\!\{X, Z\}\!\}$, to give the equations

$$[\underline{\rho}, \underline{H}_{\mathrm{SCF}}(\underline{\rho})] = 0 , \tag{III.35b}$$

where $\underline{H}_{\mathrm{SCF}}$, defined by

$$(\underline{H}_{\mathrm{SCF}})_{ab} = \epsilon_{ab} + \sum_{cd} V_{ac,bd}\rho_{dc} , \tag{III.36}$$

has the form of the matrix of the Hartree Hamiltonian (III.18). The Eq. (III.35b) is the familiar density-matrix form of the self-consistent field equations. It is important to note that we were able to go from Eqs. (III.29) to (III.35b) only because the conditions (III.34) hold. However, the proof that we have the Hartree approximation will not be complete until Eqs. (III.31) and (III.32) are proven.

It is sufficient to prove that Eqs. (III.31) and (III.32) are true when the special BZ expansion is utilized; it then follows that they will also be true for any expansion related to the special one by a canonical transformation. Let us examine this point in more detail. The special BZ expansion (III.6) may be summarized by writing

$$\eta_b^\dagger \eta_a = \hat{\rho}_{ab}(B_{i\alpha}, B_{i\alpha}^\dagger) . \tag{III.6'}$$

The shift transformation (III.23) for the special case will be written as

$$B_{i\alpha} \to e^{-iS_B} B_{i\alpha} e^{iS_B} = \sigma_{i\alpha} + B_{i\alpha} ,$$

$$B_{i\alpha}^\dagger \to e^{-iS_B} B_{i\alpha}^\dagger e^{iS_B} = \sigma_{i\alpha}^* + B_{i\alpha}^\dagger , \tag{III.37}$$

where

$$S_B = -i \sum_{i\alpha} (\sigma_{i\alpha} B_{i\alpha}^\dagger - \sigma_{i\alpha}^* B_{i\alpha}) . \tag{III.38}$$

The set of particle-hole bosons $(B_{i\alpha}, B_{i\alpha}^\dagger)$ may be expanded in the general set $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$ related to it by a canonical transformation:

$$B_{i\alpha} = g_{i\alpha}(\tilde{B}_\mu, \tilde{B}_\mu^\dagger) ,$$

$$B_{i\alpha}^\dagger = g_{i\alpha}^\dagger(\tilde{B}_\mu, \tilde{B}_\mu^\dagger) . \tag{III.39}$$

The functional dependences $\hat{\rho}_{ab}$ and $g_{i\alpha}$ are determined as usual by requiring c-ordered expansions. The general boson expansion of fermion pairs is thus obtained by substituting (III.39) into (III.6'):

$$\eta_b^\dagger \eta_a = \hat{\rho}_{ab}(g_{i\alpha}(\tilde{B}_\mu, \tilde{B}_\mu^\dagger), g_{i\alpha}^\dagger(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)) = \hat{\rho}'_{ab}(\tilde{B}_\mu, \tilde{B}_\mu^\dagger) . \tag{III.40}$$

We therefore have the c-number relations

$$\rho_{ab}(\sigma_{i\alpha}, \sigma_{i\alpha}^*) = \rho'_{ab}(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*) , \tag{III.41}$$

where

$$\sigma_{i\alpha} = g_{i\alpha}(\tilde{\sigma}_\mu, \tilde{\sigma}_\mu^*) . \tag{III.42}$$

Consequently, if the conditions

$$\underline{\rho}^2(\sigma_{i\alpha}, \sigma_{i\alpha}^*) - \underline{\rho}(\sigma_{i\alpha}, \sigma_{i\alpha}^*) = 0 \tag{III.43}$$

and

$$\mathrm{Tr}\underline{\rho}(\sigma_{i\alpha}, \sigma_{i\alpha}^*) = N \tag{III.44}$$

hold identically, they will obviously hold when the substitution (III.42) is made.

Let us proceed with the proof of Eqs. (III.43) and

(III.44). Corresponding to the special BZ expansion, we have from Eqs. (III.4) and (III.6)

$$\rho_{ji}=\sum_{\alpha}\sigma_{i\alpha}^{*}\sigma_{j\alpha},\quad \rho_{\alpha\beta}=\delta_{\beta\alpha}-\sum_{i}\sigma_{i\alpha}^{*}\sigma_{i\beta}, \tag{III.45a}$$

$$\rho_{i\alpha}=\sigma_{i\alpha}-\tfrac{1}{2}\sum_{j\beta}\sigma_{j\beta}^{*}\sigma_{j\alpha}\sigma_{i\beta} - \tfrac{1}{8}\sum_{j\beta k\gamma}\sigma_{j\beta}^{*}\sigma_{j\alpha}\sigma_{k\gamma}^{*}\sigma_{k\beta}\sigma_{i\gamma}+\cdots . \tag{III.45b}$$

From Eq. (III.45a), it is easily seen that the condition (III.44) is in fact satisfied. It is readily checked that Eq. (III.43) is also satisfied order by order. To extend the proof to all orders, we introduce the matrix $\underline{Z}$:

$$\underline{Z}=\underline{\rho}^{2}-\underline{\rho}\,. \tag{III.46}$$

From the bracket relations (III.34), one computes the brackets

$$[\![\rho_{ba}, Z_{dc}]\!]=\delta_{cb}Z_{da}-\delta_{da}Z_{bc}\,. \tag{III.47}$$

The values of the brackets are, of course, independent of the choice of canonical variables, i.e., one may choose the set $(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$ or any other set $(\tilde{\sigma}_{\mu}, \tilde{\sigma}_{\mu}^{*})$ related to the former by a canonical transformation. It is convenient, however, to choose the special set $(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$. Then, from the operator relation (III.11) one obtains, upon making the c-number replacement $B_{i\alpha}\to\sigma_{i\alpha}$, $B_{i\alpha}^{\dagger}\to\sigma_{i\alpha}^{*}$, the equation

$$\sum_{j}\rho_{ij}\rho_{j\alpha}+\sum_{\beta}\rho_{i\beta}\rho_{\beta\alpha}-\rho_{i\alpha}=0, \tag{III.48a}$$

holding identically in the variables $(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$. This is just the statement that the particle-hole matrix elements of $\underline{Z}$ vanish identically:

$$Z_{i\alpha}=0\,. \tag{III.49}$$

Taken together with Eq. (III.47), Eq. (III.49) also implies the vanishing of other matrix elements. We have, for example,

$$[\![\rho_{j\beta}^{*}, Z_{i\alpha}]\!]=\delta_{\beta\alpha}Z_{ij}-\delta_{ij}Z_{\beta\alpha}=0\,. \tag{III.50}$$

Therefore,

$$\begin{aligned} &Z_{ij}=0, \quad j\neq i;\\ &Z_{\beta\alpha}=0, \quad \beta\neq\alpha;\\ &Z_{ii}=Z_{\alpha\alpha}, \quad \text{all } i,\alpha\,. \end{aligned} \tag{III.51}$$

Thus, one can only conclude that all diagonal elements are equal. However, from Eqs. (III.47), (III.49), and (III.51) it is easily shown that

$$[\![\rho_{ab}, Z_{ii}]\!]=[\![\rho_{ab}, Z_{\alpha\alpha}]\!]=0, \quad \text{all } a, b\,. \tag{III.52}$$

As shown below, this is sufficient to prove that the diagonal matrix elements are constant, i.e., independent of the set $(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$. The constant is easily evaluated from Eqs. (III.45) by setting all $\sigma_{i\alpha}=\sigma_{i\alpha}^{*}=0$ and is then found to vanish. Therefore,

$$Z_{ii}=Z_{\alpha\alpha}=0\,, \tag{III.53}$$

corresponding to the condition $\underline{Z}=0$. The proof of Eqs. (III.43) and (III.44) and therefore of our theorem is thus essentially complete. We wish, however, to make two further comments.

First of all, we have made the assumption that if all the brackets of a function $A(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$ with the $\rho_{ab}(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$ vanish, then that function is independent of the canonical variables. Actually, it is sufficient to show that the brackets $[\![\rho_{i\alpha}, A]\!]$ and $[\![\rho_{i\alpha}^{*}, A]\!]$ vanish. The remaining variables $\rho_{ij}, \rho_{\alpha\beta}$ are redundant. Now, Eqs. (III.45) can be considered as a change of variables from the set $(\sigma_{i\alpha}, \sigma_{i\alpha}^{*})$ to the set $(\rho_{i\alpha}, \rho_{i\alpha}^{*})$. It is easy to see that the Jacobian is nonzero in some neighborhood of the point at which all $\sigma_{i\alpha}=0$. One may then properly conclude that within this neighborhood $[\![\rho_{i\alpha}, A]\!]=[\![\rho_{i\alpha}, A]\!]=0$ implies that

$$\frac{\partial A}{\partial\sigma_{i\alpha}}=\frac{\partial A}{\partial\sigma_{i\alpha}^{*}}=0\,.$$

The second comment is that since the proof greatly hinged on the boson operator identity (III.11), it would be reassuring to know that it corresponds to a meaningful identity in the fermion space. Such need not be the case from general principles, since Eq. (III.11) is not a commutator relationship. However, Eq. (III.11) can indeed be considered as the boson image of a fermion identity as will now be shown:

$$\begin{aligned} &\sum_{j}(a_{j}^{\dagger}a_{i})(b_{\alpha}a_{j})-\sum_{\beta}(b_{\beta}^{\dagger}b_{\alpha})b_{\beta}a_{i}\\ &\quad=-\Big(\sum_{j}a_{j}^{\dagger}a_{j}\Big)b_{\alpha}a_{i}+\Big(\sum_{\beta}b_{\beta}^{\dagger}b_{\beta}\Big)b_{\alpha}a_{i}\\ &\quad=(N-\hat{N})b_{\alpha}a_{i}=0 \quad (\text{in the } N\text{-particle subspace}). \end{aligned}$$

Here, $\hat{N}$ is the number operator, and the last term obviously vanishes in the N-particle subspace.

In summary, it is possible to find the ground-state energy of the Hartree approximation, and the expectation value of one-body operators with respect to the Hartree ground state, in the boson picture, starting with an arbitrary single-particle basis and any BZ expansion related to the special one by a canonical transformation, by adhering to the following prescription: Linear boson terms in the c-ordered expansion of H are removed by a unitary transformation which amounts to a simple shift in the origin of each oscillator. The constant term in the c-ordered transformed Hamiltonian is the Hartree energy E_{SCF}. The same unitary transformation may then be carried out on one-body op-

erators written in c order, and the constant arising after the shift is the expectation value of the operator in the Hartree ground state. It must be noted that if $|\tilde{0}\rangle$ is the vacuum of the bosons $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$, then $e^{iS_B}|\tilde{0}\rangle$ is not in general the boson image of the Hartree ground state.

C. Higher-Order Cranking Model in the Boson Picture

We are now in a position to analyze the cranking model for deformed nuclei in the boson representation. This was already done to first order in Ref. 1, where it was explained why the cranking model must give the same moment of inertia as the RPA. In this section, the argument is first of all carried in detail one step further to show that the cranking model also gives the expression (II.43) for the $\mathcal{B}$ coefficient, which had been derived from the boson expansion through quartic terms. Next, an argument is sketched which shows that the cranking model to all orders gives the ground-state-band rotational energy with an error of the size of the boson-expansion-parameter squared. As explained in Sec. III B, the self-consistent cranking model used here is based on the Hartree approximation rather than the Hartree-Fock approximation as in Ref. 1. Therefore, antisymmetrized two-body matrix elements are replaced by unantisymmetrized ones in the Thouless-Valatin equations for the moment of inertia. Also, one should take Eq. (III.1b) into account in the single-particle energies. For the case of a velocity-independent two-body interaction, one then obtains the Inglis form of the moment of inertia $\mathcal{I}_0$.

We begin with the cranking-model Hamiltonian H_λ defined by

$$H_\lambda = H - \lambda J, \tag{III.54}$$

where λ is a Lagrange multiplier, usually interpreted as the angular velocity. The Hartree theory in the boson picture is to be applied to H_λ. It is assumed that H_λ has been first expressed in the Hartree single-particle basis corresponding to a deformed solution for H and then expanded in the special BZ series (III.6) in c order. Therefore, H contains no linear boson terms, but $(-\lambda J)$ does contribute linear boson terms, which must be removed by the shift transformation. For added convenience, let H and J be expressed in terms of the set of normal-mode bosons $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$ as given by Sec. II A.

The shift transformation is the following:

$$\begin{aligned}
&\Phi_B \to e^{-iS_B}\Phi_B e^{iS_B} = \Phi_B,\\
&J_B \to e^{-iS_B}J_B e^{iS_B} = k(\lambda) + J_B,\\
&\mathcal{O}_\mu \to e^{-iS_B}\mathcal{O}_\mu e^{iS_B} = \xi_\mu(\lambda) + \mathcal{O}_\mu,\\
&\mathcal{O}_\mu^\dagger \to e^{-iS_B}\mathcal{O}_\mu^\dagger e^{iS_B} = \xi_\mu(\lambda)^* + \mathcal{O}_\mu^\dagger,
\end{aligned} \tag{III.55}$$

where the constants $k(\lambda)$, $\xi_\mu(\lambda)$ are chosen to eliminate linear boson terms in each power of λ and thus may be expanded in λ:

$$\begin{aligned}
&k(\lambda) = k^{(1)}\lambda + k^{(3)}\lambda^3 + \cdots,\\
&\xi_\mu(\lambda) = \xi_\mu^{(2)}\lambda^2 + \xi_\mu^{(3)}\lambda^3 + \cdots.
\end{aligned} \tag{III.56}$$

It was already seen in Ref. 1 that $\xi_\mu^{(1)} = 0$. There is no need to shift Φ_B, since terms linear in this quantity automatically drop out by the requirement of rotational invariance. The generator of the transformation is the operator

$$S_B = k(\lambda)\Phi_B - i\sum_\mu [\xi_\mu(\lambda)\mathcal{O}_\mu^\dagger - \text{H.c.}] \tag{III.57}$$

Since the cranking energy is needed to order λ^4, the boson expansion of H is needed through quartic terms, and that of J is needed through cubic terms. First, consider the transformation of the relevant parts of J. From Eqs. (II.5)–(II.7) we obtain:

$$\lambda J_B \to \lambda J_B + k^{(1)}\lambda^2 + k^{(3)}\lambda^4 + \cdots; \tag{III.58a}$$

$$\begin{aligned}
\lambda J_{II} \to{}& \lambda J_{II} + \lambda^2\{k^{(1)}\sum_\mu [j_\mu^{(2)}(11)\mathcal{O}_\mu^\dagger + \text{H.c.}] + k^{(1)}j^{(2)}(10)\Phi_B\} + \lambda^3\{J_B\sum_\mu [j_\mu^{(2)}(11)\xi_\mu^{(2)*} + \text{c.c.}] + \text{linear phonons}\}\\
&+ \lambda^4\{k^{(1)}\sum_\mu [j_\mu^{(2)}(11)\xi_\mu^{(2)*} + \text{c.c.}] + \text{linear bosons}\} + \text{constant and linear boson terms of order } \lambda^5\\
&\text{and higher};
\end{aligned} \tag{III.58b}$$

$$\begin{aligned}
\lambda J_{III} \to{}& \lambda J_{III} + \lambda^2 \times \text{quadratic bosons} + \lambda^3[3(k^{(1)})^2 j^{(3)}(30)J_B + \text{linear phonons} + \text{quadratic bosons}]\\
&+ \lambda^4[(k^{(1)})^3 j^{(3)}(30) + \text{linear and quadratic bosons}] + \text{constant, linear, and quadratic boson terms}\\
&\text{of order } \lambda^5 \text{ and higher}.
\end{aligned} \tag{III.58c}$$

The transformation of the relevant parts of H is obtained from Eqs. (II.1)–(II.4) as follows:

$$H_B \to H_B + \lambda k^{(1)} g_0^{-1} J_B + \lambda^2[(2g_0)^{-1}(k^{(1)})^2 + \sum_\mu E_\mu (\xi_\mu^{(2)} \mathcal{O}_\mu^\dagger + \text{H.c.})] + \lambda^3[k^{(3)} g_0^{-1} J_B + \text{linear phonons}]$$
$$+ \lambda^4[\sum_\mu E_\mu |\xi_\mu^{(2)}|^2 + g_0^{-1} k^{(1)} k^{(3)} + \text{linear phonons}] + \text{constant and linear boson terms of order } \lambda^5$$
$$\text{and higher ;} \qquad \text{(III.59a)}$$

$$H_{\rm III} \to H_{\rm III} + \lambda \times \text{quadratic boson terms} + \lambda^2\{(k^{(1)})^2 \sum_\mu [h_\mu^{(3)}(21)\mathcal{O}_\mu^\dagger + \text{H.c.}] + (k^{(1)})^2 h^{(3)}(20)\Phi_B + \text{quadratic bosons}\}$$
$$+ \lambda^3\{2k^{(1)} J_B \sum_\mu [h_\mu^{(3)}(21)\xi_\mu^{(2)*} + \text{c.c.}] + \text{linear phonons} + \text{quadratic bosons}\} + \lambda^4\{(k^{(1)})^2 \sum_\mu [h_\mu^{(3)}(21)\xi_\mu^{(2)*}$$
$$+ \text{c.c.}] + \text{linear and quadratic bosons}\} + \text{constant, linear, and quadratic boson terms of order } \lambda^5$$
$$\text{and higher;} \qquad \text{(III.59b)}$$

$$H_{\rm IV} \to H_{\rm IV} + \lambda \times \text{cubic bosons} + \lambda^2 \times \text{quadratic and cubic bosons} + \lambda^3[4(k^{(1)})^3 h^{(4)}(40) J_B + \text{linear phonons}$$
$$+ \text{quadratic and cubic bosons}] + \lambda^4[(k^{(1)})^4 h^{(4)}(40) + \text{linear, quadratic, and cubic bosons}]$$
$$+ \text{constant, linear, quadratic, and cubic boson terms of order } \lambda^5 \text{ and higher .} \qquad \text{(III.59c)}$$

Of course, the constant terms in Eqs. (III.58) and (III.59) involve only even powers of λ.

Elimination of linear bosons proportional to λ from Eqs. (III.58a) and (III.58b) requires that

$$k^{(1)} = g_0 . \qquad \text{(III.60)}$$

The linear boson terms proportional to λ^2 arising from the shift of H_B, $H_{\rm III}$, and $-\lambda J_{\rm II}$ add up to

$$\lambda^2\{\sum_\mu E_\mu (\xi_\mu^{(2)} \mathcal{O}_\mu^\dagger + \text{H.c.}) - g_0 \sum_\mu [j_\mu^{(2)}(11)\mathcal{O}_\mu^\dagger + \text{H.c.}] + g_0^2 \sum_\mu [h_\mu^{(3)}(21)\mathcal{O}_\mu^\dagger + \text{H.c.}] + g_0[g_0 h^{(3)}(20) - j^{(2)}(10)]\Phi_B\} . \qquad \text{(III.61)}$$

Note, however, that Eq. (II.9c), expressing rotational invariance, requires that the coefficient of Φ_B in the above equation vanish. The rest of the term is eliminated by choosing

$$\xi_\mu^{(2)} = -g_0^2[h_\mu^{(3)}(21) - g_0^{-1} j_\mu^{(2)}(11)]/E_\mu . \qquad \text{(III.62)}$$

In order to obtain the energy to order λ^4, it is only necessary to remove $\lambda^3 J_B$ terms but not $\lambda^3 \times$(phonon) terms. The $\lambda^3 J_B$ terms arising from shifting H_B, $H_{\rm III}$, $H_{\rm IV}$, and $-\lambda(J_{\rm II} + J_{\rm III})$ are eliminated by choosing

$$k^{(3)} = -4g_0^4 h^{(4)}(40) + 3g_0^3 j^{(3)}(30) - 2g_0^2 \sum_\mu [h_\mu^{(3)}(21)\xi_\mu^{(2)*} + \text{c.c.}] + g_0 \sum_\mu [j_\mu^{(2)}(11)\xi_\mu^{(2)*} + \text{c.c.}] . \qquad \text{(III.63)}$$

Now that the shift constants $k(\lambda)$ and $\xi_\mu(\lambda)$ have been determined to the order of interest, the cranking-model energy may be written down. Since the cranking term $-\lambda J$ is to be interpreted as a constraint, the energy is the total constant arising from the shift in H. Thus, adding up the constants in Eqs. (III.59) and using Eqs. (III.62) and (III.63), one obtains the shift constant $\langle\lambda|H|\lambda\rangle$ (in the notation of Ref. 1):

$$\langle\lambda|H|\lambda\rangle = E_{\rm SCF} + \tfrac{1}{2} g_0 \lambda^3 - 3g_0^4 \left[h^{(4)}(40) - g_0^{-1} j^{(3)}(30) - \sum_\mu \frac{|h_\mu^{(3)}(21) - g_0^{-1} j_\mu^{(2)}(11)|^2}{E_\mu}\right]\lambda^4 + O(\lambda^6) + \cdots , \qquad \text{(III.64)}$$

where $E_{\rm SCF}$ is the Hartree energy corresponding to $\lambda = 0$. The expectation value of J in the Hartree ground state, denoted by $\langle\lambda|J|\lambda\rangle$, is likewise obtained by adding up the shift constants in Eq. (III.58), making use of Eqs. (III.62) and (III.63):

$$\langle\lambda|J|\lambda\rangle = g_0\lambda - 4g_0^4 \left[h^{(4)}(40) - g_0^{-1} j^{(3)}(30) - \sum_\mu \frac{|h_\mu^{(3)}(21) - g_0^{-1} j_\mu^{(2)}(11)|^2}{E_\mu}\right]\lambda^3 + O(\lambda^5) + \cdots . \qquad \text{(III.65)}$$

The Lagrange multiplier λ is determined by prescribing the value of $\langle\lambda|J|\lambda\rangle$, say

$$\langle\lambda|J|\lambda\rangle = M , \qquad \text{(III.66)}$$

with M an integer. We note from Eqs. (III.64) and (III.65) that the condition

$$\frac{\partial}{\partial\lambda}\langle\lambda|H|\lambda\rangle = \lambda \frac{\partial}{\partial\lambda}\langle\lambda|J|\lambda\rangle ,$$

which can be derived from the Hellmann-Feynman theorem, is satisfied.[6] Therefore, one may eliminate λ, just as in Ref. 6, to obtain an expansion of

$\langle\lambda|H|\lambda\rangle$ in powers of the angular momentum M:

$$\langle\lambda|H|\lambda\rangle = E_{\mathrm{SCF}} + \frac{M^2}{2\mathcal{I}_0} + \mathcal{C}_0 M^4 + O(M^6) + \cdots , \tag{III.67}$$

where the $\mathcal{C}$ coefficient is exactly the expression $\mathcal{C}_0$ given by Eq. (II.43). This completes the demonstration.

As discussed in Sec. II, the rotational coefficients $\mathcal{I}$, $\mathcal{C}$, $\mathcal{E}$, etc., for the ground-state band are each expansions in the parameter ϵ and, as we have just seen, the cranking model gives the leading-order values $\mathcal{I}_0$ and $\mathcal{C}_0$. To extend this "theorem" to all orders requires a radical simplification in the bookkeeping. Such a simplification can be accomplished by introducing a new set of bosons via a canonical transformation. It will be recalled that the shift transformation can be properly applied to any set of bosons related to the particle-hole bosons of Eq. (III.6) by a canonical transformation. Following Sec. II, one may introduce the general set $(J, \Phi, \tilde{\mathcal{O}}_\mu, \tilde{\mathcal{O}}_\mu{}^\dagger)$, which includes the total angular momentum. Since H is independent of Φ, we already have one simplification. The ultimate simplification, however, is brought about by a transformation to the set $(J, \Phi, \tilde{\mathcal{O}}_\mu^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)\dagger})$, which eliminates all couplings of the ground-state band to higher-lying bands. For our purposes, it is even sufficient only to suppose that all terms of the form $J^n \times$(linear phonons) have been transformed away. In either case, the leading-order contributions to the ground-state rotational parameters will come from terms of the form (constant)$\times J^{2n}$, i.e., the piece of the Hamiltonian H_{ROT} given by

$$H_{\mathrm{ROT}} = \sum_{n=1}^{\infty} b_n J^{2n} . \tag{III.68}$$

In the representation in which all couplings of the ground-state band with higher-lying bands have been eliminated, it is clear that the lowest-order correction to the coefficient b_n comes from the expectation value of a term of the form $J^{2n}\tilde{\mathcal{O}}^{(d)}\tilde{\mathcal{O}}^{(d)\dagger}$. This correction is therefore down by a factor of ϵ^2 relative to the leading-order term b_n. It is expected that ϵ is of the order of Ω^{-1} in the two-dimensional case, and of the order of $\Omega^{-1/2}$ in the three-dimensional case. In shifting H_λ to eliminate linear boson terms, it is obviously sufficient to shift J, leaving the phonons alone. This is because all terms of the form $J^n \times$ (linear phonons) have been eliminated, so no linear phonon terms can arise from shifting J. The only linear terms consist of $-\lambda J$ and those coming from the shift $J \to J + k(\lambda)$ inserted into H_{ROT}. The particular form of the function $k(\lambda)$ is determined from the condition that these terms cancel. But how $k(\lambda)$ is chosen becomes irrelevant now that the coupling terms have been eliminated, since λ is anyhow determined from the condition $\langle\lambda|J|\lambda\rangle = k(\lambda) = M$ and the energy increment is just

$$\langle\lambda|H|\lambda\rangle - E_{\mathrm{SCF}} = \sum_{n=1}^{\infty} b_n k(\lambda)^{2n} = \sum_{n=1}^{\infty} b_n M^{2n} . \tag{III.69}$$

This result is all that is needed to extend the theorem to all orders.

Why are the values of the shift constants immaterial in this second case and not in the first case discussed? The answer is that in the first case H contains coupling terms of the form $J^n \times$ (linear phonons) and the choice of shift constants reflects the effect of diagonalizing the coupling terms. In the second case, all of the coupling terms in question have been removed and the rotational energy is diagonal to begin with. The only function of the shift is to push the information on the rotational energy from the higher orders down into the Hartree order, and any value of $k(\lambda)$ will do for this purpose.

In order to see more clearly the diagonalization of band-mixing terms in the first case, we consider the kinematic expansion of H and restrict ourselves to the vibration-rotation term $J^2 \times$ (linear phonons). From Eqs. (II.39c) and (II.41a) we have

$$H = \text{constant} + \sum_\mu E_\mu \tilde{\mathcal{O}}_\mu^{(k)\dagger}\tilde{\mathcal{O}}_\mu^{(k)} + \frac{J^2}{2\mathcal{I}_0} + J^2 \sum_\mu \{[h_\mu^{(3)}(21) - \mathcal{I}_0{}^{-1} j_\mu^{(2)}(11)]\,\tilde{\mathcal{O}}_\mu^{(k)\dagger} + \text{H.c.}\} + \cdots . \tag{III.70}$$

Let us now eliminate the vibration-rotation term in lowest order by the unitary transformation

$$H \to H' = e^{-iF_d} H e^{iF_d} , \tag{III.71}$$

which is equivalent to a transformation from the set of variables $(J, \Phi^{(k)}, \tilde{\mathcal{O}}_\mu^{(k)}, \tilde{\mathcal{O}}_\mu^{(k)\dagger})$ to the set $(J, \Phi^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)\dagger})$. The generator is

$$F_d = iJ^2 \sum_\mu \left[\frac{h_\mu^{(3)}(21) - \mathcal{I}_0{}^{-1} j_\mu^{(2)}(11)}{E_\mu}\right] \tilde{\mathcal{O}}_\mu^{(k)\dagger} + \text{H.c.} \tag{III.72}$$

Next perform the shift transformation $J \to J + g_0\lambda$:

$$H' \to H'' = e^{-ig_0\lambda\Phi^{(k)}} H' e^{ig_0\lambda\Phi^{(k)}} \tag{III.73}$$

The product of the two transformations corresponds to the procedure used in the second case, and to the given order is equivalent to a single unitary transformation generated by the operator

$$g_0\lambda\Phi^{(k)} + iJ^2\left\{\sum_\mu\left[\frac{h_\mu^{(3)}(21) - g_0^{-1}j_\mu^{(2)}(11)}{E_\mu}\right]\tilde{\mathcal{O}}_\mu^{(k)\dagger} - \text{H.c.}\right\} . \tag{III.74}$$

Since J commutes with H, it could just as well be replaced by a c number, say $g_0\lambda$, in Eqs. (III.72) and (III.74). In addition, to lowest order, $\Phi^{(k)} \approx \Phi_B$, $\tilde{\mathcal{O}}_\mu^{(k)} \approx \mathcal{O}_\mu$. If one makes these changes in Eq. (III.74), the result is the generator S_B,

$$S_B = g_0\lambda\Phi_B + i(g_0\lambda)^2\left\{\sum_\mu\left[\frac{h_\mu^{(3)}(21) - g_0^{-1}j_\mu^{(2)}(11)}{E_\mu}\right]\mathcal{O}_\mu^{\dagger} - \text{H.c.}\right\}, \tag{III.75}$$

as is seen from Eqs. (III.57), (III.60), and (III.62). This shows explicitly that diagonalization of the band-mixing term in question is built into the cranking-model procedure used in the first case.

D. Rotation-Vibration Coupling to Individual Bands

The cranking-model expression for the $\mathcal{B}$ coefficient, Eq. (II.43a), adds together all the contributions from the couplings of the ground-state band with higher-lying bands which occur through the vibration-rotation-type term $J^2 \times$ (linear phonons), together with the diagonal term proportional to J^4. In one sense, it is an advantage of the cranking model that it effectively provides sum rules which eliminate the need to consider explicitly the mixing with individual bands in calculating the ground-state-band rotational energy. In another sense, there is a disadvantage – what is one to do if one is interested in the strength of the coupling to individual bands, such as the parameter $\Gamma_\mu^{(3)}$ defined in Eqs. (II.39c)? We shall show that this can be found within the framework of the cranking model, thus obviating the need to explicitly introduce boson expansions. Of course, as was already discussed in Sec. II, there is nothing absolute in the division between a vibration-rotation term and a diagonal J^4 term; one can switch back and forth between the two by means of a unitary transformation, or, equivalently, with a suitable choice of the f coefficients in Eqs. (II.40a) and (II.40d). In order to make the problem well defined, we consider the vibration-rotation term corresponding to the kinematic choice $\Phi = \Phi^{(k)}$ and $\tilde{\mathcal{O}}_\mu = \tilde{\mathcal{O}}_\mu^{(k)}$, as given by Eq. (II.41a).

One way to extract the desired information is by means of a generalized cranking model in which phonons are constrained, as well as the angular momentum. Such an approach in lowest order has already been discussed elsewhere,[24] and is easily transcribed into the boson picture.[1] However, we shall instead describe an equivalent but simpler procedure which does not require additional constraints. First, note that the information of interest is already contained in the phonon shift constants $\xi_\mu^{(2)}$ given by Eq. (III.62). One then has

$$\Gamma_\mu^{(3)} = -E_\mu\xi_\mu^{(2)}/g_0^2 . \tag{III.76}$$

Since the practical implementation of the cranking model is made in the fermion representation, one must relate the phonon shift constant $\xi_\mu^{(2)}$ to the expectation value of a one-body operator in the cranked ground state. Now, the phonon operator $\mathcal{O}_\mu = \sum_{i\alpha}[X_{i\alpha}(\mu)^* B_{i\alpha} + Y_{i\alpha}(\mu)^* B_{i\alpha}^\dagger]$ is not a one-body operator. To the order of interest, however, it is sufficient to define the one-body operator $\hat{\mathcal{O}}_\mu$:

$$\hat{\mathcal{O}}_\mu = \sum_{i\alpha}[X_{i\alpha}(\mu)^* b_\alpha a_i + Y_{i\alpha}(\mu)^* a_i^\dagger b_\alpha^\dagger], \tag{III.77}$$

where the $X_{i\alpha}(\mu)^*$ and $Y_{i\alpha}(\mu)^*$ are the normal-mode amplitudes. This will do, since the special BZ expansion of $\hat{\mathcal{O}}_\mu$ contains only odd numbers of bosons:

$$\hat{\mathcal{O}}_\mu = \mathcal{O}_\mu + (\hat{\mathcal{O}}_\mu)_{\text{III}} + \cdots . \tag{III.78}$$

Upon performing the shift transformation (III.55), the cubic term $(\hat{\mathcal{O}}_\mu)_{\text{III}}$ can only contribute terms of order λ^3 or higher to the shift constant so that

$$e^{-iS_B}\hat{\mathcal{O}}_\mu e^{iS_B} = [\xi_\mu^{(2)}\lambda^2 + O(\lambda^3) + \cdots] + \text{linear and higher-order bosons} . \tag{III.79}$$

Therefore, if one wishes to find the quantities $\xi_\mu^{(2)}$ without explicitly introducing the BZ expansion, one need only find the cranking-model wave function (in the fermion representation) to order λ^2 and then compute the expectation value $\langle\lambda|\hat{\mathcal{O}}_\mu|\lambda\rangle$ to order λ^2 to give the result

$$\langle\lambda|\hat{\mathcal{O}}_\mu|\lambda\rangle = \lambda^2\xi_\mu^{(2)} = -(g_0\lambda)^2\frac{h_\mu^{(3)}(21) - g_0^{-1}j_\mu^{(2)}(11)}{E_\mu} . \tag{III.80}$$

It is interesting to note that the $(g_0\lambda)$ dependence in Eq. (III.80) reflects the J^2 dependence of the pho-

non operator $\mathcal{O}_\mu$ arising from the diagonalization of all vibration-rotation terms to first order. To see this, choose the value of $f_\mu^{(2)}(11)$ given by Eq. (II.42a); this is the choice which eliminates $J^2 \times$ (linear phonon) terms. From Eq. (II.33) one then obtains

$$\mathcal{O}_\mu = \mathcal{O}_\mu - J^2 \frac{h_\mu^{(3)}(21) - g_0^{-1} j_\mu^{(2)}(11)}{E_\mu} + \cdots , \tag{III.81}$$

omitting terms which are of no concern at the moment. Since in the relevant order of the cranking model $\langle\lambda|J|\lambda\rangle = g_0\lambda$, the correspondence between Eqs. (III.80) and (III.81) is complete. This result is not an accident, but rather an indication of the fact that the cranking model can be used to trace the angular momentum dependence of any operator, not just the Hamiltonian. And the angular momentum dependence involved is associated with the diagonalization of the coupling terms. This is easy to see if one writes the operator in terms of the set of variables $(J, \Phi^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)\dagger})$. In that case, the shift constant for the operator arises entirely from inserting $J \to J + k(\lambda)$ in that part of the operator which depends on J alone, just as in the case of the Hamiltonian. This idea will be illustrated in Sec. III E.

E. Cranking Model Applied to Transition Operators

In terms of the set of bosons $(J, \Phi^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)\dagger})$, the transition operator $Q^{(M)}$ may be written as

$$Q^{(M)} = \tfrac{1}{2}\{e^{iM\Phi^{(d)}}, \mathcal{Q}^{(M)}\},$$

where the scalar $\mathcal{Q}^{(M)}$ is expanded in the set $(J, \tilde{\mathcal{O}}_\mu^{(d)}, \tilde{\mathcal{O}}_\mu^{(d)\dagger})$ alone.[24a] To leading order, the transitions within the ground-state band are determined by the part of $\mathcal{Q}^{(M)}$ which depends on J alone:

$$\mathcal{Q}^{(M)} = \sum_{n=0}^{\infty} q_n J^n + \cdots \tag{III.82}$$

The expansion contains either all even or all odd powers of J, depending on the time-reversal properties of $Q^{(M)}$. There are other parts of $\mathcal{Q}^{(M)}$ which also contribute to these transitions. For example, there is a term of the form $J^n \tilde{\mathcal{O}}_\mu^{(d)} \tilde{\mathcal{O}}_\mu^{(d)\dagger}$. This provides a renormalization of q_n which is smaller by a factor of ϵ^2 compared with the leading term. The cranking model neglects such small renormalizations. In the representation under discussion, the cranking model requires only the shift of the angular momentum: $J \to k(\lambda) + J$, where $k(\lambda) = \langle\lambda|J|\lambda\rangle$, the prescribed value. The shift in $Q^{(M)}$ is then easily seen to be

$$\langle\lambda|Q^{(M)}|\lambda\rangle = \sum_{n=0}^{\infty} q_n k(\lambda)^n = \sum_{n=0}^{\infty} q_n \langle\lambda|J|\lambda\rangle^n . \tag{III.83}$$

Once the constants q_n are identified from the cranking-model expectation value of the operator, one may easily calculate moments and transition matrix elements between members of the ground-state band using the wave functions (II.62a).

As an example, let us check that the cranking model, when formulated in terms of the set $(J_B, \Phi_B, \mathcal{O}_\mu, \mathcal{O}_\mu^\dagger)$ gives the expected results, at least through order J^2. It was already shown in Ref. 1 that the linear J dependence for operators odd under time reversal is correctly given by the cranking model. Therefore, let $Q^{(M)}$ be even under time reversal. Performing the shift transformation (III.55), using the expansion of $Q^{(M)}$ defined by Eqs. (II.51) and (II.53), and the shift constants (III.60) and (III.62), one obtains the shift constant for $Q^{(M)}$:

$$\langle\lambda|Q^{(M)}|\lambda\rangle = \langle 0|Q^{(M)}|0\rangle + (g_0\lambda)^2 \Lambda^{(M)(2)}(20), \tag{III.84}$$

where the constant $\Lambda^{(M)(2)}(20)$ is just that given by Eq. (II.63a).

The present version of the cranking model does not permit calculation of transitions involving other than the ground-state band. In order to treat these, one must either use boson expansions directly, or, possibly, the generalized cranking model in which phonon operators are constrained.

IV. SUMMARY AND CONCLUSIONS

We hope to have demonstrated, first of all, that boson-expansion techniques can provide a straightforward formal solution to the problem of deriving a microscopic collective Hamiltonian for strongly deformed even-even nuclei, including rotational band-mixing effects, as well as vibrational anharmonicities. Transition operators are also easily expressed in the collective representation. An important feature of the technique is the treatment of rotation and vibration on an equal footing.

Additional justification has also been provided for the higher-order cranking model by formulating it in the boson "representation." The mechanism behind its success then becomes clearly evident: The inhomogeneous shift transformation eliminating linear boson terms carries information on the rotational energy from the higher orders of the boson expansion down into the Hartree order. In this way, it is seen that the cranking model approximates the energies of the members of the ground-state band with an error of the order of the square of the boson-expansion parameter. This accuracy is much better than previously supposed.

For purposes of the proof, the cranking model was formulated in the boson picture. Practical implementation requires the use of the fermion representation as usual. If one is content with its accuracy, especially for heavy nuclei, the cranking

model provides a handy tool for computing properties of the ground-state band while circumventing the explicit introduction of tedious boson expansions. There are two more important advantages which are readily exploited in the fermion representation. First of all, as stressed in the Appendix, the cranking model adds together the effects of all band mixings on the ground-state band, effectively providing sum rules for the rotational parameters. Second, the model can be diagonalized exactly in order to describe high-spin states, a region in which the angular momentum expansion is inadequate.

The scope of the cranking model is not limited to the computation of rotational energies. We have seen that transition operators can also be "cranked," permitting the calculation of transition probabilities between members of the ground-state band. In a forthcoming publication it will be shown that the cranking model can also be applied to nuclei with spherical ground states to calculate properties of those vibrational states which meld into rotational ones as the strength of the long-range force is increased. We therefore have a unified calculational tool which can be applied to the harmonic-vibrational, transitional (quasirotational), and rotational regions. Its implementation only requires application of the presently existing computational technology of the self-consistent-field method.

Why should there be this connection between the (Hartree) cranking model and the BZ boson expansion? The answer which we propose is that the BZ technique may be regarded as a quantized version of the nonlinear time-dependent Hartree method. It is well known that the cranking model can be derived by transforming the time-dependent equations to a frame rotating with the self-consistent field. In order to see the connection between the two methods, note that the boson images $\hat{\rho}_{ba}$ of fermion pairs $\eta_a^\dagger \eta_b$ obey the exact equations of motion:

$$i\frac{d}{dt}\hat{\rho}_{ba} = \sum_c (\varepsilon_{bc}\hat{\rho}_{ca} - \hat{\rho}_{bc}\varepsilon_{ca}) - \tfrac{1}{2}\sum_{def}(V_{de,af}\{\hat{\rho}_{bd},\hat{\rho}_{fe}\} - V_{bd,fe}\{\hat{\rho}_{ed},\hat{\rho}_{fa}\}) . \tag{IV.1}$$

If the bosons are replaced by classical canonical variables, so that $\hat{\rho}_{ba}$ is replaced by the c number ρ_{ba}, the result is

$$i\frac{d}{dt}\rho_{ba} = \sum_c (\varepsilon_{bc}\rho_{ca} - \rho_{bc}\varepsilon_{ca}) - \sum_{def}(V_{de,af}\,\rho_{bd}\rho_{fe} - V_{bd,fe}\,\rho_{ed}\rho_{fa}) . \tag{IV.2}$$

Moreover, as was seen in Sec. III B, the conditions $\underline{\rho}^2 = \underline{\rho}$ and $\mathrm{Tr}\underline{\rho} = N$ can be satisfied. In that case, Eqs. (IV.2) may be fully identified with the time-dependent Hartree (not Hartree-Fock) equations. In applications to bound states, the density matrix elements are normally expressed in terms of canonical variables and then quantized; the energy, given by Eq. (III.28), being interpreted as the Hamiltonian. The quantization is usually accomplished by means of the Pauli prescription, an *ad hoc* choice. The quantization can be achieved instead by requiring that the fermion-pair algebra be satisfied, and then one is back to the BZ method.

As a final point, we note that the present results can be generalized in a number of directions and work on this is in progress. Three-dimensional rotations and inclusion of pairing correlations require straightforward if tedious extensions. The method for two-dimensional rotation can then also be easily applied to the so-called "pairing rotation." The possibility of developing boson expansions about Hartree-Fock rather than Hartree minima is also under investigation. In this way, it might be possible to assay the significance of the Thouless-Valatin corrections to the cranking model. These have been considered in the lowest cranking order in Ref. 1. As an illustration of the ideas introduced here, direct applications are made to an exactly soluble model in a companion paper.

APPENDIX. APPLICATIONS TO THE TWO-DIMENSIONAL QUADRUPOLE-FORCE HAMILTONIAN

The boson-expansion techniques will be applied to a system of particles moving in a spherical potential well and interacting *via* the two-dimensional analog of the quadrupole-quadrupole force. The Hamiltonian is

$$H = \sum_{ab}\varepsilon_{ab}\eta_a^\dagger\eta_b - \tfrac{1}{2}\kappa Q^{(2)\dagger}Q^{(2)} , \tag{A1a}$$

where the first term corresponds to the spherical well, κ is the strength of the interaction, and $Q^{(2)}$ is defined by

$$Q^{(2)} = \sum_{ab}\langle a|(x+iy)^2|b\rangle\eta_a^\dagger\eta_b . \tag{A2}$$

It is convenient to rewrite (A1a) in terms of the Hermitian operators $R^{(\pm)}$ defined by

$$R^{(+)}=\tfrac{1}{2}(Q^{(2)}+Q^{(-2)})=\sum_{ab}\langle a|x^2-y^2|b\rangle\eta_a{}^\dagger\eta_b=\sum_{ab}R^{(+)}_{ab}\eta_a{}^\dagger\eta_b\,,$$
$$R^{(-)}=\tfrac{1}{2}i(Q^{(-2)}-Q^{(2)})=\sum_{ab}\langle a|2xy|b\rangle\eta_a{}^\dagger\eta_b=\sum_{ab}R^{(-)}_{ab}\eta_a{}^\dagger\eta_b\,, \tag{A3}$$

so that

$$H=\sum_{ab}\epsilon_{ab}\eta_a{}^\dagger\eta_b-\tfrac{1}{2}\kappa\sum_r(R^{(r)})^2,\quad r=\pm. \tag{A1b}$$

The self-consistent-field Hamiltonian is

$$H_{\rm SCF}=\tfrac{1}{2}\kappa\sum_r\langle 0|R^{(r)}|0\rangle^2+\sum_{ab}\epsilon_{ab}\eta_a{}^\dagger\eta_b-\kappa\sum_r\langle 0|R^{(r)}|0\rangle R^{(r)}\,, \tag{A4}$$

corresponding to an elliptically deformed potential well with arbitrary orientation. The state $|0\rangle$ is the ground state of (A4) determined self-consistently, with ground-state energy

$$E_{\rm SCF}=\langle 0|H_{\rm SCF}|0\rangle=\sum_{ab}\epsilon_{ab}\langle 0|\eta_a{}^\dagger\eta_b|0\rangle-\tfrac{1}{2}\kappa\sum_r\langle 0|R^{(r)}|0\rangle^2\,. \tag{A5}$$

It is assumed that the single-particle basis has already been chosen to diagonalize (A4):

$$\sum_{ab}\epsilon_{ab}\eta_a{}^\dagger\eta_b-\kappa\sum_r\langle 0|R^{(r)}|0\rangle R^{(r)}=\sum_a\epsilon_a\eta_a{}^\dagger\eta_a\,. \tag{A6}$$

We are free to orient the deformed field so that the condition

$$\langle 0|R^{(-)}|0\rangle=0 \tag{A7}$$

is satisfied. The total Hamiltonian may be split up as follows:

$$H=H_{\rm SCF}-\tfrac{1}{2}\kappa\sum_r(R^{(r)}-\langle 0|R^{(r)}|0\rangle)^2\,, \tag{A8}$$

where the second term is the residual interaction.

The particle-hole notation will be used from now on, in terms of which

$$R^{(\pm)}=\langle 0|R^{(\pm)}|0\rangle+\sum_{i\alpha}(R^{(\pm)}_{i\alpha}a_i{}^\dagger b_\alpha{}^\dagger+\text{H.c.})+\sum_{ij}R^{(\pm)}_{ij}a_i{}^\dagger a_j-\sum_{\alpha\beta}R^{(\pm)}_{\alpha\beta}b_\beta{}^\dagger b_\alpha\,. \tag{A9}$$

The special BZ expansion (III.6) can now be inserted into the Hamiltonian. The Hartree Hamiltonian remains finite:

$$H_{\rm SCF}=E_{\rm SCF}+\sum_{i\alpha}(\epsilon_i-\epsilon_\alpha)B_{i\alpha}{}^\dagger B_{i\alpha}\,. \tag{A10}$$

The expansion of $R^{(\pm)}$, however, is infinite:

$$R^{(\pm)}=R^{(\pm)}_B+R^{(\pm)}_{\rm II}+R^{(\pm)}_{\rm III}+\cdots\,. \tag{A11}$$

We only need the expansion of $R^{(\pm)}$ through cubic terms in order to obtain the expansion of H through quartic terms. Explicitly, we have

$$R^{(\pm)}_B=\langle 0|R^{(\pm)}|0\rangle+\sum_{i\alpha}(R^{(\pm)}_{i\alpha}B_{i\alpha}{}^\dagger+\text{H.c.})\,, \tag{A12}$$

$$R^{(\pm)}_{\rm II}=\sum_{ij\alpha}R^{(\pm)}_{ij}B_{i\alpha}{}^\dagger B_{j\alpha}-\sum_{i\alpha\beta}R^{(\pm)}_{\alpha\beta}B_{i\beta}{}^\dagger B_{i\alpha}\,, \tag{A13}$$

and

$$R^{(\pm)}_{\rm III}=-\tfrac{1}{2}\sum_{ij\alpha\beta}(R^{(\pm)}_{i\alpha}B_{i\beta}{}^\dagger B_{j\alpha}{}^\dagger B_{j\beta}+\text{H.c.})\,. \tag{A14}$$

It may be noted that beyond $R^{(\pm)}_{\rm II}$, there are only terms with an odd number of bosons. The expansion of H is then given by

$$H=H_B+H_{\rm III}+H_{\rm IV}+\cdots\,, \tag{A15}$$

where

$$H_B=E_{\rm SCF}+\sum_{i\alpha}(\epsilon_i-\epsilon_\alpha)B_{i\alpha}{}^\dagger B_{i\alpha}-\tfrac{1}{2}\kappa\sum_r(R^{(r)}_B-\langle 0|R^{(r)}|0\rangle)^2\,, \tag{A16}$$

$$H_{\mathrm{III}} = -\tfrac{1}{2}\kappa \sum_r \{R_B^{(r)} - \langle 0|R^{(r)}|0\rangle, R_{\mathrm{II}}^{(r)}\}$$
$$= -\tfrac{1}{2}\kappa \sum_r \sum_{ijk\alpha\beta} (R_{i\alpha}^{(r)} R_{jk}^{(r)} \{B_{i\alpha}^{\dagger}, B_{j\beta}^{\dagger} B_{k\beta}\} + \mathrm{H.c.}) + \tfrac{1}{2}\kappa \sum_r \sum_{ij\alpha\beta\gamma} (R_{i\alpha}^{(r)} R_{\beta\gamma}^{(r)} \{B_{i\alpha}^{\dagger}, B_{j\gamma}^{\dagger} B_{j\beta}\} + \mathrm{H.c.}), \tag{A17}$$

and

$$H_{\mathrm{IV}} = -\tfrac{1}{2}\kappa \sum_r \{R_B^{(r)} - \langle 0|R^{(r)}|0\rangle, R_{\mathrm{III}}^{(r)}\} - \tfrac{1}{2}\kappa \sum_r (R_{\mathrm{II}}^{(r)})^2$$
$$= \tfrac{1}{4}\kappa \sum_r \sum_{ijk\alpha\beta\gamma} (R_{i\alpha}^{(r)} R_{j\beta}^{(r)} \{B_{i\alpha}^{\dagger}, B_{j\gamma}^{\dagger} B_{k\beta}^{\dagger} B_{k\gamma}\} + \mathrm{H.c.}) + \tfrac{1}{4}\kappa \sum_r \sum_{ijk\alpha\beta\gamma} (R_{i\alpha}^{(r)*} R_{j\beta}^{(r)} \{B_{j\gamma}^{\dagger} B_{k\beta}^{\dagger} B_{k\gamma}, B_{i\alpha}\} + \mathrm{H.c.})$$
$$-\tfrac{1}{2}\kappa \sum_r (\sum_{ij\alpha} R_{ij}^{(r)} B_{i\alpha}^{\dagger} B_{j\alpha} - \sum_{i\alpha\beta} R_{\alpha\beta}^{(r)} B_{i\beta}^{\dagger} B_{i\alpha})^2 . \tag{A18}$$

The next task is to express (A17) and (A18) in terms of the normal-mode bosons which diagonalize H_B. These are given by

$$\begin{aligned}
\mathcal{O}_{\mu s}^{\dagger} &= \sum_{i\alpha} [X_{i\alpha}(\mu s) B_{i\alpha}^{\dagger} + Y_{i\alpha}(\mu s) B_{i\alpha}], \\
\mathcal{O}_{\mu s} &= \sum_{i\alpha} [Y_{i\alpha}(\mu s)^* B_{i\alpha}^{\dagger} + X_{i\alpha}(\mu s)^* B_{i\alpha}], \\
J_B &= \sum_{i\alpha} (J_{i\alpha} B_{i\alpha}^{\dagger} + \mathrm{H.c.}), \\
\Phi_B &= \frac{-i}{g_0} \sum_{i\alpha} \left(\frac{J_{i\alpha}}{\epsilon_i - \epsilon_\alpha} B_{i\alpha}^{\dagger} - \mathrm{H.c.} \right),
\end{aligned} \tag{A19}$$

in terms of which

$$H_B = E_B + \sum_{\mu s} E_{\mu s} \mathcal{O}_{\mu s}^{\dagger} \mathcal{O}_{\mu s} + \frac{J_B^2}{2g_0} , \tag{A20}$$

where E_B is a constant, the zero-point energy, and g_0 is the usual Inglis cranking moment of inertia,

$$g_0 = 2 \sum_{i\alpha} \frac{|J_{i\alpha}|^2}{\epsilon_i - \epsilon_\alpha} . \tag{A21}$$

There are no self-consistent corrections to Eq. (A21), since we are starting with the Hartree rather than the Hartree-Fock approximation used in the Thouless-Valatin method. From time-reversal considerations, one can show that the corrections in the latter come from the omitted exchange term. The additional indices s in Eqs. (A19) and (A20) denote different branches of the eigenvalue problem. In general, there may be single-particle branches for which $\mathcal{O}_{\mu s}^{\dagger}$ coincides with a particle-hole excitation $B_{i\alpha}^{\dagger}$ not affected by the two-body interaction. In addition, there are two collective branches with eigenvalues given by the dispersion equations

$$2\kappa \sum_{i\alpha} \frac{|R_{i\alpha}^{(\pm)}|^2 (\epsilon_i - \epsilon_\alpha)}{(\epsilon_i - \epsilon_\alpha)^2 - E_{\mu\pm}^2} = 1. \tag{A22}$$

As a consequence of the choice of orientation (A7), the minus branch has an $E = 0$ root. Comparing with the three-dimensional quadrupole-quadrupole-force problem, one sees that the plus branch resembles the β-vibrational branch, while the minus branch corresponds to the $K = 1$ branch. There is, of course, nothing corresponding to a γ vibration in the two-dimensional case. The amplitudes which correspond to Eqs. (A22) are

$$\begin{aligned}
X_{i\alpha}(\mu\pm) &= N_{\mu\pm} \frac{\kappa R_{i\alpha}^{(\pm)}}{\epsilon_i - \epsilon_\alpha - E_{\mu\pm}} , \\
Y_{i\alpha}(\mu\pm) &= -N_{\mu\pm} \frac{\kappa R_{i\alpha}^{(\pm)*}}{\epsilon_i - \epsilon_\alpha + E_{\mu\pm}} ,
\end{aligned} \tag{A23}$$

where $N_{\mu\pm}$ is a normalization factor:

$$N_{\mu\pm} = \left\{ 4E_{\mu\pm}\kappa^2 \sum_{i\alpha} \frac{|R_{i\alpha}^{(\pm)}|^2 (\epsilon_i - \epsilon_\alpha)}{[(\epsilon_i - \epsilon_\alpha)^2 - E_{\mu\pm}^2]^2} \right\}^{-1/2} . \tag{A24}$$

The inverse of Eqs. (A19) is

$$B_{i\alpha}^{\dagger}=\sum_{\mu s}[X_{i\alpha}(\mu s)^{*}\mathcal{O}_{\mu s}^{\dagger}-Y_{i\alpha}(\mu s)\mathcal{O}_{\mu s}]+g_0^{-1}\frac{J_{i\alpha}^{*}}{\epsilon_i-\epsilon_\alpha}J_B+iJ_{i\alpha}^{*}\Phi_B,$$

$$B_{i\alpha}=\sum_{\mu s}[-Y_{i\alpha}(\mu s)^{*}\mathcal{O}_{\mu s}^{\dagger}+X_{i\alpha}(\mu s)\mathcal{O}_{\mu s}]+g_0^{-1}\frac{J_{i\alpha}}{\epsilon_i-\epsilon_\alpha}J_B-iJ_{i\alpha}\Phi_B. \tag{A25}$$

Substitution of Eq. (A25) into Eqs. (A17) and (A18) gives H_{III} and H_{IV} in the form of Eqs. (II.3) and (II.4). We shall not write down all of the coefficients, only those which enter into the $\mathfrak{G}$ coefficient.

First of all, consider the $J_B^2\times$(phonon) term of H_{III}. Since $R_B^{(\pm)}$ is independent of J_B by time-reversal symmetry, the $J_B^2\times$(phonon) term can only come from a linear phonon term of $R_B^{(\pm)}$ combining with a J_B^2 term from $R_{\mathrm{II}}^{(\pm)}$. Actually, it will be shown that the J_B^2 term of $R_{\mathrm{II}}^{(-)}$ vanishes. One therefore obtains the coefficients of the $J_B^2\mathcal{O}_{\mu s}^{\dagger}$ terms as

$$h_{\mu s}^{(3)}(21)=-\delta_{s,+}\kappa\frac{N_{\mu+}}{g_0^2}\left[\sum_{ij\alpha}\frac{J_{i\alpha}^{*}R_{ij}^{(+)}J_{j\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)}-\sum_{i\alpha\beta}\frac{R_{\alpha\beta}^{(+)}J_{i\beta}^{*}J_{i\alpha}}{(\epsilon_i-\epsilon_\beta)(\epsilon_i-\epsilon_\alpha)}\right]. \tag{A26}$$

The expression obtained from (A26) by replacing $R^{(+)}$ by $R^{(-)}$ is seen to vanish by noting that for each term in the sum, the complex conjugate also occurs in the sum, and then employing the identity

$$J_{ab}(\epsilon_a-\epsilon_b)=2i\kappa\langle 0|R^{(+)}|0\rangle R_{ab}^{(-)}, \tag{A27}$$

which follows from the rotational invariance of H and the commutation rule

$$[J,R^{(-)}]=-2iR^{(+)}. \tag{A28}$$

Next, consider the J_B^4 term from H_{IV}. Since $R_{\mathrm{III}}^{(\pm)}$ cannot contain a J_B^3 term by time-reversal symmetry, and we have shown that $R_{\mathrm{II}}^{(-)}$ does not contain a J_B^2 term, it follows that the J_B^4 term of H_{IV} can only arise from $-\frac{1}{2}\kappa(R_{\mathrm{II}}^{(+)})^2$. We therefore obtain the coefficient

$$h^{(4)}(40)=-\tfrac{1}{2}\frac{\kappa}{g_0^4}\left[\sum_{ij\alpha}\frac{J_{i\alpha}^{*}R_{ij}^{(+)}J_{j\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)}-\sum_{i\alpha\beta}\frac{R_{\alpha\beta}^{(+)}J_{i\beta}^{*}J_{i\alpha}}{(\epsilon_i-\epsilon_\beta)(\epsilon_i-\epsilon_\alpha)}\right]^2. \tag{A29}$$

We note that the term in brackets in Eq. (A29) is the square of the bracketed term in Eq. (A26).

In order to obtain the $\mathfrak{G}$ coefficient, we also need the boson expansion of the angular momentum,

$$J=\sum_{i\alpha}(J_{i\alpha}a_i^{\dagger}b_\alpha^{\dagger}+\mathrm{H.c.})+\sum_{ij}J_{ij}a_i^{\dagger}a_j-\sum_{\alpha\beta}J_{\alpha\beta}b_\beta^{\dagger}b_\alpha, \tag{A30}$$

given by

$$J=J_B+J_{\mathrm{II}}+J_{\mathrm{III}}+\cdots, \tag{A31}$$

where

$$J_{\mathrm{II}}=\sum_{ij\alpha}J_{ij}B_{i\alpha}^{\dagger}B_{j\alpha}-\sum_{i\alpha\beta}J_{\alpha\beta}B_{i\beta}^{\dagger}B_{i\alpha}, \tag{A32}$$

and

$$J_{\mathrm{III}}=-\tfrac{1}{2}\sum_{ij\alpha\beta}(J_{i\alpha}B_{i\beta}^{\dagger}B_{j\alpha}^{\dagger}B_{j\beta}+\mathrm{H.c.}). \tag{A33}$$

Insertion of Eqs. (A25) identifies the coefficients of the $J_B\mathcal{O}_{\mu s}^{\dagger}$ terms of J_{II} as

$$j_{\mu s}^{(2)}(11)=g_0^{-1}\{\sum_{ij\alpha}(\epsilon_j-\epsilon_\alpha)^{-1}[X_{i\alpha}(\mu s)^{*}J_{ij}J_{j\alpha}-Y_{i\alpha}(\mu s)^{*}J_{ji}J_{j\alpha}^{*}]+\sum_{i\alpha\beta}(\epsilon_i-\epsilon_\beta)^{-1}[J_{\alpha\beta}J_{i\beta}^{*}Y_{i\alpha}(\mu s)^{*}-X_{i\alpha}(\mu s)^{*}J_{i\beta}J_{\beta\alpha}]\}. \tag{A34}$$

The coefficient of the J_B^3 term of J_{III} is given by

$$j^{(3)}(30)=-\frac{1}{g_0^3}\sum_{ij\alpha\beta}\frac{J_{i\alpha}^{*}J_{i\beta}J_{j\beta}^{*}J_{j\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)(\epsilon_j-\epsilon_\beta)}. \tag{A35}$$

With the aid of time-reversal symmetry considerations, it may readily be shown that all the coefficients are real. In accordance with the discussion in Sec. II, for the kinematic choice of bosons the vibration-rotation coefficients are given by $[h_{\mu s}^{(3)}(21)-g_0^{-1}j_{\mu s}^{(2)}(11)]$, while the coefficient of the J^4 term is $[h^{(4)}(40)$

$-\mathcal{I}_0^{-1}j^{(3)}(30)]$. The total $\mathfrak{B}$ coefficient is then given by

$$\mathfrak{B} = h^{(4)}(40) - \mathcal{I}_0^{-1}j^{(3)}(30) - \sum_{\mu s} \frac{|h^{(3)}_{\mu s}(21) - \mathcal{I}_0^{-1} j_{\mu s}(11)|^2}{E_{\mu s}} \quad . \tag{A36}$$

The cranking model must give exactly the result (A36), but the formal expression is simplified by a sum rule for the summation over phonon modes. In order to obtain this result, we work with the Hamiltonian H_λ:

$$H_\lambda = H - \lambda J \, . \tag{A37}$$

The usual procedures of the cranking model in the fermion picture may then be followed. One may, for example, remove all $a_i^\dagger b_\alpha^\dagger$ and $b_\alpha a_i$ terms in Eq. (A37) by the transformation

$$H_\lambda \rightarrow e^{-iS} H_\lambda e^{iS} \, , \tag{A38}$$

where S is a one-body operator:

$$S = -i \sum_{i\alpha} (S_{i\alpha} a_i^\dagger b_\alpha^\dagger + \text{H.c.}) \, . \tag{A39}$$

Alternatively, we can use the boson picture and follow the procedures described in Sec. III. In order to obtain the sum rule, however, the Hamiltonian H_λ must be expressed in terms of the bosons $B_{i\alpha}, B_{i\alpha}^\dagger$ rather than the normal modes. The linear boson terms, proportional to $B_{i\alpha}$ and $B_{i\alpha}^\dagger$, are then removed by the shift transformation

$$\begin{aligned} B_{i\alpha} &\rightarrow e^{-iS_B} B_{i\alpha} e^{iS_B} = B_{i\alpha} + \sigma_{i\alpha} \, , \\ B_{i\alpha}^\dagger &\rightarrow e^{-iS_B} B_{i\alpha}^\dagger e^{iS_B} = B_{i\alpha}^\dagger + \sigma_{i\alpha}^* \, , \end{aligned} \tag{A40}$$

where S_B is the operator

$$S_B = -i \sum_{i\alpha} (\sigma_{i\alpha} B_{i\alpha}^\dagger - \sigma_{i\alpha}^* B_{i\alpha}) \, . \tag{A41}$$

The constants $\sigma_{i\alpha}$ are then expanded in powers of λ:

$$\sigma_{i\alpha} = \lambda \sigma_{i\alpha}^{(1)} + \lambda^2 \sigma_{i\alpha}^{(2)} + \lambda^3 \sigma_{i\alpha}^{(3)} + \cdots \, . \tag{A42}$$

The expansion of the density matrix, $\underline{\rho} = \underline{\rho}^{(0)} + \lambda \underline{\rho}^{(1)} + \lambda^2 \underline{\rho}^{(2)} + \lambda^3 \underline{\rho}^{(3)}$, may then be found from Eq. (III.45). In this way, we obtain

$$\rho_{i\alpha}^{(1)} = \sigma_{i\alpha}^{(1)} = S_{i\alpha}^{(1)} = J_{i\alpha}/(\epsilon_i - \epsilon_\alpha) \, ; \tag{A43}$$

$$\rho_{ij}^{(1)} = \rho_{\alpha\beta}^{(1)} = 0 \, ; \tag{A44}$$

$$\rho_{i\alpha}^{(2)} = \sigma_{i\alpha}^{(2)} = S_{i\alpha}^{(2)} = \sum_j \frac{J_{ij} J_{j\alpha}}{(\epsilon_i - \epsilon_\alpha)(\epsilon_j - \epsilon_\alpha)} - \sum_\beta \frac{J_{i\beta} J_{\beta\alpha}}{(\epsilon_i - \epsilon_\beta)(\epsilon_i - \epsilon_\alpha)} + \frac{\delta\langle R^{(+)}\rangle}{\lambda^2} \kappa \frac{R_{i\alpha}^{(+)}}{\epsilon_i - \epsilon_\alpha} \, . \tag{A45}$$

The quantity $\delta\langle R^{(+)}\rangle$ is the second-order change in the deformation due to the centrifugal stretching ($\delta\langle R^{(+)}\rangle = \langle \lambda | R^{(+)} | \lambda \rangle - \langle 0 | R^{(+)} | 0 \rangle$) given by

$$\delta\langle R^{(+)}\rangle = \frac{1}{2} \frac{\lambda^2}{C} \frac{d\mathcal{I}}{d\langle R^{(+)}\rangle} \, , \tag{A46}$$

where

$$C = \kappa \left(1 - 2\kappa \sum_{i\alpha} \frac{|R_{i\alpha}^{(+)}|^2}{\epsilon_i - \epsilon_\alpha} \right) , \tag{A47}$$

and the quantity $d\mathcal{I}/d\langle R^{(+)}\rangle$ is the derivative of the cranking moment of inertia with respect to deformation, given by the expression

$$\frac{1}{2\kappa} \frac{d\mathcal{I}}{d\langle R^{(+)}\rangle} = \sum_{ij\alpha} \frac{J_{i\alpha}^* R_{ij}^{(+)} J_{j\alpha}}{(\epsilon_i - \epsilon_\alpha)(\epsilon_j - \epsilon_\alpha)} + 2 \sum_{ij\alpha} \frac{R_{i\alpha}^{(+)*} J_{ij} J_{j\alpha}}{(\epsilon_i - \epsilon_\alpha)(\epsilon_j - \epsilon_\alpha)} - \sum_{i\alpha\beta} \frac{J_{i\alpha}^* J_{i\beta} R_{\beta\alpha}^{(+)}}{(\epsilon_i - \epsilon_\alpha)(\epsilon_i - \epsilon_\beta)} - 2 \sum_{i\alpha\beta} \frac{R_{i\alpha}^{(+)*} J_{i\beta} J_{\beta\alpha}}{(\epsilon_i - \epsilon_\alpha)(\epsilon_i - \epsilon_\beta)} \, . \tag{A48}$$

Although $\sigma_{i\alpha}$ and $S_{i\alpha}$ coincide through second order, they no longer do so in third order. In fact, we obtain

$$\rho^{(3)}_{i\alpha} = \sigma^{(3)}_{i\alpha} - \tfrac{1}{2}\sum_{j\beta}\sigma^{(1)}_{i\beta}\sigma^{(1)}_{j\beta}{}^{*}\sigma^{(1)}_{j\alpha} = S^{(3)}_{i\alpha} - \tfrac{2}{3}\sum_{j\beta}\sigma^{(1)}_{i\beta}\sigma^{(1)}_{j\beta}{}^{*}\sigma^{(1)}_{j\alpha}$$

$$= -\sum_{j\beta}\frac{J_{i\beta}J_{j\beta}{}^{*}J_{j\alpha}}{(\epsilon_i-\epsilon_\beta)(\epsilon_j-\epsilon_\alpha)}\left(\frac{1}{\epsilon_i-\epsilon_\alpha}+\frac{1}{\epsilon_j-\epsilon_\beta}\right)-\sum_{j\beta}\frac{J_{ij}J_{j\beta}J_{\beta\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\beta)}\left(\frac{1}{\epsilon_i-\epsilon_\beta}+\frac{1}{\epsilon_j-\epsilon_\alpha}\right)$$

$$+\sum_{jk}\frac{J_{ij}J_{jk}J_{k\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)(\epsilon_k-\epsilon_\alpha)}+\sum_{\beta\gamma}\frac{J_{i\beta}J_{\beta\gamma}J_{\gamma\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)(\epsilon_i-\epsilon_\gamma)}$$

$$+\frac{\delta\langle R^{(+)}\rangle}{\lambda^2}\kappa\left[\sum_j\frac{R^{(+)}_{ij}J_{j\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)}+\sum_j\frac{J_{ij}R^{(+)}_{j\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)}-\sum_\beta\frac{J_{i\beta}R^{(+)}_{\beta\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)}-\sum_\beta\frac{R^{(+)}_{i\beta}J_{\beta\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)}\right]. \quad \text{(A49)}$$

The other density matrix elements are

$$\rho^{(3)}_{ji} = \sum_\alpha(\sigma^{(1)}_{j\alpha}\sigma^{(2)}_{i\alpha}{}^{*}+\sigma^{(2)}_{j\alpha}\sigma^{(1)}_{i\alpha}{}^{*}),$$

$$\rho^{(3)}_{\alpha\beta} = -\sum_i(\sigma^{(2)}_{i\alpha}{}^{*}\sigma^{(1)}_{i\beta}+\sigma^{(1)}_{i\alpha}{}^{*}\sigma^{(2)}_{i\beta}). \quad \text{(A50)}$$

From Eqs. (III.65) and (III.67), one sees that the $\mathfrak{B}$ coefficient is obtained from the shift in J, i.e., the expectation value in the cranked ground state, as follows:

$$\mathfrak{B} = -\tfrac{1}{4}g_0{}^{-4}\langle\lambda|J|\lambda\rangle^{(3)} = -\tfrac{1}{4}g_0{}^{-4}\mathrm{Tr}\underline{\rho}^{(3)}\underline{J}$$

$$= \frac{1}{g_0{}^4}\left[\sum_{ij\alpha\beta}\frac{J_{i\alpha}{}^{*}J_{i\beta}J_{j\beta}{}^{*}J_{j\alpha}}{(\epsilon_i-\epsilon_\beta)(\epsilon_j-\epsilon_\beta)(\epsilon_j-\epsilon_\alpha)}+2\sum_{ij\alpha\beta}\frac{J_{i\alpha}{}^{*}J_{ij}J_{j\beta}J_{\beta\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\beta)(\epsilon_j-\epsilon_\alpha)}\right.$$

$$\left.-\sum_{i\alpha\beta\gamma}\frac{J_{i\alpha}{}^{*}J_{i\beta}J_{\beta\gamma}J_{\gamma\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)(\epsilon_i-\epsilon_\gamma)}-\sum_{ijk\alpha}\frac{J_{i\alpha}{}^{*}J_{ij}J_{jk}J_{k\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)(\epsilon_k-\epsilon_\alpha)}-\frac{1}{8}\left(\frac{dg}{d\langle R^{(+)}\rangle}\right)^2\frac{1}{C}\right]. \quad \text{(A51)}$$

The first four terms in Eq. (A51) correspond to the "Coriolis" term $\mathfrak{B}_C$ of Ref. 6. This term arises only from $H_{\mathrm{SCF}}-\lambda J$. The last term of Eq. (A51) arises from the residual interaction and represents the centrifugal stretching; it corresponds to the term $\mathfrak{B}_{\mathrm{vib}}$ of Ref. 6. It was assumed in that work that $\mathfrak{B}_{\mathrm{vib}}$ is the contribution of the vibration-rotation interaction, and that therefore $\mathfrak{B}_C$ is the coefficient of the J^4 term. While such a division is perfectly correct for a proper choice of Φ (or, equivalently, of the f coefficients in Sec. II B) it is hardly unique, and, in fact, does not correspond to the kinematic choice. The kinematic vibration-rotation term contributes to both $\mathfrak{B}_C$ and $\mathfrak{B}_{\mathrm{vib}}$, as shown by comparison of Eqs. (A51), (A35), and (A36), giving the sum rule:

$$-\sum_{\mu s}\frac{|h^{(3)}_{\mu s}(21)-g_0{}^{-1}j^{(2)}_{\mu}(11)|^2}{E_{\mu s}} = -h^{(4)}(40)-\frac{1}{8g_0{}^4C}\left(\frac{dg}{d\langle R^{(+)}\rangle}\right)^2+\frac{1}{g_0{}^4}\left[2\sum_{ij\alpha\beta}\frac{J_{i\alpha}{}^{*}J_{ij}J_{j\beta}J_{\beta\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\beta)(\epsilon_j-\epsilon_\alpha)}\right.$$

$$\left.-\sum_{i\alpha\beta\gamma}\frac{J_{i\alpha}{}^{*}J_{i\beta}J_{\beta\gamma}J_{\gamma\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_i-\epsilon_\beta)(\epsilon_i-\epsilon_\gamma)}-\sum_{ijk\alpha}\frac{J_{i\alpha}{}^{*}J_{ij}J_{jk}J_{k\alpha}}{(\epsilon_i-\epsilon_\alpha)(\epsilon_j-\epsilon_\alpha)(\epsilon_k-\epsilon_\alpha)}\right]. \quad \text{(A52)}$$

It is seen from Eqs. (III.58b) and (III.59b) that this sum rule may also be obtained by computing the constant term of order λ^4 arising from $H_{\mathrm{III}}-\lambda J_{\mathrm{II}}$.

One of the big advantages of the cranking model as a calculational tool is that it sums together the effects of all band mixings on the ground-state rotational band, thus eliminating the need to solve for each RPA band-head excitation explicitly. We also note that although the quantity C given by Eq. (A47) resembles the adiabatic vibrational force constant, the $\mathfrak{B}$ coefficient (A51) has nothing to do with the adiabatic approximation. On the contrary, $\mathfrak{B}_{\mathrm{vib}}$ actually includes summation of effects due to all RPA solutions.

As a bonus, we note that the λ^2 dependence of $\langle R^{(+)}\rangle$ identifies the J^2 dependence of the operator $Q^{(2)}$ in accordance with the discussion in Sec. III E. From Eqs. (II.63a) and (III.84), we may make the following identification (with $M=2$):

$$\Lambda^{(2)(2)}(20) = \tfrac{1}{2}q^{(2)(2)}(20) - 2\sum_{\mu} q_{\mu}^{(2)(1)}(0)\frac{h_{\mu}^{(3)}(21) - g_0^{-1}j_{\mu}^{(2)}(11)}{E_{\mu}}$$

$$= \frac{1}{g_0^2}\frac{dg}{d\langle R^{(+)}\rangle}\frac{1}{C} \ . \tag{A53}$$

Finally, let us consider the orders of magnitude of the parameters. This will only be done very crudely here. First of all, from Eqs. (A26) and (A34) it is immediately apparent that $h_{\mu s}^{(3)}(21)$ and $g_0^{-1}j_{\mu s}^{(2)}(11)$ are roughly of the same order of magnitude. It is not so apparent that $h^{(4)}(40)$, given by Eq. (A29), and $g_0^{-1}j^{(3)}(30)$, given by Eq. (A35) are of the same order of magnitude, but this can, in fact, be verified by more detailed considerations. Comparing Eqs. (A26) and (A34) with Eq. (A48) one obtains the rough estimates:

$$h_{\mu s}^{(3)}(21) \sim g_0^{-1}j_{\mu s}^{(2)}(11) \sim N_{\mu +}\frac{1}{g_0^2}\frac{dg}{d\langle R^{(+)}\rangle} \ ,$$

$$h^{(4)}(40) \sim g_0^{-1}j^{(3)}(30) \sim \frac{1}{\kappa}\left(\frac{1}{g_0^2}\frac{dg}{d\langle R^{(+)}\rangle}\right)^2 \ . \tag{A54}$$

The $N_{\mu +}$ are just zero-point amplitudes. The largest amplitude is expected for the lowest eigenmode, for which one may make the adiabatic estimate

$$E^2 2\kappa^2 \sum_{i\alpha}\frac{|R_{i\alpha}^{(+)}|^2(\epsilon_i - \epsilon_{\alpha})}{[(\epsilon_i - \epsilon_{\alpha})^2 - E^2]^2} \sim C \sim \kappa \ .$$

Therefore,

$$N_{\mu +} \sim (E_{\mu +}/2\kappa)^{1/2} \ ,$$

so that one indeed obtains

$$\frac{|h_{\mu s}^{(3)}(21) - g_0^{-1}j_{\mu s}^{(2)}(11)|^2}{E_{\mu s}} \sim h^{(4)}(40) - g_0^{-1}j^{(3)}(30) \ .$$

We may now write (with $\hbar = 1$)

$$h_{\mu s}^{(3)}(21) - g_0^{-1}j_{\mu s}^{(2)}(11) \sim \frac{1}{2g_0}\left(\frac{\text{zero-point amplitude}}{\langle 0|R^{(+)}|0\rangle}\right)\left(\frac{dg}{d\langle R^{(+)}\rangle}\frac{\langle 0|R^{(+)}|0\rangle}{g_0}\right) \ , \tag{A55a}$$

$$h^{(4)}(40) - g_0^{-1}j^{(3)}(30) \sim \frac{1}{2g_0}\frac{(2g_0)^{-1}}{E}\left(\frac{\text{zero-point amplitude}}{\langle 0|R^{(+)}|0\rangle}\right)^2\left(\frac{dg}{d\langle R^{(+)}\rangle}\frac{\langle 0|R^{(+)}|0\rangle}{g_0}\right)^2 \ . \tag{A55b}$$

Based on experience with the three-dimensional case, we expect that

$$\frac{dg}{d\langle R^{(+)}\rangle}\frac{\langle 0|R^{(+)}|0\rangle}{g_0} \sim 1 \ . \tag{A56}$$

Thus, the vibration-rotation coefficient is reduced relative to the leading-order rotational-energy parameter $(2g_0)^{-1}$ by the ratio of the zero-point amplitude to the equilibrium deformation. This ratio must be small if the RPA is to be a good approximation for the deformed system. The square of this parameter occurs in the coefficient of the J^4 term, which is further diminished by the ratio of the rotational to vibrational energy.

In a similar manner, it may be shown that the coefficient $\Lambda^{(2)(2)}(20)$ is reduced relative to the leading term $\langle 0|R^{(+)}|0\rangle$ by a factor of order

$$\frac{(2g_0^{-1})}{E}\left(\frac{\text{zero-point amplitude}}{\langle 0|R^{(+)}|0\rangle}\right)^2 \ .$$

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[13]In this case, no generality is lost by writing the quadratic phonon terms in normal order.

[14]If the shape of the ground state is reflection symmetric, only even values of M occur.

[15]Strictly speaking, the original Hartree approximation subtracted out a self-interaction term which is usually included as part of the so-called exchange term that we drop. The procedure used in our work has the advantage that the single-particle states are orthogonal as in the Hartree-Fock approximation.

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[19]For convenience, we continue to use the same symbol for fermion operators and their boson images where no confusion will occur. The equality sign should, of course, be interpreted more precisely as a mapping $\eta_b^\dagger \eta_a \to \hat{\rho}_{ab}$.

[20]The appellation "c-ordered" has no intrinsic significance – we simply needed a name and this one seemed as good as any.

[21]It is understood that any pair of bosons $(\tilde{B}_\mu, \tilde{B}_\mu^\dagger)$ may be replaced by a generalized coordinate-momentum pair.

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[24a]Although this form is adequate for present purposes, one may have to use the more general form $Q^{(m)} = \frac{1}{2}(e^{im\Phi} \times \mathcal{Q}^{(m)} + \mathcal{Q}'^{(m)} e^{im\Phi})$, $\mathcal{Q}^{(m)}$, $\mathcal{Q}'^{(m)}$ being scalars.

[24b]While it is not needed here, it may be shown that C_n is given by the recursion formula: $C_1 = -\frac{1}{2}$, $C_n = -\frac{1}{2} \times \sum_{m=1}^{n-1} C_m C_{n-m}$, $n \geq 2$.