Collective Motion in Finite Many-Particle Systems. III. Foundations of a Theory of Rotational Spectra of Deformed Nuclei*

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The generalized Hartree-Fock approximation developed in previous papers is here applied to provide a microscopic and fully quantum-mechanical self-consistent theory of the rotational spectra of deformed nuclei. Starting from a rotation- and inversion-invariant Hamiltonian, the equations of the method are derived for the present application, including the effect of pairing correlations. The equations of motion yield the description of a quasiparticle (hole) self-consistently coupled to a rotator. Within a consistent approximation, all the usual observables associated with the notion of deformed nuclei—moments of inertia, collective gyromagnetic ratios, quadrupole moments, and transition probabilities—can be obtained in terms of the solutions of these equations, which are developed as a power series in the reciprocal of the moment of inertia. The zero-order theory is equivalent to the best current theory of nuclear shapes and also describes, therefore, the quadrupolar properties of the nucleus. The first-order solution suffices for the calculation of the moment of inertia and the collective gyromagnetic ratio. Here again familiar results are obtained in the only case considered in detail, that of a single band with unlimited angular-momentum states available. The second-order solution is also found and used to study the spectrum of the neighboring odd nuclei. The main new results of this paper are contained in the formulas for the moment of inertia and decoupling parameter for odd-particle or hole-based bands, where the self-consistency requirements yield terms not hitherto noticed in the case of an odd nucleus.

I. INTRODUCTION

OUR aim in this paper is the reconstruction of the foundations for a theory of the spectra of deformed nuclei. There has been, in recent years, notable progress in this area,[1] leading for *practical* purposes to a reasonable solution of many of the outstanding problems, such as the moment of inertia and the collective gyromagnetic ratio (at least for the rare earths and the actinides). Nevertheless, there remain conceptual objections to current theories and, as well, problems concerned with the applicability of their concepts to lighter nuclei[2] (s-d shell for example), higher order effects of rotation-particle coupling and rotation-vibration interaction,[3] etc. Some of these problems will be dealt with in subsequent papers. In this one, we deal largely with the conceptual ones, deriving from our standpoint many known results, though we do obtain new results for the spectra of odd nuclei and point the way toward new results for other properties of the latter.

The best current theory of rotations[1] is based on the self-consistent cranking of a deformed nucleus whose wave function is determined by the long-range average quadrupole field and by the pairing interaction. By cranking, we understand the *imposition* of an external field which forces the nucleus to rotate about a given axis. It is thereby assumed that the inertial parameter characterizing this constrained, continuously variable motion is the same as that which determines the actually observed discrete rotational spectrum. Though plausible, this has never been demonstrated prior to the current work.[4]

In the previous papers of this series,[5] the basic ideas of the generalized Hartree-Fock approximation (GHFA) were described in some detail and applied with success to the characteristic testing grounds of uniform translational motion and rotations in a plane. In this paper we

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[1] For recent discussions of theoretical concepts and full references to the literature, see the following reviews: V. G. Soloviev, in *Selected Topics in Nuclear Physics* (International Atomic Energy Agency, Vienna, 1963), p. 233; S. T. Belyaev, *ibid.*, p. 291; M. Baranger, *1962 Cargese Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963), Chap. V; K. T. Hecht, in *Selected Topics in Nuclear Spectroscopy* (Interscience Publishers, Inc., New York, 1964), p. 51; C. J. Gallagher, *ibid.*, p. 133; A. M. Lane, *Nuclear Theory* (W. A. Benjamin, Inc, New York, 1964); J. G. Valatin, *Lectures in Theoretical Physics* (Interscience Publishers, Inc., New York, 1962), Vol. IV, p. 1; Vol. VI, p. 292.

[2] C. A. Levinson, Phys. Rev. **132**, 2184 (1963); I. Kelson, *ibid.* **132**, 2189 (1963); I. Kelson and C. A. Levinson, *ibid.* **134**, B269 (1964); W. H. Bassichis, C. A. Levinson, and I. Kelson, *ibid.* **136**, B300 (1964).

[3] A. Faessler, W. Greiner, and R. K. Sheline, Technical Report 345, Department of Physics and Astronomy, University of Maryland, 1963 (unpublished); Phys. Rev. **135**, B591 (1964); I. M. Pavlichenkov, Nucl. Phys. **55**, 225 (1964); S. M. Harris, Phys. Rev. Letters **13**, 663 (1964); V. Radojevic, A. Sobiczewski, and Z. Szymanski, Nucl. Phys. **38**, 607 (1962); Yu. T. Grin and I. M. Pavlichenkov, Zh. Eksperim. i Teor. Fiz. **43**, 465 (1962) [English transl.: Soviet Phys.—JETP **16**, 333 (1963)]; A. Faessler and W. Greiner, Z. Physik **177**, 190 (1964); A. Faessler, Nucl. Phys. **59**, 177 (1964); A. Faessler and H. G. Wahsweiler, *ibid.* **59**, 202 (1964); Yu. N. Devyatko, V. V. Lomonsov, and M. G. Vrin, Zh. Eksperim. i Teor. Fiz. **46**, 2070 (1964) [English transl.: Soviet Phys.—JETP **19**, 1396 (1964)].

[4] The basic idea was first described in A. K. Kerman and A. Klein, Phys. Letters **1**, 185 (1962). A preliminary report of some of the contents of the present paper was given in A. Klein and A. K. Kerman, Proceedings of the Eastern Conference on Theoretical Physics, University of North Carolina, 1963 (unpublished).

[5] A. K. Kerman and A. Klein, Phys. Rev. **132**, 1326 (1963), referred to as I; A. Klein and A. K. Kerman, Phys. Rev. **138**, B1323 (1965).

extend the theory to the study of axially symmetric rotations in three dimensions, including pairing correlations. The contents are arranged as follows: Section II contains a concise self-contained statement of the fundamental equations of the theory including pairing. The physical content of the equations is transparent: In the simple version of the theory to which we restrict ourselves they describe a quasihole (particle) coupled self-consistently to a rotator. The theory is thus a microscopic version of the core-particle coupling model.

The major part of our program consists in obtaining the solution of the equations as a power series in the reciprocal of the moment of inertia. The zeroth-order solution, as derived in Sec. III is equivalent to the best available theory of nuclear shapes.[6] The first- and second-order solutions are derived in Secs. IV and VI, respectively, subject to restrictions which have been studied in the previous paper of this series. It is these restrictions to a semiclassical limit that lead us back to familiar results. The moment of inertia of the ground-state band of an even-even nucleus is obtained in Sec. V. The energy levels of single-particle bands of the neighboring odd nuclei are studied in Sec. VI. Here the formulas for both the moment of inertia and the decoupling parameter contain new terms arising from the self-consistency requirements of the theory. Finally, Sec. VII contains calculations of some standard formulas for $B(E2)$ values, requiring a slight extension of the ideas of the previous text, and of a formula for the collective gyromagnetic ratio, similar to that for the moment of inertia. The material of this section is to be considered as introductory to a more extensive investigation of one-particle observables in odd-deformed nuclei.

With this paper we have essentially completed the first phase of our investigation—the derivation from a more satisfactory point of veiw of the simplest parts of the theory of deformed nuclei. In future accounts, we shall report techniques for avoiding the major practical limitation of the current work (which is also the essential assumption for making connection with previous work), namely, that each rotational band is assumed to extend without limit.[7] In this way we hope to obtain a theory applicable also to lighter deformed nuclei.

II. GENERALIZED HARTREE-FOCK THEORY WITH PAIRING INTERACTION

We take as our Hamiltonian the general form

$$H=\int \psi^\dagger(x_1)h(x_1,x_2)\psi(x_2) +\frac{1}{4}\int \psi^\dagger(x_1)\psi^\dagger(x_2)V(x_1x_2;x_3x_4)\psi(x_4)\psi(x_3)\,, \quad (2.1)$$

where x represents a complete set of coordinates of a single particle, and

$$\begin{aligned} h^*(x_1,x_2)&=h(x_2,x_1)\,,\\ V(x_1x_2;x_3x_4)&=-V(x_1x_2;x_4x_3)\\ &=-V(x_2x_1;x_3x_4)=V^*(x_3x_4;x_1x_2)\,. \end{aligned} \quad (2.2)$$

In (2.1) one may consider either that h is the kinetic-energy operator and V is the total interaction or that h is an appropriate spherical-shell-model Hamiltonian and V is the residual interaction. We shall beg the question of making a definite choice here, though in the current state of the art, it is usually the latter or model Hamiltonian that is treated. We note simply that in writing (2.2), we have already made use of the exclusion principle.

We shall moreover, make the fundamental assumption that H is invariant under rotations, expressed by the statements

$$\begin{aligned} h(x_1,x_2)&=h(x_{1R},x_{2R})\,,\\ V(x_1x_2;x_3x_4)&=V(x_{1R}x_{2R};x_{3R}x_{4R})\,, \end{aligned} \quad (2.3)$$

where the subscript R indicates the performance of a definite rotation. We also assume invariance under space inversion.

We use the equations of motion

$$[\psi(x),H]=\int h(x,x_1)\psi(x_1) +\frac{1}{2}\int V(xx_1;x_2x_3)\psi^\dagger(x_1)\psi(x_3)\psi(x_2)\,, \quad (2.4a)$$

$$-[\psi^\dagger(x),H]=\int \psi^\dagger(x_1)h(x_1,x) +\frac{1}{2}\int \psi^\dagger(x_2)\psi^\dagger(x_3)\psi(x_1)V(x_2x_3;xx_1) \quad (2.4b)$$

to study matrix elements of the type

$$\Psi_i(xI)\equiv\langle i|\psi(x)|I\rangle\,, \quad (2.5)$$

where $|I\rangle$ (magnetic quantum number suppressed) is a member of the ground-state rotational band of an even-even nucleus with A nucleons and $|i\rangle$ is some state of the A-1 nucleus which can be reached from it with appreciable amplitude by the destruction of a single particle. For $|I\rangle=|0\rangle$, (2.5) is the field-theoretical definition of the Hartree-Fock single-particle wave function. From (2.4a) we obtain

$$[\mathcal{E}_i+E(I)]\Psi_i(x,I) =\int h(x,x_1)\Psi_i(x_1I)+\frac{1}{2}\int V(xx_1;x_2x_3) \times\langle i|\psi^\dagger(x_1)\psi(x_3)\psi(x_2)|I\rangle\,, \quad (2.6)$$

[6] The most recent account has been given by M. Baranger, *Proceedings of the Paris Conference on Nuclear Physics, 1964* (Éditions du Centre National de la Recherche Scientifique, Paris, 1964), Vol. I, p. 49.

[7] A tentative approach to a generalized theory can be found in R. Dreizler and A. Klein, Nucl. Phys. (to be published).

where, in an obvious notation in which W stands for the total energy of a state,

$$W_A(I)-W_{A-1}(i)=[W_A(0)-W_{A-1}(i)] +[W_A(I)-W_A(0)]\equiv[\mathcal{E}_i+\mu]+E(I), \quad (2.7)$$

and μ, the separation energy, has been incorporated in (2.6) by the replacement $h\to h-\mu$.

To see how to proceed, we note that in the Hartree-Fock theory (including "superconductivity" or pairing effects) we would write

$$\begin{aligned}\langle i|\psi^\dagger(1)\psi(3)\psi(2)|0\rangle &\cong\langle i|\psi(2)|0\rangle\langle 0|\psi^\dagger(1)\psi(3)|0\rangle \\ &-\langle i|\psi(3)|0\rangle\langle 0|\psi^\dagger(1)\psi(2)|0\rangle \\ &+\langle i|\psi^\dagger(1)|0\rangle\langle 0|\psi(3)\psi(2)|0\rangle. \quad (2.8)\end{aligned}$$

We note that if $|0\rangle$ and $\langle 0|$ were Bardeen-Cooper-Schrieffer (BCS) wave functions (2.8) would be exact; if $|0\rangle$ and $|i\rangle$ were Hartree-Fock wave functions, we would omit the last term which describes pairing. For the last term of (2.8) one may either go over to a particle-nonconserving representation or remember that $|0\rangle$ does not always refer to the same nucleus.

As the generalization of (2.8) we shall now write

$$\begin{aligned}\langle i|\psi^\dagger(1)\psi(3)\psi(2)|I\rangle &\cong\sum_{I'}\{\langle i|\psi(2)|I'\rangle\langle I'|\psi^\dagger(1)\psi(3)|I\rangle \\ &-\langle i|\psi(3)|I'\rangle\langle I'|\psi^\dagger(1)\psi(2)I\rangle \\ &+\langle i|\psi^\dagger(1)|I'\rangle\langle I'|\psi(3)\psi(2)|I\rangle\}. \quad (2.9)\end{aligned}$$

Though in contrast to (2.8), we do not (yet) know a set of wave functions for which (2.9) is exact, it should be remarked in its justification that (2.8) can be derived by a physical argument about large matrix elements which can be immediately generalized to (2.9). The essential reasoning, but for the minor complication of pairing, has been described in generous detail in Paper I, and will not be repeated here. We emphasize, however, that these expressions *cannot* be derived by a simple sum-over-states argument only. Moreover, the development to which we here allude has the distinct advantage that we can write an essentially exact reminder to the approximation in each case.

Upon substituion of (2.9) into (2.6), we find

$$\begin{aligned}[\mathcal{E}_i+E(I)]\Psi_i(xI) &=\int h(x,x')\Psi_i(x'I)+\int (xI|\Gamma|x'I')\Psi_i(x'I') \\ &+\int (xI|\Delta|x'I')\Phi_i^*(x'I'), \quad (2.10)\end{aligned}$$

where

$$(xI|\Gamma|x'I')=\int V(xy;x'y')(y'I|\rho|yI'), \quad (2.11)$$

$$(xI|\Delta|x'I')=\frac{1}{2}\int V(xx';yy')(yI|\sigma|y'I'), \quad (2.12)$$

with

$$(xI|\rho|x'I')=\langle I'|\psi^\dagger(x')\psi(x)|I\rangle, \quad (2.13)$$

$$(xI|\sigma|x'I')=\langle I'|\psi(x')\psi(x)|I\rangle, \quad (2.14)$$

and

$$\Phi_i^*(xI)=\langle i|\psi^\dagger(x)|I\rangle. \quad (2.15)$$

Here Γ is the generalized Hartree-Fock potential, Δ the generalized pairing potential, ρ the generalized single-particle density, and σ the generalized pair wave function.

To obtain a closed set of equations, we must find an equation for the amplitude (2.15). This can be done starting from (2.4b). Proceeding as before, we find without difficulty

$$\begin{aligned}[\mathcal{E}_i+E(I)]\Phi_i^*(xI) &=-\int h^*(x,x')\Phi_i^*(x'I)-\int (xI'|\Gamma|x'I)^*\Phi_i^*(x'I') \\ &-\int (xI'|\Delta|x'I)^*\Psi_i(x'I'). \quad (2.16)\end{aligned}$$

Since from (2.13) and (2.14), we have

$$(xI|\rho|x'I')=\textstyle\sum_i \Psi_i(xI)\Psi_i^*(x'I'), \quad (2.17)$$

$$(xI|\sigma|x'I')=\textstyle\sum_i \Psi_i(xI)\Phi_i(x'I'), \quad (2.18)$$

we see that (2.10) and (2.16) constitute a set of closed equations. We emphasize their significance by introducing a matrix notation,

$$\Theta_i(xI)=\begin{pmatrix}\Psi_i(xI)\\ \Phi_i^*(xI)\end{pmatrix}, \quad (2.19)$$

$$(xI|\mathcal{H}|x'I')=\begin{pmatrix}-E(I)\delta_{II'}\delta(x-x')+h(x,x')\delta_{II'}+(xI|\Gamma|x'I') & (xI|\Delta|x'I') \\ -(xI'|\Delta|x'I)^* & -E(I)\delta_{II'}\delta(x-x')-h^*(x,x')\delta_{II'}-(xI'|\Gamma|x'I)^*\end{pmatrix}. \quad (2.20)$$

With the aid of (2.19) and (2.20), (2.10) and (2.16) are equivalent to the equation

$$\mathcal{E}_i\Theta_i(xI)=\int (xI|\mathcal{H}|x'I')\Theta_i(x'I'). \quad (2.21)$$

Our point of view is that (2.21) is to be solved for the $\mathcal{E}_i$, Θ_i, given $\mathcal{H}$, but this means that there are two elements of self-consistency; the potentials Γ and Δ defined by (2.11) and (2.12) together with (2.17) and (2.18) constitute one of these, with nothing new in principle, but only an enlarged space. The other element of self-consistency, which arises because we must prescribe the excitation energies $E(I)$ in order to define the Hamiltonian H, is obtained from the definition

$$E(I)=\langle I|H|I\rangle-\langle 0|H|0\rangle \tag{2.22}$$

and from the expression

$$\langle I|H|I\rangle=\int h(x,x')(x'I|\rho|xI)+\frac{1}{4}\int V(x_1x_2;\,x_3x_4)$$
$$\times\{(x_4I|\rho|x_2I')(x_3I'|\rho|x_1I)-(x_3I|\rho|x_2I')(x_4I'|\rho|x_1I)$$
$$+(x_3I|\sigma|x_4I')(x_1I|\sigma|x_2I')^*\}, \tag{2.23}$$

where the terms in curly brackets represent the factorization[5]

$$\{\ \}=\langle I|\psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_4)\psi(x_3|I)\rangle, \tag{2.24}$$

the analog of (2.9). Equations (2.22), (2.23) thus constitute equations for the energy spectrum of interest.

To complete the prescription requires several additional conditions which specify the number of solutions Θ_i to be used in the pursuit of self-consistency and the norm to be assigned to each. There is first the statement that we are studying a system with A particles, i.e.,

$$A\delta_{II'}=\langle I|\int\psi^\dagger(x)\psi(x)|I'\rangle=\int(xI'|\rho|xI)$$
$$=\sum_i\int\Psi_i(xI')\Psi_i^*(xI), \tag{2.25}$$

and second a completeness condition which can be written

$$\sum_i\{\Theta_i(xI)\Theta_i^\dagger(x'I')+(\tau_1\Theta_i^*(xI'))(\tau_1\Theta_i^*(x'I))^\dagger\}$$
$$=\delta_{II'}\delta(x-x')\begin{pmatrix}1&0\\0&1\end{pmatrix}, \tag{2.26}$$

with τ_1 referring to the appropriate Pauli matrix. Equation (2.26) is derived by combining into matrix form the commutation relations,

$$\langle I|\left\{\begin{pmatrix}\psi(x)\\ \psi^\dagger(x)\end{pmatrix},\ (\psi^\dagger(x'),\psi(x'))\right\}|I'\rangle$$
$$=\delta_{II'}\delta(x-x')\begin{pmatrix}1&0\\0&1\end{pmatrix}. \tag{2.27}$$

We complete this section with a few comments on the properties of our equations. It can be seen that $\mathcal{H}$, Eq. (2.20), is Hermitian and thus for two different solutions of (2.21) we have

$$(\Theta_i,\Theta_{i'})=0,\quad \mathcal{E}_i\neq\mathcal{E}_{i'}. \tag{2.28}$$

If, with normalizations ultimately determined by (2.25), (2.26), we define a matrix $\mathcal{R}$ [the same as appears in the first term of (2.26)],

$$\mathcal{R}=\sum_i\Theta_i\Theta_i^\dagger. \tag{2.29}$$

Then from (2.21), we can deduce that

$$[\mathcal{R},\mathcal{H}]=0. \tag{2.30}$$

Finally, with reference to Eq. (2.26), it should be remarked that this equation represents the generalization of the statement that for the self-consistent well, the filled plus unfilled states (holes plus particles) together constitute a complete set. In the present case however the particles, represented by the "wave functions" $(\tau_1\Theta_i^*(xI))$ do not satisfy the same equations as the holes, Eq. (2.21), but as one can show, satisfy instead

$$-\mathcal{E}_i(\tau_1\Theta_i^*(xI))=\int(xI|\mathcal{H}|x'I')(\tau_1\Theta_i^*(x'I')), \tag{2.31}$$

where

$$(xI|\mathcal{H}|x'I')=\begin{pmatrix}E(I)\delta_{II'}\delta(x-x')+h(x,x')\delta_{II'}+(xI'|\Gamma|x'I)-(xI|\Delta|x'I')^* & (xI'|\Delta|x'I)\\ & E(I)\delta_{II'}\delta(x-x')-h^*(x,x')\delta_{II'}-(xI|\Gamma|x'I')^*\end{pmatrix}$$
$$=-\tau_1(xI|\mathcal{H}|x'I')^*\tau_1. \tag{2.32}$$

In the present theory, where there is no sharp Fermi surface, particles and holes use the same set of labels.

III. ZEROTH APPROXIMATION: THEORY OF NUCLEAR SHAPES

We turn to the problem of solving Eqs. (2.21) and (2.31) restricted by the various subsidiary and consistency conditions. We shall study only the simplest example of direct physical interest, that in which the ground-state band of the nucleus behaves like an axially symmetric rigid rotator. This problem is defined by choosing an excitation spectrum of the form

$$E(I)=(4\mathcal{J})^{-1}I(I+1)[1+(-)^I] \tag{3.1}$$

appropriate to an even-even nucleus.

We shall concentrate on the solution of Eq. (2.21). It is convenient for purposes of illustration to suppose that the spectrum (3.1) continues to arbitrarily large values of I. Our theory then describes a "quasiparticle" in interaction with a rotator, the interaction between the two being determined self-consistently. Its essential content is best illustrated by the change of variables defined by

$$\Theta_i(x\hat{n})=\sum_{IM}\Theta_i(xIM)Y_M{}^{I*}(\hat{n}),\qquad(3.2)$$

$$(x\hat{n}|\mathcal{H}|x'\hat{n}')=\sum_{IMI'M'}Y_M{}^{I*}(\hat{n})\times(xIM|\mathcal{H}|x'I'M')Y_{M'}{}^{I'}(\hat{n}'),\qquad(3.3)$$

where $Y_M{}^I(\hat{n})$ is a normalized spherical harmonic of the angles defining the unit vector $\hat{n}$. According to (3.1) the summations in (3.2), (3.3) are restricted to even I. This is most conveniently expressed by replacing the spherical harmonics by a function symmetrized under inversion

$$Y_M{}^I(\hat{n})\to\tfrac{1}{2}[Y_M{}^I(\hat{n})+Y_M{}^I(-\hat{n})]=\tfrac{1}{2}Y_M{}^I(\hat{n})[1+(-1)^I]\equiv[\hat{n}|IM],\qquad(3.4)$$

the square brackets denoting that the symmetrization has been carried out.

Under the symmetrized version of the transformation (3.2),

$$E(I)\to I^2/2\mathcal{I},\qquad(3.5)$$

the differential operator $\mathbf{I}$ now acting on the variables $\hat{n}=(\alpha,\beta)$ where α is the aximuthal, β the polar angle. In terms of these new variables, we notice that the components of the wave function $\Theta_i[x\hat{n}]$ retain an abstract definition, for example

$$\Psi_i[x\hat{n}]=\sum_{IM}\langle i|\psi(x)|IM\rangle[IM|\hat{n}]=\langle i|\psi(x)|\hat{n}].\qquad(3.6)$$

A general representation of this amplitude is obtained by remarking that the $|\hat{n}\rangle$ are a complete set of states localized in angle

$$[\hat{n}|\hat{n}']=\tfrac{1}{4}\{\langle\hat{n}|\hat{n}'\rangle+\langle\hat{n}|-\hat{n}'\rangle+\langle-\hat{n}|\hat{n}'\rangle+\langle-\hat{n}|-\hat{n}'\rangle\}=\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}+\hat{n}')],\qquad(3.7)$$

and that

$$|\hat{n}\rangle=U(R)|\hat{o}\rangle,\quad U(R)=\exp[-iJ_z\alpha]\times\exp[-iJ_y\beta]\exp[-iJ_z\gamma],\qquad(3.8)$$

$$U^{-1}(R)\psi(x)U(R)=\psi(Rx),\qquad(3.9)$$

where $\hat{o}$ defines the "intrinsic" coordinate system, the rotation R taking us from the laboratory system to this system. The transformation R is here defined by the set of Euler angles $R=R(\hat{n},\gamma)=R(\alpha,\beta,\gamma)$.

With $U(\pm\hat{n})\equiv U[R(\pm\hat{n},0)]$, and restricting ourselves henceforth to such transformations, since γ is arbitrary, a consequence of (3.8) is

$$U^{-1}[\pm\hat{n}]|\hat{n}]=|\hat{o}]=\sum_{IM}|IM\rangle Y_M{}^{I*}(\hat{o})\tfrac{1}{2}[1+(-1)^I].\qquad(3.10)$$

To apply these statements we suppose the comparison state $|i\rangle$ to be specified more closely as $|iJ-\mu\rangle$, where J, $-\mu$ are angular-momentum quantum numbers and i represents the remaining quantum numbers. With the help of (3.9) and (3.10), we may thus write

$$\begin{aligned}\Psi_{iJ\mu}[x,\hat{n}]&\equiv\langle iJ-\mu|\psi(x)|\hat{n}]\\&=\langle iJ-\mu|U(\hat{n})U^{-1}(\hat{n})\psi(x)U(\hat{n})U^{-1}(\hat{n})|\hat{n}]\\&=\textstyle\sum_K\langle iJ-\mu|U(\hat{n})|iJ-K\rangle\langle iJ-K|\psi(Rx)|\hat{o}]\\&=\textstyle\sum_K D_{-\mu-K}{}^{J*}(\hat{n})\langle iJ-K|\psi(Rx)|\hat{o}].\end{aligned}\qquad(3.11)$$

By means of the relation[8]

$$D_{-\mu-K}{}^{J*}(\hat{n})=(-1)^{K-\mu}D_{\mu K}{}^J(\hat{n}),\qquad(3.12)$$

and separating positive from negative K, we have instead

$$\Psi_{iJ\mu}[x,\hat{n}]=\sum_{K>0}(-)^{K-\mu}\{D_{\mu K}{}^J(\hat{n})\langle iJ-K|\psi(Rx)|\hat{o}]-D_{\mu-K}{}^J(\hat{n})\langle iJK|\psi(Rx)|\hat{o}]\}.\qquad(3.13)$$

Still another useful form of (3.13) follows from the utilization of the relation

$$\langle iJK|\psi(Rx)|\hat{o}]=-(-)^J\langle iJ-K|\psi(R_1x)|\hat{o}],\qquad(3.14)$$

where $R_1=R(-\hat{n})$; the proof of (3.14) requires (3.10) as well as the equation[8]

$$D_{\mu K}{}^J(-\hat{n})=(-1)^JD_{\mu-K}{}^J(\hat{n}).\qquad(3.15)$$

In place of (3.13) we thus have

$$\Psi_{iJ\mu}[x,\hat{n}]=\sum_{K>0}(-)^{K-\mu}\{D_{\mu K}{}^J(\hat{n})\langle iJ-K|\psi(Rx)|\hat{o}]+(-)^JD_{\mu-K}{}^J(\hat{n})\langle iJ-K|\psi(R_1x)|\hat{o}],\qquad(3.16)$$

or for the matrix function,

$$\Theta_{iJ\mu}[x,\hat{n}]=\sum_{K>0}(-)^{K-\mu}\{D_{\mu K}{}^J(\hat{n})\theta_{iJK}[Rx]+(-)^JD_{\mu-K}{}^J(\hat{n})\theta_{iJK}[R_1x]\}=\Theta_{iJ\mu}[x,-\hat{n}],\qquad(3.17)$$

as follows by noting (3.15). In (3.17) we have

$$\theta_{iJK}[Rx]=\langle iJ,-K|\begin{Bmatrix}\psi(Rx)\\\psi^\dagger(Rx)\end{Bmatrix}|\hat{o}].\qquad(3.18)$$

Equation (3.17) is now substituted into the transform of (2.21) and due notice is taken of the action of the operator $\mathbf{I}^2$,

$$\mathbf{I}^2=(\mathbf{J}-\mathbf{j})^2\to J(J+1)+j^2-2J_3j_3-(J_+j_-+J_-j_+),\qquad(3.19)$$

where $\mathbf{J}$ as a differential operator[9] acts on the function

[8] Many properties are conveniently summarized in the Appendix of M. A. Preston, *Physics of the Nucleus* (Addison-Wesley Publishing Company, Inc., New York, 1962). We employ, however, the definition of $D_{\mu K}{}^J$ used by Wigner and Edmonds (as defined by Preston).

[9] $\mathbf{J}$, for example, is a specialization of the customary differential operator $\mathbf{J}$ $(\alpha,\beta,\partial_\alpha,\partial_\beta,\partial_\gamma)$ in that $\partial_\gamma\to iK$.

$D_{\mu K}{}^J(\hat{n})$, while j acts on $Rx=x_R$, and we understand the components of $\mathbf{J}$ and $\mathbf{j}$ shown in (3.19) to be those in the intrinsic coordinate system. This means that we may set $j_3{}^2-2J_3j_3=-K^2$ when acting on each term in the sum (3.17). Furthermore, in accordance with the scheme of approximation discussed in Paper II, we drop the term $j_1{}^2+j_2{}^2$ since this leads to a small correction to the energies independent of the collective coordinates and of a small order of magnitude for which our method cannot be guaranteed to be self-consistent. Finally, we shall restrict our further considerations of this section to the limit in which we ignore the Coriolis coupling

$$\mathcal{H}_c\equiv(J_-j_++J_+j_-)/2\mathcal{I}\equiv J_{-i}j_i/2\mathcal{I} \qquad (3.20)$$

arising from the last term of (3.10). We shall then show that in this limit our equations possess self-consistent solutions of the form (defined only for positive K)

$$\Theta_{iJK\mu}[x\hat{n}]\cong 2^{-1/2}\{\theta_{iK}(Rx)(\hat{n}|J\mu K) + \theta_{iK}(R_1x)(-\hat{n}|J\mu K)\}, \qquad (3.21)$$

where, as indicated, the single-particle functions are *independent of* J and $(\hat{n}|J\mu K)$ is a suitable normalized version of $D_{\mu K}{}^J(\hat{n})$ defined below.

Before verifying this assertion it is necessary to investigate the phase relations which (3.14) implies for (3.21). To reach (3.21) we assume

$$\theta_{iJK}[Rx]\cong 2^{-1/2}(2J+1/4\pi)^{1/2}\eta(J,K)\theta_{iK}(Rx), \quad |\eta|=1. \qquad (3.22)$$

From (3.14) now follows

$$\begin{aligned}\theta_{iJ-K}[Rx]&\cong 2^{-1/2}(2J+1/4\pi)^{1/2}\eta(J,-K)\theta_{i-K}(Rx)\\ &=(-)(-)^J2^{-1/2}(2J+1/4\pi)^{1/2}\\ &\quad\times\eta(J,K)\theta_{iK}(R_1x). \end{aligned}\qquad (3.23)$$

With the choice

$$\eta(J,K)=i^{(JK/|K|)}, \qquad (3.24)$$

we therefore have the convenient relation

$$\theta_{i-K}(Rx)=\theta_{iK}(R_1x). \qquad (3.25)$$

It remains only to supply the definition

$$(\hat{n}|J\mu K)=(2J+1/4\pi)^{1/2}D_{\mu K}{}^J(\hat{n}) \qquad (3.26)$$

for a *single* term of (3.17) to assume the form (3.21). In the definition (3.26) we have dropped a phase factor $i^J(-)^{|K|-\mu}$ which is implied by the previous considerations. This corresponds to a unitary change of basis, which affects none of the physical results of this paper.

We next show that (3.21) constitutes an approximate solution of the self-consistent equations. To establish this assertion, we consider the density and pairing matrices, Eqs. (2.17), (2.18) associated with the ansatz (3.21). Thus, utilizing the completeness relation

$$\sum_{J\mu}(J\mu K|\hat{n})(\hat{n}'|J\mu K)=\delta(\hat{n}-\hat{n}') \qquad (3.27)$$

and the definitions

$$\begin{aligned}\rho(Rx,Rx')&=\tfrac{1}{2}\sum_{i,K>0}\{\psi_{iK}(Rx)\psi_{iK}{}^*(Rx')\\ &\quad+\psi_{iK}(R_1x)\psi_{iK}{}^*(R_1x')\}\\ &=\sum_{i,K}\psi_{iK}(Rx)\psi_{iK}{}^*(Rx'), \end{aligned}\qquad (3.28)$$

$$\begin{aligned}\sigma(Rx,Rx')&=\tfrac{1}{2}\sum_{i,K>0}\{\psi_{iK}(Rx)\phi_{iK}(Rx')\\ &\quad+\psi_{iK}(R_1x)\phi_{iK}(R_1x')\}\\ &=\sum_{i,K}\psi_{iK}(Rx)\phi_{iK}(Rx'), \end{aligned}\qquad (3.29)$$

the last equalities following from (3.25), we find ($\hat{n}_1=-\hat{n}$)

$$(x\hat{n}|\rho|x'\hat{n}')=\rho(Rx,Rx')\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}-\hat{n}_1{}')], \qquad (3.30)$$

$$(x\hat{n}|\sigma|x'\hat{n}')=\sigma(Rx,Rx')\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}-\hat{n}_1{}')]. \qquad (3.31)$$

From (2.11) and (2.12), we then find for the self-consistent potentials,

$$(x\hat{n}|\Gamma|x'\hat{n}')=\Gamma(Rx,Rx')\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}-\hat{n}_1{}')], \qquad (3.32)$$

$$(x\hat{n}|\Delta|x'\hat{n}')=\Delta(Rx,Rx')\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}-\hat{n}_1{}')], \qquad (3.33)$$

$$\Gamma(x,x')=\int V(xy;x'y')\rho(y',y), \qquad (3.34)$$

$$\Delta(x,x')=\frac{1}{2}\int V(xx';yy')\sigma(y,y'), \qquad (3.35)$$

where we have used the rotational invariance of the Hamiltonian. With the definitions

$$\mathcal{E}_{iK}\equiv\mathcal{E}_{iKJ}+[J(J+1)-K^2]/2\mathcal{I}, \qquad (3.36)$$

$$\mathcal{H}^{(0)}(x,x')=\begin{pmatrix}h(x,x')+\Gamma(x,x') & \Delta(x,x')\\ -\Delta^*(x,x') & -h^*(x,x')-\Gamma^*(x,x')\end{pmatrix}, \qquad (3.37)$$

Eq. (2.21) becomes in this approximation

$$\mathcal{E}_{iK}\Theta_{iKJ\mu}[x,\hat{n}]=\int\mathcal{H}^{(0)}(Rx,Rx')\Theta_{iKJ\mu}[x',\hat{n}]. \qquad (3.38)$$

We may finally obtain an equation for the intrinsic function $\theta_{iK}(x)$ by noting that (3.38) depends on but a single arbitrary direction in space which we now choose as our z axis. Thus we set $\hat{n}=\hat{o}$, $R=1$, $R_1=R(\pi,\pi,0)$.

Using standard properties of the representations of the rotation group,[8] we have

$$\Theta_{iKJ\mu}[x,\hat{\sigma}]=[(2J+1)/8\pi]^{1/2} \times\{\delta_{\mu K}\theta_{iK}(x)+(-1)^J\delta_{\mu,-K}\theta_{i,-K}(x)\}, \quad (3.39)$$

and thus finally obtain the equation

$$\mathcal{E}_{iK}\theta_{iK}(x)=\int \mathcal{H}^{(0)}(x,x')\theta_{iK}(x'). \quad (3.40)$$

Before discussing the significance of (3.40) let us obtain the remaining equations which specify this approximate theory: (a) Together with any set of solutions $\theta_{iK}(x)$ of (3.40), there exists another set $\tau_1\theta_{iK}^*(x)$ with eigenvalues $-\mathcal{E}_{iK}$, (τ_1 is the Pauli matrix). These are the "particle" solutions, which can be obtained directly from (3.40) or by applying the approximations of this section to (2.31). Since $\mathcal{H}^{(0)}$ is Hermitian, the solutions θ_{iK} and $\tau_1\theta_{iK}^*$ are orthogonal to one another. (b) The condition that the system contains an average of A particles, as expressed by Eq. (2.25), becomes

$$A=\int dx\,\rho(x,x). \quad (3.41)$$

(c) The sum rule or completeness condition (2.26) takes the matrix form

$$\mathcal{R}(x,x')+\mathcal{T}(x,x')=\delta(x-x')\mathbf{1}, \quad (3.42)$$

where

$$\mathcal{R}(x,x')=\sum_{iK}\theta_{iK}(x)\theta_{iK}^\dagger(x'), \quad (3.43)$$

$$\mathcal{T}(x,x')=\sum_{iK}[\tau_1\theta_{iK}^*(x)][\tau_1\theta_{iK}^*(x')]^\dagger. \quad (3.44)$$

It follows that

$$\mathcal{R}^2=\mathcal{R},\quad \mathcal{R}\mathcal{T}=\mathcal{T}\mathcal{R},\quad \mathcal{T}^2=\mathcal{T}. \quad (3.45)$$

We now consider the significance of the results obtained in this section. In Eq. (3.40) we have a self-consistent field problem of now conventional type, including the pairing effect. Exactly this equation has been proposed[1] and utilized[6] as the basis for a theory of nuclear shapes, previous derivations having been based on a generalized Bogoliubov-Valantin transformation or related methods. One is, in principle, directed to seek all possible self-consistent solutions of (3.40) subject to (3.34), (3.35), (3.41), and (3.42). One then calculates the ground-state energy from the density and pairing matrix thus obtained, utilizing for this purpose Eq. (2.23). If the lowest energy is achieved for a spherical solution then one's task is complete as far as this problem is concerned: The moment of inertia vanishes and there is no rotational spectrum. If one finds on the other hand that the energy minimum is achieved with a nonspherical solution, for example, by an axially symmetric solution, as we have explicitly assumed to be the case in this section, then to this point we have two important results: (i) We have derived in a fundamental way, i.e., based on an original Hamiltonian invariant under rotations, the existence of a self-consistent deformed well. (ii) In the same approximation, Eq. (3.36) informs us that if the even-even nucleus with which we start has a rotational spectrum, so do the neighboring odd nuclei, with effectively the same moment of inertia. (The correction to the moment of inertia due to the odd particle or hole requires the higher order theory of Sec. VI.)

The present approximation, however, contains no information about the value of the moment of inertia. (The energy is independent of I.) We remedy this defect starting in the next section by noting that the solution given here corresponds to the limit $\mathcal{I}\to\infty$. The next step is therefore to develop the solution in powers of $\mathcal{I}^{-1}$, as will be done for the remainder of this paper.

For the method of studying numerically the equations derived in this section we refer the reader to Ref. 1.

We append here a useful property of the solutions. We expand $\theta_{iK}(Rx)$ in eigenfunctions of the angular momentum,

$$\theta_{iK}(Rx)=\sum_j c_{iK}{}^j\theta_K{}^j(Rx) =\sum_{jm} c_{iK}{}^j\theta_m{}^j(x)D_{mK}{}^{j*}(\hat{n}). \quad (3.46)$$

But we also have from (3.15)

$$\theta_{iK}(R_1x)=\sum_{jm} c_{iK}{}^j\theta_m{}^j(x)(-)^{j+1}D_{m-K}{}^{j*}(\hat{n}). \quad (3.47)$$

Thus, from (3.25), (3.46), and (3.47), we find

$$C_{i-K}{}^j=(-)^{j+1}C_{iK}{}^j. \quad (3.48)$$

IV. FIRST-ORDER SOLUTION FOR AXIALLY SYMMETRIC NUCLEI

We imagine ourselves to be in the region of the Periodic Table where the equations of the previous section yield an axially symmetric self-consistent field. Our aim becomes to obtain a sufficiently improved solution to the fundamental equations (2.21), (2.31) and associated conditions as to permit calculation of the moment of inertia. We shall also be interested in studying the change in the single-particle energies, since these can be applied to the interpretation of the spectra of neighboring odd nuclei.

We suppose that we have in hand a complete set of solutions of Eq. (3.38) of the form of Eq. (3.21). In what follows we shall combine the pair of indices (iK) into a single index K, whose inclusive nature will be understood. The equation we propose to solve is

$$(\mathcal{E}_K+\delta\mathcal{E}_{KJ})(\Theta_{KJ\mu}{}^{(0)}+\delta\Theta_{KJ\mu}) =(\mathcal{H}^{(0)}+\mathcal{H}_c+\delta\mathcal{H})(\Theta_{KJ\mu}{}^{(0)}+\delta\Theta_{KJ\mu}), \quad (4.1)$$

the superscript zero referring to solutions proportional to (3.21) and the zero-order Hamiltonian (3.37), respectively. Whereas $\mathcal{H}_c$ is a fixed perturbation, $\delta\mathcal{H}$ arises from the functional dependence of the self-consistent potential on the solutions. The most general form of $\delta\Theta_{KJ\mu}$ other than a change in normalization is

$$\delta\Theta_{KJ\mu}[x,\hat{n}]=\sum_{L\neq K}\Theta_{LJ\mu}{}^{(0)}[x,\hat{n}]G_{LK}{}^{J}+\sum_L \Theta_{\bar{L}J\mu}{}^{(0)}[x,\hat{n}]F_{LK}{}^{J}, \quad (4.2)$$

where the function $\Theta_{\bar{L}J\mu}$ is obtained from $\Theta_{LJ\mu}$ by replacing in (3.18) θ_K by $\tau_1\theta_{-K}{}^*$. According to (3.42) it requires both sets of functions utilized in (4.2) to form a complete set. The omission of the term $L=K$ in the first sum is compensated by a change in normalization of $\Theta_{KJ\mu}$,

$$\Theta_{KJ\mu}{}^{(0)}\rightarrow A_K{}^J\Theta_{KJ\mu}(0). \quad (4.3)$$

From (4.1), (4.2), and (4.3), we obtain easily, using the orthogonality of different solutions of (3.30),

$$\delta\mathcal{E}_{KJ}=(\Theta_{KJ\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\Theta_{KJ\mu})+(A_K{}^J)^{-1}(\Theta_{KJ\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\delta\Theta_{KJ\mu}), \quad (4.4)$$

where, henceforth dropping the superscript (0), we have also utilized the fact that (Appendix A)

$$(\Theta_{KJ\mu},\Theta_{KJ\mu})=1, \quad (4.5)$$

and

$$(\mathcal{E}_K+\delta\mathcal{E}_{KJ}-\mathcal{E}_L)G_{LK}{}^J=(\Theta_{LJ\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\Theta_{KJ\mu})A_K{}^J+(\Theta_{LJ\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\delta\Theta_{KJ\mu}), \quad (4.6)$$

$$(\mathcal{E}_K+\delta\mathcal{E}_{KJ}+\mathcal{E}_L)F_{LK}{}^J=(\Theta_{\bar{L}J\mu}(\mathcal{H}_c+\delta\mathcal{H})\Theta_{KJ\mu})A_K{}^J+(\Theta_{\bar{L}J\mu}(\mathcal{H}_c+\delta\mathcal{H})\delta\Theta_{KJ\mu}). \quad (4.7)$$

Except for the nonlinearity buried in $\delta\mathcal{H}$ and the fact that there are constraints, we are, of course, simply doing perturbation theory.

In the sequel, it is of considerable aid to recognize that the matrix

$$[x\hat{n}|\,\delta\mathcal{H}\,|x'\hat{n}']=\delta\begin{pmatrix}[x\hat{n}|\Gamma|x'\hat{n}'] & [x\hat{n}|\Delta|x'\hat{n}']\\ -[x\hat{n}'|\Delta|x'\hat{n}]^* & -[x\hat{n}'|\Gamma|x'\hat{n}]^*\end{pmatrix} \quad (4.8)$$

is of the form

$$[x\hat{n}|\,\delta\mathcal{H}\,|x'\hat{n}']=\int \mathbf{V}(xy;x'y')\delta\sum_{KJ\mu}\Theta_{KJ\mu}[y'\hat{n}]\Theta_{KJ\mu}{}^\dagger[y\hat{n}'], \quad (4.9)$$

where

$$\mathbf{V}(12;34)=\begin{matrix}11\\12\\21\\22\end{matrix}\begin{bmatrix}V(12;34) & 0 & 0 & 0\\ 0 & 0 & -\frac{1}{2}V(13;24) & 0\\ 0 & -\frac{1}{2}V^*(13;24) & 0 & 0\\ 0 & 0 & 0 & V^*(12;34)\end{bmatrix}. \quad (4.10)$$

Thus by the integration symbol in (4.9) we mean not only the integral with respect to y and y', but also the trace over the two-valued associated discrete matrix indices. The equivalence of (4.8) and (4.9) follows by straightforward identification of terms and the use of the completeness relation (2.26).

Turning now to the solution of (4.4), (4.6), and (4.7), we begin by showing that the first-order contribution of $\mathcal{H}_c$ in (4.4) is the now familiar contribution to the odd-particle energy involving the decoupling parameter. The contribution coming from two equal cross terms can be put into the form

$$=(2\mathcal{I})^{-1}\int d\hat{n}\langle J\mu K|\hat{n}\rangle J_{-i}\langle\hat{n}|J\mu-K\rangle(-1)^J\times\sum_j|c_{jK}|^2(-1)^j\int\theta_{jK}(x)j_i\theta_{j-K}(x) \quad (4.11)$$

by simply doubling one of the contributions and by utilizing Eqs. (3.15) and (3.48). The further evaluation of (4.11) is straightforward (see Appendix A) and yields

$$=-(2\mathcal{I})^{-1}a(-)^{J+1/2}(J+\tfrac{1}{2})\delta_{K,1/2}, \quad (4.12)$$

where

$$a=-\sum_j(j+\tfrac{1}{2})(-1)^{j+\frac{1}{2}}|c_{j\frac{1}{2}}|^2 \quad (4.13)$$

is the well-known decoupling parameter. In contrast to the usual theory, there will be an additional first-order contribution, to be derived below.

We next study the solutions of Eqs. (4.6) and (4.7) to first order. In this approximation these simplify to

$$(\mathcal{E}_K-\mathcal{E}_L)G_{LK}{}^J=(\Theta_{LJ\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\Theta_{KJ\mu}), \quad (4.14)$$

$$(\mathcal{E}_K+\mathcal{E}_L)F_{LK}{}^J=(\Theta_{\bar{L}K\mu},\,(\mathcal{H}_c+\delta\mathcal{H})\Theta_{KJ\mu}). \quad (4.15)$$

From (4.17), it follows that

$$G_{LK}{}^J+G_{KL}{}^{J*}=0, \quad (4.16)$$

indicating that the $G_{LK}{}^J$ define an infinitesmal unitary transformation. It follows from (4.16) that the first-order contribution to $\delta\mathcal{H}$ arises only from the coefficients $F_{LK}{}^J$.

The form of solution of (4.14) and (4.15) is suggested by the forms of the inhomogeneous terms, the matrix elements of $\mathcal{H}_c$. By the means employed in reaching (4.12), we find, for example,

$$(\Theta_{\bar{L}J\mu},\mathcal{H}_c\Theta_{KJ\mu}) = (2\mathcal{I})^{-1}(J\mu L|J_{-i}|J\mu K)(\bar{L}|j_i|K), \quad (4.17)$$

where

$$(\bar{L}|j_i|K)\equiv\int dx(\tau_1\theta_{-L}(x)^*)^\dagger j_i\theta_K(x) \equiv\int dx\theta_{\bar{L}}^\dagger j_i\theta_K(x). \quad (4.18)$$

Equation (4.17) is demonstrated briefly in Appendix A.

The form of (4.17) suggests the solutions

$$F_{LK}{}^J=(2\mathcal{I})^{-1}(J\mu L|J_{-i}|J\mu K)(\bar{L}|f_i|K), \quad (4.19)$$

$$G_{LK}{}^J=(2\mathcal{I})^{-1}(J\mu L|J_{-i}|J\mu K)(L|g_i|K). \quad (4.20)$$

The manipulations designed to demonstrate the correctness of (4.19) and (4.20) and to derive from (4.14) and (4.15) equations for the coefficients $(\bar{L}|f_i|K)$ and $(L|g_i|K)$ are outlined in Appendix A. The resulting equations are

$$(\mathcal{E}_K+\mathcal{E}_L)(\bar{L}|f_i|K)=(\bar{L}|j_i|K)+\sum_{K'\bar{L}'}\{(\bar{L}K'|\mathbf{V}|K\bar{L}')(\bar{L}'|f_i|K')+(\bar{L}\bar{L}'|\mathbf{V}|KK')(\bar{L}'|f_{-i}|K')^*\}, \quad (4.21)$$

$$(\mathcal{E}_K-\mathcal{E}_L)(L|g_i|K)=(L|j_i|K)+\sum_{K'\bar{L}'}\{(LK'|\mathbf{V}|K\bar{L}')(\bar{L}'|f_i|K')+(\bar{L}\bar{L}'|\mathbf{V}|KK')(\bar{L}'|f_{-i}|K')^*\}, \quad (4.22)$$

with, for example,

$$(\bar{L}K'|\mathbf{V}|K\bar{L}')=\int\theta_{\bar{L}}^\dagger(x)\theta_{K'}^\dagger(y)\mathbf{V}(xy;x'y')\theta_K(x')\theta_{\bar{L}'}(y'). \quad (4.23)$$

With respect to (4.21) in particular we notice that if we adjoin to it its complex conjugate, the two equations may be written in the matrix form

$$M\mathfrak{F}_i=\mathcal{G}_i, \quad (4.24)$$

where

$$(L|\mathfrak{F}_i|K)=\begin{pmatrix}(\bar{L}|f_i|K)\\(\bar{L}|f_{-i}|K)^*\end{pmatrix}, \quad (4.25)$$

with a similar expression for $(\bar{L}|\mathcal{G}_i|K)$, and

$$(\bar{L}K|M|\bar{L}'K')=\begin{pmatrix}-(\mathcal{E}_K+\mathcal{E}_L)\delta_{LL'}\delta_{KK'}+(\bar{L}K'|\mathbf{V}|K\bar{L}') & (\bar{L}\bar{L}'|\mathbf{V}|KK')\\(KK'|\mathbf{V}|\bar{L}\bar{L}') & -(\mathcal{E}_K+\mathcal{E}_L)\delta_{KK'}\delta_{LL'}+(K\bar{L}'|\mathbf{V}|\bar{L}K')\end{pmatrix}. \quad (4.26)$$

The matrix M is the same one that plays a role in the stability theory of Eq. (3.32), and in the random phase approximation with pairing.

The solutions of (4.21) enable us to go back to obtain from (4.4) the full expression for the first-order change in the single-particle (or rather hole) energy. To (4.12) we must add the contribution of the second term of (4.4), i.e., the first-order diagonal effect of $\delta\mathcal{H}$. The details are again relegated to Appendix A. The result is

$$\delta\mathcal{E}_{KJ}{}^{(1)}=-\delta_{K,1/2}(2\mathcal{I})^{-1}(-)^{J+1/2}(J+\tfrac{1}{2})[a+\delta a] \quad (4.27)$$

where a is given by Eq. (4.13) and $[(R\tfrac{1}{2})\equiv\theta_{1/2}(Rx)$, etc.],

$$\delta a=-i\sum_{\text{all }K'L'}\{([R\tfrac{1}{2}]K'|V|\tfrac{1}{2}\bar{L}')(\bar{L}|f_-|K') -([R\tfrac{1}{2}]K'|V|\tfrac{1}{2}L')^*(\bar{L}'|f_-|K')^*\}. \quad (4.28)$$

From a phenomenological point of view $a+\delta a$ may be viewed as the effective decoupling parameter. From a fundamental point of view, however, this represents a definite change compared to the usual unified model.

We shall return in Sec. VI to the problem of obtaining solutions of (4.4)–(4.6) to higher order. As we know from the study of the corresponding problem in two dimensions, however, and as we shall see again, the solutions of (4.21) together with the renormalization coefficient A_{KJ} of the zero-order solution—to be derived imminently—suffice to determine the moment of inertia $\mathcal{I}$ of the even nucleus with which we started. This calculation will be carried out in the next section. For the remainder of this section we shall obtain to first order the consequences of the remaining conditions of the theory.

In the present case we do not have to study the equation for the "particle" excitation, Eq. (2.31) separately. The solution of (2.31) to first order is simply $\delta\tau_1\Theta_{KJ\mu}{}^*\times[x,\hat{n}]=\tau_1(\delta\Theta_{KJ\mu}[x,\hat{n}])^*$ and is therefore determined by the same coefficients $G_{LK}{}^J$ and $F_{LK}{}^J$, first appearing in Eq. (4.2). Concerning Eq. (2.25), the condition for the average number of particles, there is no change to first order from its expression by Eq. (3.41). There remains to be determined only the consequences of the completeness condition or sum rule (T means transposed):

$$\sum_{KJ\mu}\{\Theta_{KJ\mu}[x,\hat{n}]\Theta_{KJ\mu}^{\dagger}[x',\hat{n}'] +\tau_1\Theta_{KJ\mu}^*[x,\hat{n}']\tau_1\Theta_{KJ\mu}^T[x',\hat{n}]\} =\tfrac{1}{2}\delta(x-x')[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}+\hat{n}')]. \quad (4.29)$$

The consequences of (4.29) to second order in $\mathcal{I}^{-1}$ are deduced in Appendix B. For immediate purposes, i.e., for the calculation of the next section we need the following results: In first order we find

$$\langle K|g_i|L\rangle=-\langle L|g_{-i}|K\rangle^*, \quad (4.30)$$

$$\langle \bar{L}|f_i|K\rangle=\langle\bar{K}|f_{-i}|L\rangle. \quad (4.31)$$

Of these conditions, we already know that (4.30) is compatible with the equations of motion, since it is in fact equivalent to Eq. (4.16). To establish the compatibility of (4.31) with (4.21) requires the recognition that

$$\langle\bar{L}|j_i|K\rangle=\langle\bar{K}|j_{-i}|L\rangle, \quad (4.32)$$

and that a number of equalities obtain among the matrix elements of the potential-energy matrix V. We require, for instance, that

$$\begin{aligned}(\bar{K}L'|\mathbf{V}|L\bar{K}')&=(\bar{L}K'|\mathbf{V}|K\bar{L}'),\\ (\bar{L}\bar{L}'|\mathbf{V}|KK')&=(\bar{K}\bar{K}'|\mathbf{V}|LL'),\end{aligned} \quad (4.33)$$

which, in turn, follow from the identity

$$(\tau_1)_1\mathbf{V}(\tau_1)_2=(\tau_1)_2\mathbf{V}^*(\tau_1)_1. \quad (4.34)$$

We also quote here some second-order "diagonal" results. We obtain the normalization condition

$$\begin{aligned}|A_K{}^J|^2&=1-\sum_L\{|F_{KL}{}^J|^2+|G_{KL}{}^J|^2\}\\ &=1-(2\mathcal{I})^2[J(J+1)-K^2]\\ &\quad\times\sum_{Li}\{|(\bar{K}|f_i|L)|^2+|(K|g_i|L)|^2\}\\ &\quad-(2\mathcal{I})^{-2}K\sum_L\{|(\bar{K}|f_+|L)|^2-|(\bar{K}|f_-|L)|^2\\ &\quad+|(K|g_+|L)|^2-|(K|g_-|L)|^2\},\end{aligned} \quad (4.35)$$

where we have utilized (4.19) and (4.20).

V. CALCULATION OF THE MOMENT OF INERTIA

In this section we utilize the results of the previous sections for the evaluation of $\langle I|H|I\rangle$, Eq. (2.23). It is convenient to utilize an alternative version of this expression, namely,

$$\langle I|H|I\rangle=\int dxdx'\sum_{I'}[\tfrac{1}{2}(xI|(\eta+\lambda+\tfrac{1}{2}\gamma)|x'I')(x'I'|\mathcal{R}|xI)]+\frac{1}{2}\int dx\,h(x,x)+\frac{1}{4}\int dxdy\,V(xy;xy)$$
$$-\frac{1}{4}\int dxdx'\sum_{I'}\{(xI|\Delta|x'I')^*(x'I|\sigma|xI')-(xI'|\Delta|x'I)^*(x'I'|\sigma|xI)\}. \quad (5.1)$$

The new quantities in (5.1) are

$$(xI|\eta|x'I')=\delta_{II'}\begin{pmatrix}h(x,x') & 0\\ 0 & -h^*(x,x')\end{pmatrix}, \quad (5.2)$$

$$(xI|\lambda|x'I')=\delta_{II'}\begin{bmatrix}0 & 0\\ 0 & -\int dy\,V^*(xy;x'y)\end{bmatrix}, \quad (5.3)$$

and

$$(xI|\gamma|x'I')=\begin{pmatrix}(xI|\Gamma|x'I') & (xI|\Delta|x'I')\\ -(xI'|\Delta|x'I)^* & (xI|\Lambda|x'I')\end{pmatrix}=\int V(xy;x'y')(y'I|\mathcal{R}|yI'), \quad (5.4)$$

where

$$(xI|\Lambda|x'I')=\int dydy'\,V^*(xy;x'y')(y'I|\tau|yI'), \quad (5.5)$$

and

$$(y'I|\tau|yI')=\sum_{KJ\mu}\Phi_{KJ\mu}^*(y'I)\Phi_{KJ\mu}(yI'). \quad (5.6)$$

In fact

$$(xI|\mathcal{R}|x'I')=\sum_{KJ\mu}\Theta_{KJ\mu}(xI)\Theta_{KJ\mu}^{\dagger}(x'I')=\begin{pmatrix}(xI|\rho|x'I') & (xI|\sigma|x'I')\\ -(xI'|\sigma|x'I)^* & (xI|\tau|x'I')\end{pmatrix}. \quad (5.7)$$

In terms of the quantities defined in (5.2)–(5.4), the equation of motion (2.21) may be written

$$\int(xI|(\eta+\lambda+\gamma)|x'I')\Theta_{KJ\mu}(x'I')=[\mathcal{E}_{KJ}+E(I)]\Theta_{KJ\mu}(xI). \quad (5.8)$$

The advantage of the form (5.1) is that the first term is as simple to treat as in the absence of pairing, the second and third terms are, of course, constants, and the last term, as we now argue, can be dropped. We are interested in that portion of it proportional to $I(I+1)$: The coefficient must be zero since the term itself vanishes upon summation over I. Our assertion can, of course, be verified by direct calculation. It can also be verified that this term does not destroy the self-consistency.

We therefore write

$$\langle I|H|I\rangle=\int d\hat{n}d\hat{n}'[I|\hat{n}]\langle\hat{n}|H|\hat{n}'\rangle[\hat{n}'|I], \quad (5.9)$$

where

$$\begin{aligned}\langle\hat{n}|H|\hat{n}'\rangle=&\operatorname{tr}\tfrac{1}{2}(\eta+\lambda)(\hat{n}'|\mathcal{R}|\hat{n})\\&+\tfrac{1}{4}\operatorname{tr}_{12}\mathbf{V}(\hat{n}'|\mathcal{R}|\hat{n}'')(\hat{n}''|\mathcal{R}|\hat{n})\\&+\delta(\hat{n}-\hat{n}')[\tfrac{1}{2}\operatorname{tr}h+\tfrac{1}{4}\operatorname{tr}_{12}V]. \quad (5.10)\end{aligned}$$

To obtain $\mathcal{R}$ to the required accuracy it suffices to write

$$\begin{aligned}\Theta_{KJ\mu}[x,\hat{n}]=&\{1-(2\mathcal{I})^{-2}\tfrac{1}{2}[J(J+1)-K^2]\\&\times\textstyle\sum_A|(A|c_i|K)|^2\}\Theta_{KJ\mu}{}^{(0)}[x,\hat{n}]\\&+\sum_{A\neq K,\bar{K}}\Theta_{AJ\mu}{}^{(0)}[x,\hat{n}](2\mathcal{I})^{-1}\\&\times(A|c_i|K)(J\mu A|J_{-i}|J\mu K). \quad (5.11)\end{aligned}$$

Here we have introduced a concise notation as follows:

$$(A|c_i|K)=(\bar{A}|f_i|K),$$

or

$$(A|c_i|K)=(A|g_i|K), \quad (5.12)$$

according as $\Theta_{AJ\mu}{}^{(0)}$ is a particle or a hole solution. The form (5.11) with (5.12) which follows from (4.2), (4.3), (4.19), (4.20), (4.20), and (4.35) contains only the normalization correction to second order. As for the latter, we have dropped a piece which does not contribute to the present calculation. Other second-order terms (such as computed in the next section), proportional to $\Theta_{AJ\mu}{}^{(0)}$, $A\neq K$, also do not contribute, as will be made evident below. We notice in connection with (5.12) that (4.21) and (4.22) and their complex conjugates may be written in a combined matrix form

$$\mathfrak{M}\mathcal{C}=\mathcal{J} \quad (5.13)$$

with suitably enlarged definitions of $\mathfrak{M}$ and $\mathcal{J}$.

Utilizing now the solution (5.11), we substitute in (5.9) and (5.10) the sum

$$\mathcal{R}=\mathcal{R}^{(0)}+\mathcal{R}^{(1)}+\mathcal{R}^{(20)}+\mathcal{R}^{(21)}, \quad (5.14)$$

where

$$(x\hat{n}|\mathcal{R}^{(0)}|x'\hat{n}')=\tfrac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}+\hat{n}')]\textstyle\sum_K\theta_K(Rx)\theta_K{}^\dagger(Rx'), \quad (5.15)$$

$$(x\hat{n}|\mathcal{R}^{(1)}|x'\hat{n}')=\sum_{L,K>0,J,\mu}\{\Theta_{\bar{L}J\mu}[x\hat{n}]\Theta_{KJ\mu}{}^\dagger[x'\hat{n}']F_{LK}{}^J+\Theta_{KJ\mu}[x,\hat{n}]\Theta_{\bar{L}J\mu}{}^\dagger[x',\hat{n}']F_{LK}{}^{J*}\}, \quad (5.16)$$

$$(x\hat{n}|\mathcal{R}^{(20)}|x'\hat{n}')=\sum_{A,K>0,J\mu}(-)(2\mathcal{I})^{-2}[J(J+1)-K^2]\Theta_{KJ\mu}{}^{(0)}[x,\hat{n}]\Theta_{KJ\mu}{}^\dagger[x',\hat{n}']|(A|c_i|K)|^2, \quad (5.17)$$

$$(x,\hat{n}|\mathcal{R}^{(21)}|x',\hat{n}')=\sum_{K,A,A'>0,J,\mu}\Theta_{AJ\mu}[x,\hat{n}]\Theta_{A'J\mu}{}^\dagger[x',\hat{n}']C_{AK}{}^JC_{A'K}{}^{J*}. \quad (5.18)$$

In (5.18) $C_{AK}{}^J=F_{LK}{}^J$ or $G_{LK}{}^J$ according as $A=\bar{L}$, $A=L$, respectively. According to (5.16) only the $F_{LK}{}^J$ occur in $\mathcal{R}^{(1)}$.

We now utilize (5.15)–(5.18) for the evaluation of (5.9). The zero-order energy, independent of the state of rotation, is

$$W_0=\int[h(x,x')+\tfrac{1}{2}\Gamma(x,x')]\rho(x',x)+\frac{1}{2}\int\Delta(x,x')\sigma^\dagger(x'x)=\operatorname{tr}[(h+\tfrac{1}{2}\Gamma)\rho+\tfrac{1}{2}\Delta\sigma^\dagger], \quad (5.19)$$

the usual expression associated with the theory of the self-consistent field with pairing. The first-order contribution, from $\mathcal{R}^{(1)}$,

$$(2\mathcal{I})^{-1}\langle IM|J_{-i}|IM\rangle\sum_{K,A>0}\mathcal{E}_K\delta_{KA}[(A|c_i|K)+(A|c_{-i}|K)^*]=0 \quad (5.20)$$

thus vanishes doubly, both because of the matrix element in front and because of an orthogonality integral which yields the factor δ_{KA}. For the latter reason also the second-order terms omitted from the solution (5.11) do not contribute to the moment of inertia calculation.

For the physically interesting second-order terms, we find first as the contribution from $\mathcal{R}^{(20)}$ and $\mathcal{R}^{(21)}$, Eqs. (5.17) and (5.18),

$$-(2\mathcal{I})^{-2}I(I+1)\sum_{K,A>0}(\mathcal{E}_K-\mathcal{E}_A)|(A|c_i|K)|^2=-(2\mathcal{I})^{-2}I(I+1)\sum_{K,L>0}(\mathcal{E}_K+\mathcal{E}_L)|(A|f_i|K)|^2, \quad (5.21)$$

the final result following from (4.30) and because $\mathcal{E}_{\bar{L}}=-\mathcal{E}_L$. There is finally the action of Eq. (5.16) in the second term of (5.10). Here we find after some calculation of the type exemplified in Appendix A, the contribution

$$(2\mathcal{I})^{-2}\tfrac{1}{2}I(I+1)\sum_{KL>0}\sum_{K'L'}\{(\bar{L}|f_{-i}|K)(\bar{L}'|f_i|K')(KK'|\mathbf{V}|\bar{L}\bar{L}')+(\bar{L}|f_i|K)^*(\bar{L}'|f_i|K')(\bar{L}K'|\mathbf{V}|K\bar{L}')$$
$$+(\bar{L}|f_{-i}|K)(\bar{L}'|f_{-i}|K')^*(K\bar{L}'|\mathbf{V}|\bar{L}K')+(\bar{L}|f_i|K)^*(\bar{L}'|f_{-i}|K')^*(\bar{L}\bar{L}'|\mathbf{V}|KK')\}. \quad (5.22)$$

For the sum of (5.21) and (5.22), we find

$$E(I)=\tfrac{1}{2}(2\mathcal{I})^{-1}I(I+1)\sum_{KL>0}\sum_{K'L'}(L|\mathfrak{F}|K)^\dagger(LK|M|L'K')(L'|\mathfrak{F}|K'). \quad (5.23)$$

Thus, utilizing Eq. (5.13), we find

$$\mathcal{I}=\frac{1}{4}\sum_{KL>0}(L|\mathfrak{F}_i|K)^\dagger(L|\mathcal{J}_i|K)$$
$$=\sum_{K,L>0}(L|\mathfrak{F}_x|K)^\dagger(L|\mathcal{J}_x|K), \quad (5.24)$$

where x refers to *some* component orthogonal to the axis of symmetry. This is the self-consistent cranking result derived several times previously.[10] If we ignore the self-consistency aspect, we obtain the cranking-model formula with pairing,

$$\mathcal{I}\cong-\sum_{K,L>0}\frac{|(L|\mathcal{J}_x|K)|^2}{\mathcal{E}_K+\mathcal{E}_L}. \quad (5.25)$$

[The positive value of (5.25) is not in doubt since $\mathcal{E}_K$ and $\mathcal{E}_L$ as hole energies are negative.] Equation (5.25) is known to yield good agreement with experiment.[11]

Before leaving this subject, we wish to emphasize once again that the derivation of this section is valid only under the assumption that we can ignore terms of order $\langle j\rangle/\mathcal{I}$, relative to those of order $J/\mathcal{I}$, where $\langle j\rangle$ is an average of the component of angular momentum of a single particle normal to the figure axis, and J is a similar component of the collective angular momentum. This assumption is more plausible if rephrased to assert that we can lend credence to small terms in the energy if and only if they have a characteristic dependence on the collective coordinates.

VI. SECOND-ORDER SOLUTION: SELF-CONSISTENT SINGLE-PARTICLE ENERGIES

We return to the job begun in Sec. IV, and carry the solution of Eqs. (4.6) and (4.7) to second order. According to Eq. (4.4), this is necessary to obtain the single-particle energies to second order. From (4.6) and (4.7), the equations to be solved are

$$(\mathcal{E}_K-\mathcal{E}_A)C_{AK}{}^{J(2)}-(\Theta_{AJ\mu}\delta\mathcal{H}^{(22)}\Theta_{KJ\mu})$$
$$=-\delta\mathcal{E}_{KJ}{}^{(1)}C_{AK}{}^{J(1)}+(\Theta_{AJ\mu},\mathcal{H}_c\delta\Theta_{KJ\mu}{}^{(1)})$$
$$=-\delta\mathcal{E}_{KJ}{}^{(1)}C_{AK}{}^{J(1)}+(\Theta_{AJ\mu},\mathcal{H}_c\delta\Theta_{KJ\mu}{}^{(1)})$$
$$+(\Theta_{AJ\mu},\delta\mathcal{H}^{(1)}\delta\Theta_{KJ\mu}{}^{(1)})+(\Theta_{AJ\mu},\delta\mathcal{H}^{(21)}\Theta_{KJ\mu}), \quad (6.1)$$

where we have adopted the concise notation of the previous section, with

$$C_{LK}{}^J\equiv G_{LK}{}^J,$$
$$C_{\bar{L}K}{}^J\equiv F_{LK}{}^J, \quad (6.2)$$

and $\mathcal{E}_{\bar{L}}=-\mathcal{E}_L$. Here $\delta\mathcal{H}^{(21)}$ signifies the second-order change in the self-consistent single-particle Hamiltonian arising from the first-order coefficients, $\delta\mathcal{H}^{(22)}$ the corresponding change depending on the second-order coefficients. Thus, as written, the entire right-hand side of (6.1) represents the driving term, which we proceed to evaluate.

Under the assumption $A\neq|\tfrac{1}{2}|$, we obtain, utilizing the definition

$$C_{AK}{}^{J(1)}=(2\mathcal{I})^{-1}(J\mu A|J_{-i}|J\mu K)(A|c_i|K), \quad (6.3)$$

and precisely the same techniques of evaluation as in Sec. IV and Appendix A,

$$(\Theta_{AJ\mu},\mathcal{H}_c\delta\Theta_{KJ\mu}{}^{(1)})=(2\mathcal{I})^{-2}(J\mu A|J_{-i}J_{-j}|J\mu K)\sum_{A'\neq K,A}(A|j_i|A')(A'|c_j|K), \quad (6.4)$$

$$(\Theta_{AJ\mu},\delta\mathcal{H}^{(1)}\delta\Theta_{KJ\mu}{}^{(1)})=(2\mathcal{I})^{-2}(J\mu A|J_{-i}J_{-j}|J\mu K)\sum_{A'\neq K,A}(A|k_i|A')(A'|c_j|K), \quad (6.5)$$

where

$$(A|k_j|A')=\sum_{K''L''}\{(AK''|\mathbf{V}|A'\bar{L}'')(\bar{L}''|f_j|K'')+(A\bar{L}''|\mathbf{V}|A'K'')(\bar{L}''|f_{-j}|K'')^*\}, \quad (6.6)$$

and

$$(\Theta_{AJ\mu},\delta\mathcal{H}^{(21)}\Theta_{KJ\mu})=(2\mathcal{I})^{-2}(J\mu A|J_{-i}J_{-j}|J\mu K)\{\sum_{K'A',A''}(AA''|\mathbf{V}|KA')(A''|c_{-j}|K')^*(A'|c_i|K')$$
$$-\delta_{-j,i}\textstyle\sum_{K'}(\bar{K}_1K'|\mathbf{V}|KK')\delta_{A,\bar{K}_1}\sum_L[|(\bar{K}'|f_i|L)|^2+|(K'|g_i|L)|^2]\}, \quad (6.7)$$

[10] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **37**, 249 (1959) [English transl.: Soviet Phys.—JETP **10**, 176 (1960)]; S. T. Belyaev, Zh. Eksperim. i Teor. Fiz. **40**, 672 (1961) [English transl.: Soviet Phys.—JETP **13**, 470 (1961)]; D. J. Thouless, Nucl. Phys. **21**, 225 (1960); **22**, 78 (1961); R. E. Prange, *ibid.* **22**, 283 (1961); A. Katz and J. F. Blatt, *ibid.* **23**, 612 (1961); D. J. Thouless and J. Valatin, *ibid.* **31**, 211 (1962); R. E. Peierls and D. J. Thouless, *ibid.* **38**, 154 (1962).

[11] For numerical evaluation see J. Griffin and M. Rich, Phys. Rev. **118**, 850 (1960); S. G. Nilsson and O. Prior, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **32**, No. 16 (1960).

where K_1 is any energy level having $j_3=K$, and therefore including, but not exclusively, the level K. We shall return below to the case $A=|\frac{1}{2}|$.

With the assumption that neither A nor $K=|\frac{1}{2}|$, and in view of (6.4) to (6.7), Eq. (6.1) is satisfied by the assumption

$$C_{AK}^{J(2)}=(2\mathcal{J})^{-2}(J\mu A|J_{-i}J_{-j}|J\mu K)[(A|c_{ij}|K)+\delta_{-j,i}\delta_{A,\bar{K}_1}(\bar{K}_1|d_i|K)], \quad (6.8)$$

and we then find for $(A|c_{ij}|K)$, $(\bar{K}_1|d_i|K)$, the equations

$$(\mathcal{E}_K-\mathcal{E}_A)(A|c_{ij}|K)-\sum_{K'A'}\{(AK'|\mathbf{V}|KA')(A'|c_{ij}|K')+(AA'|\mathbf{V}|KK')(A'|c_{-j-i}|K')^*\}$$
$$=\sum_{A'\neq K,A}(A|(j_i+k_i)|A')(A'|c_j|K)+(AA''|\mathbf{V}|KA')(A''|c_{-j}^{(1)}|K')^*(A'|c_i^{(1)}|K'), \quad (6.9)$$

and

$$(\mathcal{E}_K+\mathcal{E}_{K_1})(\bar{K}_1|d_i|K)-\sum_{K',K_1'}\{(\bar{K}_1K'|\mathbf{V}|K\bar{K}_1')(\bar{K}_1'|d_i|K')+\sum_{K'K_1'}(\bar{K}_1\bar{K}_1'|\mathbf{V}|KK')(\bar{K}_1'|d_i|K')\}$$
$$=-\sum_{LK'}(\bar{K}_1K'|\mathbf{V}|KK')[|(\bar{K}'|f_i|L)|^2+|(K'|g_i|L)|^2]. \quad (6.10)$$

In the event that either $|K|=\frac{1}{2}$ or $|A|=\frac{1}{2}$, we require supplementary considerations. In the former case, the first term on the right-hand side of (6.1) must be taken into account whereas in the latter case there are additional contributions to (6.4) and (6.5). These come about as follows: In the decomposition

$$\delta\Theta_{KJ\mu}^{(1)}=\sum_{A'\neq A}\Theta_{A'J\mu}C_{A'K}^{J(1)}+\Theta_{AJ\mu}C_{AK}^{J(1)}, \quad (6.11)$$

the effect of the second term has so far been omitted. After some calculation the result, not surprisingly, is to alter the first term of the right-hand side of (6.1) to

$$-[\delta\mathcal{E}_{KJ}^{(1)}-\delta\mathcal{E}_{AJ}^{(1)}]C_{AK}^{J(1)}. \quad (6.12)$$

During the course of the demonstration it is important to recognize such relationships as

$$(\bar{K}|j_i|-\bar{K})=-(K|j_i|-K), \quad (6.13)$$

$$(\bar{K}|j_i|-K)=0. \quad (6.14)$$

The form (6.12) suggests the addition to (6.8) of the term

$$\delta C_{AK}^{J(2)}=(2\mathcal{J})^{-1}[\delta\mathcal{E}_{KJ}^{(1)}-\delta\mathcal{E}_{AJ}^{(1)}]\times(J\mu A|J_{-i}|J\mu K)(A|c_i^{(2)}|K). \quad (6.15)$$

The equation of motion (6.1) will continue to be satisfied if for $|K|$ or $|A|=\frac{1}{2}$, in addition to Eqs. (6.9), (6.10) the equation

$$(\mathcal{E}_K-\mathcal{E}_A)(A|c_i^{(2)}|K)=-(A|c_i^{(1)}|K)-\sum_{K'A'}\{(A(RK')|\mathbf{V}|(RK)A')(A'|c_i^{(2)}|K')$$
$$+(A(RA')|\mathbf{V}|(RK)K')(A'|c_i^{(2)}|K')^*\}[b_i(K')/b_i(K)] \quad (6.16)$$

is true. The derivation of (6.16) is only marginally different from that of the previous equations of motion of this section, depending, for instance, on the recognition that we can write [cf. Eq. (4.27)]

$$\delta\mathcal{E}_{KJ}^{(1)}=(-)^J(J\mu K|J_{-j}|J\mu-K)b_j(K), \quad (6.17)$$

where

$$b_{-i}(A)=b_i(A)=\mp(-)^{1/2}(2\mathcal{J})^{-1}(a_A+\delta a_A), \quad (6.18)$$

the minus (plus) sign pertaining to the case that A is a hole (particle) state. The subscript "A" on a_A is meant to describe a particular $j_3=\frac{1}{2}$ state. In consequence of (6.17), the first term of (6.15) is of the form

$$\delta C_{AK}^{J(2)}\sim(-)^J(J\mu A|J_{-i}J_{-j}|J\mu-K)\times(A|c_i^{(2)}|K)b_j(K). \quad (6.19)$$

With the help of Eq. (3.15) at appropriate junctures, the derivation of (6.15) proceeds in close analogy with that of previous equations for the first- and second-order coefficients. Let us note that the ratios $b_i(K')/b_i(K)$ appearing in (6.16) may or may not be 1 depending upon whether or not K' refers to the same $j_3=\frac{1}{2}$ level as does K [analogous to the need for an extension of notation in Eqs. (6.7), (6.8), and (6.10)]. An essential proviso must be entered with respect to (6.19), however. Since $K=\frac{1}{2}$, we necessarily have $A=\frac{3}{2}$. In contrast to $C_{AK}^{J(2)}$, therefore, $\delta C_{AK}^{J(2)}$ does not contribute to the energy calculation given below.

It is therefore possible to express the second-order contribution $\delta\mathcal{E}_{KJ}^{(2)}$ to the single-hole energy in terms of the coefficients defined by (6.9) and (6.10). The value of the expression

$$\delta\mathcal{E}_{KJ}^{(2)}=(\Theta_{KJ\mu},(\mathcal{H}_c+\delta\mathcal{H}^{(1)})\delta\Theta_{KJ\mu}^{(1)})+(\Theta_{KJ\mu},(\delta\mathcal{H}^{(21)}+\delta\mathcal{H}^{(22)})\Theta_{KJ\mu}), \quad (6.20)$$

is rendered most concisely if Eqs. (6.9) and (6.10) are rewritten in the forms

$$(\mathcal{E}_K-\mathcal{E}_A)(A|c_{ij}|K)\equiv(A|k_{ij}|K), \qquad (6.21)$$

and

$$(\mathcal{E}_K+\mathcal{E}_{K_1})(\bar{K}_1|d_i|K)\equiv(\bar{K}_1|m_i|K), \qquad (6.22)$$

thus defining the right-hand sides. We then have

$$\delta\mathcal{E}_{KJ}{}^{(2)}=(2\mathcal{I})^{-2}(J\mu K|J_{-i}J_{-j}|J\mu K)[(K|k_{ij}|K)+(\bar{K}|m_i|K)\delta_{i,-j}]$$
$$=(2\mathcal{I})^{-2}[J(J+1)-K^2][(K|[k_{+-}+k_{-+}]|K)+\sum_i(\bar{K}|m_i|K)]$$
$$+(2\mathcal{I})^{-2}K[(K|[k_{+-}-k_{-+}]|K)+(\bar{K}|[m_+-m_-]|K)]. \qquad (6.23)$$

Physically, it is more meaningful to rewrite (6.23) as

$$\delta\mathcal{E}_{KJ}{}^{(2)}=\delta\mathcal{E}_K{}^{(2)}+\delta\mathcal{E}_J{}^{(2)}, \qquad (6.24)$$

where

$$\delta\mathcal{E}_K{}^{(2)}=(2\mathcal{I})^{-2}\{-K(K-1)[(K|k_{+-}|K)+(\bar{K}|m_+|K)]-K(K+1)[(K|k_{-+}|K)+(\bar{K}|m_-|K)]\} \qquad (6.25)$$

is a change in the intrinsic energy, whereas,

$$\delta\mathcal{E}_J{}^{(2)}=(2\mathcal{I})^{-2}J(J+1)$$
$$\times[(K|k_{+-}+k_{-+}|K)+\sum_i(\bar{K}|m_i|K)] \qquad (6.26)$$

can be interpreted in accordance with the equation

$$\mathcal{E}_{KJ}=\mathcal{E}_K-[J(J+1)/2\mathcal{I}]+\delta\mathcal{E}_{KJ} \qquad (6.27)$$

as an increment in the moment of inertia $\mathcal{I}\to\mathcal{I}-\delta\mathcal{I}_K$, of the band based on the hole state $|K\rangle$:

$$\delta\mathcal{I}_K=\tfrac{1}{2}[\langle K|k_{+-}+k_{-+}|K\rangle+\sum_i(\bar{K}|m_i|K)]. \qquad (6.28)$$

In the cranking limit, Eq. (6.28) reduces to a result given by Belyaev.[12] In general, however, it contains a number of additional terms arising from the self-consistency and constitutes a new result.

As the last formal topic of this section, we consider the conditions which follow in second order from the sum rule in Appendix D, the consistency of these with the equations of this section, and any simplications resulting therefrom. The relevant equations are (B15) and (B16) which imply, respectively, in a notation which again distinguishes particle- and hole-matrix elements,

$$(\bar{K}|f_{ij}|L)-(\bar{L}|f_{-j-i}|K)$$
$$=-\sum_{L'}\{(\bar{K}|f_i|L')(L|g_{-j}|L')^*$$
$$-(K|g_i|L')^*(\bar{L}|f_{-j}|L')\}, \qquad (6.29)$$

$$(K|g_{ij}|L)+(L|g_{-j-i}|K)^*$$
$$=-\sum_{L'}\{(K|g_i|L')(L|g_{-j}|L')^*$$
$$+(\bar{K}|f_i|L')^*(\bar{L}|f_{-j}|L')\}, \qquad (6.30)$$

and

$$(\bar{K}_1|d_i|K)-(\bar{K}|d_i|K_1)=0. \qquad (6.31)$$

These are conditions on the coefficients of Eq. (6.8), relating them to first-order coefficients. There are also conditions on the coefficients defined in Eq. (6.15). These are obtained by equating to zero the right-hand sides of (B15) and (B16), applying the resulting conditions to the relevant part of (6.15), and remembering that particle and hole energies differ in sign. We thus obtain the conditions

$$(\bar{L}|f_i{}^{(2)}|K)-(\bar{K}|f_{-i}{}^{(2)}|L)=0. \qquad (6.32)$$

$$(L|g_i{}^{(2)}|K)-(K|g_{-i}{}^{(2)}|L)^*=0. \qquad (6.33)$$

We can verify the compatibility of (6.29) and (6.30) with (6.9), of (6.31) with (6.10), and of (6.32) and (6.33) with (6.16). It is a matter of forming the proper linear combinations and utilizing the sum rule conditions and their antecedents, Eqs. (4.30) and (4.31). We omit the algebra. It is worth recording one additional equation, however, which is a form taken by (6.9) after utilization of (6.30):

$$(\mathcal{E}_K-\mathcal{E}_A)(A|c_{ij}|K)$$
$$=\sum_{A'}(A|(j_i+k_i)|A')(A'|c_j|K)$$
$$+\sum_{K'L'L''}\{(A\bar{K}'|\mathbf{V}|K\bar{L}')(\bar{K}'|f_{-j}|L'')^*(\bar{L}'|f_i|L'')$$
$$-(AK'|\mathbf{V}|KL')(\bar{K}'|f_{-j}|L'')(\bar{L}'|f_i|L'')^*$$
$$+(AK'|\mathbf{V}|K\bar{L}')(K'|g_{-j}|L'')^*(\bar{L}'|f_i|L'')$$
$$+(A\bar{K}'|\mathbf{V}|KL')(\bar{K}'|f_{-j}|L'')^*(L'|g_i|L'')\}$$
$$+\sum_{K'A'}\{(AK'|\mathbf{V}|K\bar{L}')(L'|f_{ij}|K')$$
$$+(A\bar{L}'|\mathbf{V}|KK')(\bar{L}|f_{-j-i}|K')^*\}. \qquad (6.34)$$

VII. OTHER OBSERVABLES

In this section, we indicate with a few examples how observables other than the nuclear energies may be computed with the results obtained for the one-particle density matrix. The material of this section is only illustrative and introductory and will be developed more fully in later work.

[12] S. T. Belyaev, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 31, No. 11 (1959).

A. Electric-Quadrupole Moments and Quadrupole Transitions

We first show how our zero-order results are equivalent, for electrical quadrupole effects, to those of the unified model.[13] As the simplest possible quantity, we consider the reduced $E2$ transition probability for a transition within the ground-state band of an even-even nucleus.

$$B(E2;I\rightarrow I')=(2I+1)^{-1}\sum_{mMM'}|\langle I'M'|\mathfrak{M}_{2m}|IM\rangle|^2, \qquad (7.1)$$

where, using an isospin notation,

$$\mathfrak{M}_{2m}=e\int\psi^\dagger(x)\tfrac{1}{2}(1+\tau_3)r^2Y_m{}^{(2)}(\theta\phi)\psi(x). \qquad (7.2)$$

The calculation thus depends on the structure of[14]

$$\begin{aligned}\langle I'M'|\psi^\dagger(x)\psi(x)|IM\rangle &=(xIM|\rho|xI'M')\\ &=\int d\hat{n}d\hat{n}'(\hat{n}|IM0)(I'M'0|\hat{n}')(x\hat{n}|\rho|x\hat{n}')\\ &=\int d\hat{n}(\hat{n}|IM0)(I'M'0|\hat{n})\rho(RX,RX)\\ &=\int dR(R|IM0)(I'M'0|R)\rho(RX,RX), \qquad (7.3)\end{aligned}$$

utilizing Eq. (3.22) for the lowest order density matrix. The last step of (7.3) involves simply a renormalization of factors, $(R|IM0)=(2\pi)^{-1/2}(\hat{n}|IM0)$, and the subsequent extension of the integral to include the third Euler angle γ. Writing $RX=X'$ and with the help of the transformation

$$Y_m{}^{(2)}(\theta\phi)=\sum_{m'}Y_{m'}{}^{(2)}(\theta'\phi')D_{mm'}{}^{(2)}(R), \qquad (7.4)$$

we can now write

$$\begin{aligned}\langle I'M'|\mathfrak{M}_{2m}|IM\rangle &=\int dR(I'M'0|R)D_{m0}(R)(R|IM0)\\ &\quad\times e\int r^2Y_0{}^{(2)}(\theta\phi)\tfrac{1}{2}(1+\tau_3)\rho(x,x)\\ &=[(2I+1)/(2I'+1)]^{1/2}(IM,2m|I2;I'M')\\ &\quad\times(I0,20|I2;I'0)\left(\frac{5}{16\pi}\right)^{1/2}eQ_0, \qquad (7.5)\end{aligned}$$

where we have used the results and definitions

$$\frac{1}{8\pi^2}\int dR\,D_{M'K'}{}^{I'*}(R)D_{mm'}{}^{k}(R)D_{MK}{}^{I}(R)=(2I'+1)^{-1}(IMkm|IkI'M')(IKkm'|IkI'K'), \qquad (7.6)$$

and

$$Q_0=(16\pi/5)^{1/2}\int r^2Y_0{}^{(2)}(\theta\phi)\tfrac{1}{2}(1+\tau_3)\rho(x,x). \qquad (7.7)$$

Equation (7.5) yields directly the well-known result[14]

$$B(E2\!:I\rightarrow I')=\frac{5}{16\pi}e^2Q_0{}^2|(I020|I2I'0)|^2. \qquad (7.8)$$

We next consider the corresponding expression for the neighboring odd nucleus (one nucleon added), $B(E2\!:JK\rightarrow J'K)$. Basically we require the density matrix for the $A+1$ particle system

$$(xJ\mu K|\rho^{(A+1)}|xJ'\mu'K)\equiv\langle J'\mu'K|\psi^\dagger(x)\psi(x)|J\mu K\rangle, \qquad (7.9)$$

not previously computed in this paper. We here require an accuracy comparable to (7.3). Writing

$$(xJ\mu K|\rho^{(A+1)}|xJ'\mu'K)=\textstyle\sum_n\langle J'\mu'K|\psi^\dagger(x)|n\rangle\langle n|\psi(x)|J\mu K\rangle, \qquad (7.10)$$

the problem is to ascertain which intermediate states contribute. One must, of course, include the ground-state rotational band,

$$\begin{aligned}\sum_{IM}\langle J'\mu'K|\psi^\dagger(x)|IM0\rangle\langle IM0|\psi(x)|J\mu K\rangle &=\int d\hat{n}d\hat{n}'\langle J'\mu'K|\psi^\dagger(x)|\hat{n}\rangle\\ &\quad\times\langle\hat{n}'|\psi(x)|J\mu K\rangle\sum_{IM}(\hat{n}|IM0)(IM0|\hat{n}')\\ &\cong\int dR\,\phi_{\bar{K}}(Rx)\phi_{\bar{K}}{}^*(Rx)(R|J\mu K)(J'\mu'K|R), \qquad (7.11)\end{aligned}$$

where we have used completeness and the unsymmetrized zeroth approximation

$$\langle\hat{n}|\psi(x)|J\mu K\rangle\cong\phi_{\bar{K}}(Rx)(\hat{n}|J\mu K), \qquad (7.12)$$

as well as a final change in normalization.

Equation (7.11) is clearly the contribution from the odd particle. To obtain the core contribution, we must assume that to everyone of the A bands which can be reached by destroying a particle in the ground-state band of the even-even nucleus, there is a corresponding excited band of the latter which is a hole-particle excited-state band, with the particle corresponding to the state of Eq. (7.11). We thus enter as the additional

[13] For reviews, see C. J. Gallagher (Ref. 1); A. K. Kerman, *Nuclear Reactions* (Interscience Publishers, Inc., New York, 1959), Vol. 1, p. 427; S. A. Moszkowski, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 411.

[14] In this section we ignore symmetrization requirements, since they do not affect any of the results to be obtained.

contribution to (7.10)

$$\sum_{IML} \langle J'\mu'K|\psi^\dagger(x)|Im, K-L\rangle\langle IM, K-L|\psi(x)|J\mu K\rangle$$
$$=\sum_{IML}\int d\hat{n}d\hat{n}'\langle J'\mu'K|\hat{n}'\rangle\langle\hat{n}|J\mu K\rangle$$
$$\times\langle\hat{n}'K|\psi^\dagger(x)|IM, K-L\rangle\langle IM, K-L|\psi(x)|\hat{n}K\rangle$$
$$=\int dR\rho^{(A)}(Rx,Rx)(R|J\mu K)(J'\mu'K'|R), \qquad (7.13)$$

where $\rho^{(A)}(x,x)$ is the density matrix of (7.3). In reaching the obvious answer (7.13), the essential step is to ignore the particle-hole interaction and therefore to write (ignoring symmetrization)

$$\langle IM, K-L|\psi(x)|\hat{n}K\rangle\cong(\hat{n}|IM, K-L)\psi_L(Rx). \qquad (7.14)$$

By virtue of (7.11) and (7.13), we now have for (7.9)

$$\langle J'\mu'K|\psi^\dagger(x)\psi(x)J\mu K\rangle$$
$$=\int dR\,\rho^{(A+1)}(Rx,Rx)(R|J\mu K)(J'\mu'K|R), \qquad (7.15)$$

where

$$\rho^{(A+1)}(Rx,Rx)=\rho^{(A)}(Rx,Rx)+|\phi_{\bar{K}}(Rx)|^2. \qquad (7.16)$$

By completely strict analogy with the derivation of (7.8), we then find[14]

$$B(E2;JK\rightarrow J'K)$$
$$=\frac{5}{16\pi}e^2Q_0^2|(JK20|J2J'K)|^2, \qquad (7.17)$$

where Q_0 is again defined by Eq. (7.7), but with respect to the density (7.16), which includes the extra particle.

B. Collective Gyromagnetic Ratio

We calculate the magnetic moment in an excited state of the ground-state band

$$\mu=\langle II0|(\mu_0)_{\rm op}|II0\rangle, \qquad (7.18)$$

where $\mu_{\rm op}$ is the usual operator,

$$(\mu_m)_{\rm op}=\int\psi^\dagger(x)\mu_m\psi(x), \qquad (7.19)$$

$$\mu_m=\tfrac{1}{2}(1+\tau_3)(l_m+g_pS_m)+\tfrac{1}{2}(1-\tau_3)g_nS_m, \qquad (7.20)$$

and m here refers to the appropriately phased spherical components of the orbital- and spin-angular momentum. In the present case, one can see easily that a nonvanishing contribution requires at least first-order accuracy for the density matrix. We find by means already utilized

$$\int dx\langle II0|\psi^\dagger(x)\mu_0\psi(x)|II0\rangle$$
$$=-(2\mathcal{I})^{-1}\sum_{AK>0}\int dR(II0|R)D_{0m}^{(1)}(R)J_{-i}(R|II0)$$
$$\times\{(K|\mu_m|A)(A|c_i|K)+(A|\mu_m|K)(A|c_{-i}|K)^*\}. \qquad (7.21)$$

For the angular integral in (7.21), one obtains

$$\int dR=\delta_{-i,m}(II10|I1II)(I-m1m|I1I0)$$
$$\times(II-m|J_m|II0)=\mp2^{-1/2}I\delta_{-i,m}, \qquad (7.22)$$

where $\mp$ refers to $m=\pm1$, respectively. Remembering that

$$\mu_{\pm1}=\mp2^{-1/2}\mu_\pm=\mp2^{-1/2}(\mu_x\pm i\mu_y), \qquad (7.23)$$

we finally obtain

$$\mu=g_RI, \qquad (7.24)$$

$$g_R=\mathcal{I}^{-1}\sum_{KL>0}\{(K|\mu_x|\bar{L})(\bar{L}|f_x|K)+\text{c.c.}\}. \qquad (7.25)$$

In the cranking limit, this too reduces to the well-known result.[15]

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APPENDIX A

In this Appendix we provide some of the details of the calculations reported in Sec. IV. Beginning with Eq. (4.5), we study

$$(\Theta_{KJ\mu},\Theta_{KJ\mu})=\int d\hat{n}dx\;\Theta_{KJ\mu}^\dagger[x\hat{n}]\Theta_{KJ\mu}[x,\hat{n}] \qquad (A1)$$

with $\Theta_{KJ\mu}$ given by (3.21). We have from the normalization chosen in (3.12)

$$\int_0^\pi \sin\beta d\beta\int_0^{2\pi}d\alpha|(\hat{n},0|J\mu K)|^2=1 \qquad (A2)$$

and from Eq. (3.42)

$$\int dx|\theta_K(x)|^2=1. \qquad (A3)$$

The result Eq. (4.5) then follows as soon as we notice the vanishing of the cross terms proportional to

$$\int dxd\hat{n}(J\mu K|\hat{n})(-\hat{n}|J\mu K)\theta_K^\dagger(x)\theta_K(R(\pi,\pi,0)x). \qquad (A4)$$

[15] S. G. Nilsson and O. Prior, Ref. 11.

Here it is the integral over x that vanishes as one sees by utilizing Eq. (3.25).

As a result of the choice of phase in Eq. (3.26), we have

$$\int d\hat{n}(J\mu K|\hat{n})J_{\pm}(\hat{n}|J\mu K\pm 1)=(J\mu K|J_{\pm}|J\mu K\pm 1)=[(J\mp K)(J\pm K+1)]^{1/2}. \quad (A5)$$

We turn then to the derivation of (4.21) and (4.22). In this connection some prior remarks concerning the derivation of (4.17) will be helpful. Most straightforwardly the result of the calculation in (4.17) is

$$(\Theta_{\bar{L}J\mu},\mathcal{H}_c\Theta_{KJ\mu})=(4\mathcal{I})^{-1}\{(J\mu L|J_{-i}|J\mu K)(\bar{L}|j_i|K)+(J\mu-L|J_{-i}|J\mu-K)((R\bar{L})|j_i|(RK))\}, \quad (A6)$$

where one utilizes (3.15) and the definition

$$|RK\rangle=\theta_{(RK)}(x)=\theta_K(R(\pi,\pi,0)x). \quad (A7)$$

With the help of (3.48) we then find

$$((R\bar{L})|j_i|(RK))=-(-\bar{L}|j_i|-K)=(\bar{L}|j_{-i}|K). \quad (A8)$$

Similarly,

$$(J\mu-L|J_i|J\mu-K)=(J\mu L|J_{-i}|J\mu K). \quad (A9)$$

From (A8) and (A9), it follows that the two terms of (C7) are equal.

We turn now to the derivation of (4.21). To illustrate the basic technique involved we consider the quantity

$$\delta\mathcal{H}_1(x\hat{n},x'\hat{n}')=\int dydy'V(xy;x'y')\sum_{L,K>0;J,\mu}\Theta_{\bar{L}J\mu}[y'\hat{n}]\Theta_{KJ\mu}{}^{\dagger}[y\hat{n}']F_{LK}{}^{J}$$
$$=\frac{1}{2}\int dydy'V(xy;x'y')\sum_{K,L>0;J\mu}[(\hat{n}|J\mu L)(J\mu K|\hat{n}')\theta_{\bar{L}}(y'\hat{n})\theta_K{}^{\dagger}(y\hat{n}')$$
$$+(-\hat{n}|J\mu L)(J\mu K|\hat{n}')\theta_{\bar{L}}(R_1y')\theta_K{}^{\dagger}(R_1'y)+(\hat{n}\rightarrow-\hat{n})(\hat{n}'\rightarrow-\hat{n}')](JL|J_{-i}|JK)(\bar{L}|f_i|K). \quad (A10)$$

With the aid of the invariance property [(3.21) and (3.25)],

$$\Theta_{KJ\mu}[x,\hat{n}]=\Theta_{KJ\mu}[x,-\hat{n}], \quad (A11)$$

we find

$$(\Theta_{\bar{L}J\mu},\delta\mathcal{H}_1\Theta_{KJ\mu})=2\sum_{L'K'>0,J\mu}\int d\hat{n}'dxdx'dydy'\Theta_{\bar{L}J\mu}{}^{\dagger}[x,\hat{n}]V(xy;x'y')$$
$$\times(\hat{n}|J'\mu'L')(J'\mu'K'|\hat{n})\theta_{\bar{L}'}(y'\hat{n})\theta_{K'}{}^{\dagger}(y\hat{n}')\Theta_{KJ\mu}[x',\hat{n}'](JL'|J_{-i}|JK')(\bar{L}'|f_i|K'). \quad (A12)$$

From the completeness relation

$$\sum_{J\mu}(JL'|J_{-i}|JK')(\hat{n}|J\mu L')(J\mu K'|\hat{n}')=J_{-i}(\hat{n})\delta(\hat{n}-\hat{n}'), \quad (A13)$$

and after integration by parts, ignoring the contributions in which the collective angular-momentum operator J_{-i} is converted by its operation on the single-particle functions θ into j_{-i}, we obtain

$$(\Theta_{\bar{L}J\mu},\delta\mathcal{H}_1\Theta_{KJ\mu})=2\sum_{L'K'>0}\int\Theta_{\bar{L}J\mu}{}^{\dagger}[x,\hat{n}]V(xy;x'y')\theta_{\bar{L}}(Ry')\theta_K{}^{\dagger}(Ry)J_{-i}(\hat{n})\Theta_{KJ\mu}(x'\hat{n})(\bar{L}'|f_i|K')$$
$$=\sum_{L'K'>0}\{(JL|J_{-i}|JK)(\bar{L}K'|V|K\bar{L}')(\bar{L}'|f_i|K')$$
$$+(J-L|J_{-i}|J-K)(\bar{L}[RK']|V|K[R\bar{L}'])(\bar{L}'|f_i|K')\}. \quad (A14)$$

If we suppose that [cf. Eq. (A8)]

$$(\bar{L}'|f_i|K')=([R\bar{L}']|f_{-i}|[RK'])=-(-\bar{L}'|f_{-i}|-K'), \quad (A15)$$

and remember Eq. (3.25), we find with the help of (A9)

$$(\Theta_{\bar{L}J\mu},\delta\mathcal{H}_1\Theta_{KJ\mu})=\sum_{\text{all }L'K'}(JL|J_{-i}|JK)(\bar{L}K'|V|K\bar{L}')(\bar{L}'|f_i|K'). \quad (A16)$$

This result accounts for part of the right-hand side of (4.21), and the remainder can be derived in a similar manner.

We consider next the derivation of (4.28). As a representative piece, we study [cf. (A14)]

$$(\Theta_{KJ\mu}\delta\mathcal{H}_1\Theta_{KJ\mu})=\delta_{K,\frac{1}{2}}\sum\{(J\mu K|-\hat{n})J_{-i}(\hat{n})(\hat{n}|J\mu K)([RK]K'|V|K\bar{L}')(\bar{L}'|f_i|K')$$
$$+(J\mu K|\hat{n})J_{-i}(\hat{n})(-\hat{n}|J\mu K)(KK'|V|[RK]\bar{L}')(\bar{L}'|f_i|K')\}$$
$$=\delta_{K,\frac{1}{2}}\sum(-)^{J+1}(J\mu-\tfrac{1}{2}|J_{-i}|J\mu\tfrac{1}{2})([R\tfrac{1}{2}]K'|V|\tfrac{1}{2}\bar{L}')(\bar{L}'|f_i|K')$$
$$+\delta_{K,\frac{1}{2}}\sum(-)^{J}(J\mu-\tfrac{1}{2}|J_i|J\mu\tfrac{1}{2})(\tfrac{1}{2}K'|V|(R\tfrac{1}{2})\bar{L}')(\bar{L}'|f_i|K')$$
$$=(-)^{J+1}\delta_{K,\frac{1}{2}}\sum(J\mu-\tfrac{1}{2}|J_{-i}|J\mu\tfrac{1}{2})[([R\tfrac{1}{2}]K'|V|\tfrac{1}{2}\bar{L}')(\bar{L}'|f_i|K')$$
$$-(\tfrac{1}{2}K'|V|[R\tfrac{1}{2}]\bar{L}')(R\bar{L}'|f_i|RK')], \quad \text{(A17)}$$

where the sum is over K', $L'>0$. We now note that

$$(\tfrac{1}{2}K'|V|[R\tfrac{1}{2}]\bar{L}')=([R\tfrac{1}{2}][RK']|V|[R^2\tfrac{1}{2}][R\bar{L}'])=([R\tfrac{1}{2}],-K'|V|\tfrac{1}{2},-\bar{L}'), \quad \text{(A18)}$$

where we have used Eq. (3.25) in the form

$$\theta_K(Rx)=\theta_{-K}(x), \quad \text{(A19)}$$

as well as the equation

$$\theta_K(R^2x)=-\theta_K(x), \quad \text{(A20)}$$

which follows from the same considerations as yield (3.43). It follows straightforwardly now that

$$(\Theta_{\frac{1}{2}J\mu},\delta\mathcal{H}\Theta_{\frac{1}{2}J\mu})=-(-)^{J+\frac{1}{2}}(2\mathcal{I})^{-1}\delta_{K,\frac{1}{2}}(J+\tfrac{1}{2})\delta a, \quad \text{(A21)}$$

where δa is given by (4.28).

APPENDIX B

We deduce the consequences of the completeness relations or sum rule in the form given in Eq. (4.29). In general, this involves some complication beyond zero order owing to the intertwining of variables. These complications are only apparent, however, to the order of accuracy for which equations of motion and supplementary conditions are compatible.

We write

$$\Theta_{KJ\mu}[x,\hat{n}]=A_K{}^J\Theta_{KJ\mu}{}^{(0)}[x,\hat{n}]+\sum_{L\neq K}\Theta_{LJ\mu}{}^{(0)}[x,\hat{n}]G_{LK}{}^J+\sum_L\Theta_{LJ\mu}{}^{(0)}[x,\hat{n}]F_{LK}{}^J. \quad \text{(B1)}$$

To exploit (4.29), we also require the relations

$$\tau_1\Theta_{KJ\mu}{}^{(0)*}[x,\hat{n}]=(-)^{J+\mu-K}\Theta_{\bar{K}J,-\mu}{}^{(0)}[x,\hat{n}], \quad \text{(B2)}$$

$$\tau_1\Theta_{\bar{K}J_1-\mu}{}^{(0)*}[x,\hat{n}]=(-)^{J+\mu-K}\Theta_{KJ\mu}{}^{(0)}[x,\hat{n}], \quad \text{(B3)}$$

which in turn yield

$$\tau_1\Theta_{KJ\mu}{}^*[x,\hat{n}]=(-)^{J+\mu-K}\{A_K{}^{J*}\Theta_{\bar{K}J,-\mu}[x,\hat{n}]+\textstyle\sum_L(-)^{L+K}\Theta_{LJ,-\mu}{}^{(0)}[x,\hat{n}]F_{LK}{}^{J*}$$
$$+\textstyle\sum_L(-)^{K-L}\Theta_{\bar{L},J,-\mu}{}^{(0)}[x,\hat{n}]G_{LK}{}^{J*}\}. \quad \text{(B4)}$$

The proof of (B2) depends on the statements

$$D_{\mu K}{}^{J*}(\hat{n})=(-)^{\mu-K}D_{-\mu-K}{}^J(\hat{n})=(-)^{J+\mu+K}D_{-\mu K}{}^J(-\hat{n}), \quad \text{(B5)}$$

$$\theta_K(R_1x)=\theta_{-K}(Rx), \quad K>0, \quad \text{(B6)}$$

$$\theta_{-K}(R_1x)=-\theta_K(Rx), \quad K>0, \quad \text{(B7)}$$

The consequence of the sum rule (4.29) to zero order is already known [Eq. (3.42)] to be the completeness relation for the set of functions $\{\theta_K(x),\tau_1\theta_K{}^*(x)\}$. To obtain more generally the consequences of the sum rule we write it out with the aid of (B1) and (B4)

$$\frac{1}{2}[\delta(\hat{n}-\hat{n}')+\delta(\hat{n}-\hat{n}')]\delta(x-x')$$
$$=\sum_{J\mu K}|A_K{}^J|^2\{\Theta_{KJ\mu}[x,\hat{n}]\Theta_{KJ\mu}{}^\dagger[x',\hat{n}']+\Theta_{\bar{K}J\mu}[x,\hat{n}']\Theta_{\bar{K}J\mu}{}^\dagger[x',\hat{n}]\}$$
$$+\sum_{J\mu KL}\{[G_{KL}{}^{J*}+G_{LK}{}^J]\Theta_{LJ\mu}[x,\hat{n}]\Theta_{KJ\mu}[x',\hat{n}']+(-)^{K-L}[G_{KL}{}^{J*}+G_{LK}{}^J]\Theta_{\bar{K}J\mu}[x,\hat{n}']\Theta_{\bar{L}J\mu}{}^\dagger[x',\hat{n}]$$
$$+F_{LK}{}^J\Theta_{\bar{L}J\mu}[x,\hat{n}]\Theta_{KJ\mu}{}^\dagger[x'\hat{n}']+F_{LK}{}^{J*}\Theta_{KJ\mu}[x,\hat{n}]\Theta_{\bar{L}J\mu}{}^\dagger[x'\hat{n}']$$
$$+(-)^{K+L}F_{LK}{}^J\Theta_{\bar{K}J\mu}[x,\hat{n}']\Theta_{LJ\mu}{}^\dagger[x'\hat{n}]+(-)^{K+L}F_{LK}{}^{J*}\Theta_{LJ\mu}[x,\hat{n}']\Theta_{\bar{K}J\mu}{}^\dagger[x',\hat{n}]\}$$
$$+\sum_{J\mu LKK'}\{G_{LK'}{}^JG_{KK'}{}^{J*}[\Theta_{LJ\mu}[x,\hat{n}]\Theta_{KJ\mu}{}^\dagger[x'\hat{n}']+(-)^{L-K'}(-)^{K-K'}\Theta_{\bar{K}J\mu}[x,\hat{n}']\Theta_{\bar{L}J\mu}{}^\dagger[x'\hat{n}]]$$
$$+F_{LK'}{}^JF_{KK'}{}^{J*}[\Theta_{\bar{L}J\mu}[x,\hat{n}]\Theta_{\bar{K}J\mu}{}^\dagger[x'\hat{n}']+(-)^{L+K'}(-)^{K+K'}\Theta_{KJ\mu}[x,\hat{n}']\Theta_{LJ\mu}{}^\dagger[x',\hat{n}]]$$
$$+G_{LK'}{}^JF_{KK'}{}^{J*}[\Theta_{LJ\mu}[x,\hat{n}]\Theta_{\bar{K}J\mu}{}^\dagger[x'\hat{n}']+(-)^{L-K'}(-)^{K+K'}\Theta_{KJ\mu}[x,\hat{n}']\Theta_{\bar{L}J\mu}{}^\dagger[x'\hat{n}]]$$
$$+F_{LK'}{}^JG_{KK'}{}^{J*}[\Theta_{\bar{L}J\mu}[x,\hat{n}]\Theta_{KJ\mu}{}^\dagger[x'\hat{n}']+(-)^{L+K'}(-)^{K-K'}\Theta_{\bar{K}J\mu}[x,\hat{n}']\Theta_{LJ\mu}{}^\dagger[x',\hat{n}]]\}. \quad \text{(B8)}$$

We shall satisfy this relation order by order by means of the expansions

$$G_{LK}{}^J=G_{LK}{}^{J(1)}+G_{LK}{}^{J(2)}+\cdots, \quad \text{(B9)}$$

$$F_{LK}{}^J=F_{LK}{}^{J(1)}+F_{LK}{}^{J(2)}+\cdots, \quad \text{(B10)}$$

$$|A_K{}^J|^2=1-|a_K{}^{J(1)}|^2+\cdots. \quad \text{(B11)}$$

For the first-order coefficients we then find

$$G_{LK}{}^{J(1)}+G_{KL}{}^{J(1)*}=0, \quad \text{(B12)}$$

$$F_{KL}{}^{J(1)}-F_{LK}{}^{J(1)}=0. \quad \text{(B13)}$$

For the normalization change (diagonal second-order contribution) we find, remembering (B11)

$$|a_K{}^{J(1)}|^2=\sum_{K'}\{|G_{KK'}{}^{J(1)}|^2+|F_{KK'}{}^{J(1)}|^2\}, \quad \text{(B14)}$$

which is further evaluated in Eq. (4.35) of the text. In addition $F_{LL}{}^{J(2)}$ is undetermined and may be set to zero. Finally, for the off-diagonal second-order terms we obtain

$$G_{LK}{}^{J(2)}+G_{KL}{}^{J(2)}+\sum_{K'}\{G_{LK'}{}^{J(1)}G_{KK'}{}^{J(1)*}+F_{KK'}{}^{J(1)}F_{LK'}{}^{J(1)*}\}=0, \quad \text{(B15)}$$

$$F_{LK}{}^{J(2)}-F_{KL}{}^{J(2)}+\sum_{K'}F_{LK'}{}^{J(1)}G_{KK'}{}^{J(1)*}-F_{KK'}{}^{J(1)}G_{LK}{}^{J(1)*}=0. \quad \text{(B16)}$$

The verification of Eqs. (B12)–(B16) utilizes the same procedures and approximations as needed in the work of Sec. IV.