# Derivation and assessment of strong coupling core-particle model from the Kerman-Klein-Dönau-Frauendorf theory

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We review briefly the fundamental equations of a semimicroscopic core-particle coupling method that makes no reference to an intrinsic system of coordinates. We then demonstrate how an intrinsic system can be introduced in the strong coupling limit so as to yield a completely equivalent formulation. It is emphasized that the conventional core-particle coupling calculation introduces a further approximation that avoids what has hitherto been the most time-consuming feature of the full theory, and that this approximation can be introduced either in the intrinsic system, the usual case, or in the laboratory system, our preference. A new algorithm is described for the full theory that largely removes the difference in complexity between the two types of calculation. Comparison of the full and approximate theories for some representative cases provides a basis for the assessment of the accuracy of the traditional approach. We find that for well-deformed nuclei, e.g., <sup>157</sup>Gd and <sup>157</sup>Tb, the core-coupling method and the full theory give similar results. [S0556-2813(97)05501-5]

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## I. INTRODUCTION

We have recently undertaken the task of revitalizing and extending a semimicroscopic theory of collective motion for odd nuclei that we shall refer to as the Kerman-Klein-Dönau-Frauendorf (KKDF) model [1-4]. This model, aside from the elements discussed for the first time in the present paper, was introduced in close to its present form by Dönau and Frauendorf [5-9], whose work was in turn stimulated by an application [10] of the theory of collective motion developed by Kerman and Klein [11-14].

In the presentation of our work at seminars and conferences, one question that has invariably arisen is the connection between the KKDF model and the conventional coreparticle coupling model, especially for deformed nuclei, to which our published applications have so far been confined. Even if we widen the inquiry to the connection between the shell model and the core-particle model, we find that the literature on this subject is sparse. We are aware of only two publications that have been addressed specifically to this topic. The earlier of these papers [15] showed how all, then extant, core-particle coupling models could be understood as approximations to the work of Kerman and Klein. This paper appears to have gone completely unnoticed, since it is not quoted in the later work [16], which is devoted to the derivation of the strong coupling core-particle model from a schematic shell model. In the book by Ring and Schuck [17], which appeared betweentimes, the success of the strong coupling model in its domain of application is heralded but at the same time proclaimed a mystery.

The main purposes of the present work are threefold. The first is to transform the Kerman-Klein equations from the "laboratory" system in which they are derived and conveniently applied to the "intrinsic" system, when it makes sense to define such a system, as is done in the strong coupling core-particle model. The resulting theory is completely equivalent to the starting one and does not yet constitute the standard phenomenological model. A second purpose is to describe and implement the approximation that leads to the standard model. We describe in most detail how this may be done in the intrinsic system, the usual choice, but emphasize that the approximation may equally be defined in the laboratory system and that the latter approach has some advantages.

The essential point here may be described as follows. In the physical situation, which requires the inclusion of pairing interactions, the number of solutions of the full KKDF model is twice as great as the number of physical states being described. Hitherto, the major technical difficulty (and consumption of CPU time) of this method has been the application of a criterion to select the physical solutions. For the ground state problem there is the well-known property of the BCS theory that the physical solutions (quasiparticles) correspond to positive energies and the unphysical ones to negative energies. In the KKDF model the strategy is to ignore initially rotational excitation energies so as to collapse each band to a single degenerate state to which the ground state criterion can be applied. We then step up the excitation energies, returning them finally to their full values; at each step we select the physical solutions by a projection technique described in our cited work, that involves an extension of the techniques introduced by Dönau and Frauendorf.

Another way of stating the problem that is directly related to the traditional core-particle model is to remark that although only half of the solutions of the KKDF model are related to physics, the full set of solutions is necessary for mathematical completeness. The solutions of our equations at full excitation can be expanded in terms of the complete set generated at zero excitation, but this expansion will involve both physical and unphysical states of the latter limit. In the conventional core-particle model it is assumed that the physical states of the actual problem are well approximated by a superposition of the physical solutions at zero excita-

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tion. It follows from this that it suffices to solve a single eigenvalue problem for the problem of actual interest rather than having to solve a sequence of such problems.

The third purpose of this paper is to carry through several illustrative calculations using both the KKDF model and the approximation to it just described, in order to assess the validity of the latter. In the course of rethinking our algorithms in preparation for this study, we have discovered a method of simplifying the full calculation to a sufficient extent that much of the advantage of technical simplicity of the coreparticle limit has been wiped out. We shall also describe this new development.

We start in Secs. II and III with a review of the fundamental equations of the Kerman-Klein method, in order to introduce some improvements in notation and presentation, as well as to correct some phase errors made previously in the formulas for transition matrix elements. In Sec. IV we transform our equations (without approximation) to a description in terms of an intrinsic frame of reference. Starting from these equations, the definition and formulation of the strong coupling core-particle model in its usual form in the intrinsic system is given in Sec. V. It is explained in Sec. VI that an equivalent and possibly more effective version of this limit can perfectly well be carried out in the laboratory system. Turning to applications, our new algorithm is described in Sec. VII and then applied together with the standard coreparticle model to some illustrative cases in Sec. VIII. Concluding remarks are presented in Sec. IX. Two appendices provide some technical details of the derivation carried out in Sec. IV.

### II. FUNDAMENTAL EQUATIONS OF THE KERMAN-KLEIN METHOD FOR ODD NUCLEI

In this section we shall derive a version of the Kerman-Klein equations based on the Hamiltonian given below. In essence, these equations are already a special case of the formalism presented more than thirty years ago [18]. The original equations and the form of them derived in this section, when taken literally, define a nonlinear problem for the self-consistent study of the properties of an odd nucleus and of its immediate even neighbors. This is a problem of considerable complexity on which limited progress was reported in early applications [10]. Based on more recent experience in an application to the theory of skyrmions [19], we believe that the prognosis for success of such an undertaking would be much higher today than it was a quarter of a century ago.

Nevertheless, we must emphasize that the present series of papers using the KKDF version of the theory has a more modest goal. This is to make such further approximations so as to reduce the problem to a linear eigenvalue problem for the properties of odd nuclei, assuming the required properties of the neighboring even nuclei to be known. This can be done only if the Hamiltonian can be chosen of sufficiently simple form that the matrix elements of its ingredient multipole and pairing operators can be related to observed properties of the even neighbors. It is this specialization, which in the present paper is first introduced and utilized in Sec. V, that defines the KKDF version of the Kerman-Klein theory. A main contention is that even with such simplification, the resulting theory generalizes existing core-particle coupling models. The derivations that are presented in Secs. II, III, and IV are self-contained, and therefore it should be possible for any reader to reproduce them (with sufficient algebraic devotion to the task).

We start with a shell-model Hamiltonian of the form

$$H = \sum_{\alpha} h_a a^{\dagger}_{\alpha} a_{\alpha} + \frac{1}{4} \sum_{abcd} \sum_{LM_L} F_{acdb}(L) B^{\dagger}_{LM_L}(ac) B_{LM_L}(db) + \frac{1}{4} \sum_{abcd} \sum_{ML_M} G_{abcd}(L) A^{\dagger}_{LM_L}(ab) A_{LM_L}(cd).$$
(2.1)

Here  $h_a$  are the spherical single-particle energies referred to the nearest closed shell,  $\alpha$  refers to the standard set of singleparticle quantum numbers, including in particular the pair  $(j_a, m_a)$ , and *a* refers to the same set with  $m_a$  omitted.  $B_{LM_t}^{\dagger}$  is the particle-hole multipole operator,

$$B_{LM_{L}}^{\dagger}(ab) \equiv \sum_{m_{a}m_{b}} s_{\beta}(j_{a}m_{a}j_{b}-m_{b}|LM_{L})a_{\alpha}^{\dagger}a_{\beta}$$
$$= (-1)^{j_{a}+j_{b}-M_{L}+1}B_{L-M_{L}}(ba), \qquad (2.2)$$

and  $A_{LM_{I}}^{\dagger}$  is the particle-particle multipole operator,

$$A_{LM_L}^{\dagger}(ab) \equiv \sum_{m_a m_b} (j_a m_a j_b - m_b | LM_L) a_{\alpha}^{\dagger} a_{\overline{\beta}}^{\dagger}, \quad (2.3)$$

where  $(j_1m_1j_2m_2|jm)$  is a Clebsch-Gordon (CG) coefficient,  $s_{\alpha} = (-1)^{j_a - m_a}$ , and a bar indicates reversal of the sign of the magnetic quantum number. The coefficients *F* are the particle-hole matrix elements,

$$F_{acdb}(L) \equiv \sum_{m's} s_{\gamma} s_{\beta} (j_a m_a j_c - m_c | LM_L)$$
$$\times (j_d m_d j_b - m_b | LM_L) V_{\alpha\beta\gamma\delta}, \qquad (2.4)$$

which satisfies the relation

$$F_{acdb}(L) = (-1)^{j_a + j_b + j_c + j_d} F_{bdca}(L), \qquad (2.5)$$

and G the particle-particle matrix elements

$$G_{abcd}(L) \equiv \sum_{m's} (j_a m_a j_b - m_b | LM_L) \\ \times (j_c m_c j_d - m_d | LM_L) V_{\alpha \overline{\beta} \gamma \overline{\delta}}, \qquad (2.6)$$

which satisfies the conditions

$$G_{acdb}(L) = (-1)^{j_a + j_c - L + 1} G_{cadb} = (-1)^{j_b + j_d - L + 1} G_{acbd}.$$
(2.7)

Our initial task is to obtain equations for the states and energies of an odd nucleus assuming that properties of immediately neighboring even nuclei are known. The states of the odd nucleus (particle number A) are designated as  $|J\mu\nu\rangle$ , where  $\nu$  denotes all quantum numbers besides the angular momentum *J* and its projection  $\mu$ . The states of the neighboring even nuclei with particle numbers  $(A \pm 1)$  are written, in a parallel notation, as  $|IMn(A \pm 1)\rangle$ . The corre-

sponding eigenvalues are  $E_{J\nu}$  and  $E_{In}^{(A\pm 1)}$ , respectively. The operator equations of motion (EOM) are obtained by forming commutators between the single-fermion operators and the Hamiltonian,

$$[a_{\alpha},H] = h'_{a}a_{\alpha} + \frac{1}{2}\sum_{bd\gamma}\sum_{LM}s_{\gamma}(j_{a}m_{a}j_{c}-m_{c}|LM)F_{acdb}(L)a_{\gamma}B_{LM}(db) + \frac{1}{2}\sum_{bd\gamma}\sum_{LM}(j_{a}m_{a}j_{c}-m_{c}|LM)G_{acbd}(L)a^{\dagger}_{\gamma}A_{LM}(bd),$$

$$(2.8)$$

$$[a_{\overline{\alpha}}^{\dagger},H] = -h_{a}^{\prime}a_{\overline{\alpha}}^{\dagger} - \frac{1}{2}\sum_{bd\gamma}\sum_{LM} s_{\overline{\gamma}}(j_{a} - m_{a}j_{c}m_{c}|LM)F_{acdb}(L)B_{LM}^{\dagger}(db)a_{\overline{\gamma}}^{\dagger} + \frac{1}{2}\sum_{bd\gamma}\sum_{LM} (j_{a} - m_{a}j_{c}m_{c}|LM)G_{acbd}(L)A_{LM}^{\dagger}(bd)a_{\gamma}.$$

$$(2.9)$$

Here

$$h'_{a} = h_{a} - \frac{1}{4} \sum_{Lj_{c}} F_{acac}(L) \frac{2L+1}{2j_{a}+1}$$
(2.10)

are modified single-particle energies.

The matrix elements of these equations provide expressions that determine the single-particle coefficients of fractional parentage,

$$V_{J\mu\nu}(\alpha; IMn) = \langle J\mu\nu | a_{\alpha} | IMn(A+1) \rangle, \qquad (2.11)$$

$$U_{J\mu\nu}(\alpha;IMn) = \langle J\mu\nu | a_{\overline{\alpha}}^{\dagger} | IMn(A-1) \rangle.$$
 (2.12)

To find equations for these quantities, we form the necessary matrix elements of the EOM and evaluate the interaction terms by inserting the completeness relation between the single-fermion operators and the multipole or pair operators. In order to obtain equations that are expressed completely by means of the amplitudes defined in Eqs. (2.11) and (2.12), it is necessary to interchange the order of the single-fermion operator and the pair operator in the interaction terms of Eq. (2.9). This leads to further contributions to the single-particle energy in this equation, in that  $h'_a$  is replaced by  $h''_a$  with

$$h_{a}^{\prime\prime} = h_{a}^{\prime} - \sum_{Lj_{c}} \frac{2L+1}{2j_{a}+1} \left( G_{acac} + \frac{1}{2} F_{acac} \right).$$
(2.13)

In terms of a convenient and physically meaningful set of energy differences and sets of multipole fields and pairing fields defined below, we obtain generalized matrix equations of the Hartree-Bogoliubov form

$$\mathcal{E}_{J\nu}V_{J\mu\nu}(\alpha;IMn) = (\epsilon' + \omega^{(A+1)} + \Gamma^{(A+1)})_{\alpha IMn,\gamma I'M'n'}V_{J\mu\nu}(\gamma;I'M'n') + \Delta_{\alpha IMn,\gamma I'M'n'}U_{J\mu\nu}(\gamma;I'M'n'),$$
(2.14)

$$\mathcal{E}_{J\nu}U_{J\mu\nu}(\alpha;IMn) = (-\epsilon'' + \omega^{(A-1)} - \Gamma^{(A-1)\dagger})_{\overline{\alpha}IMn,\overline{\gamma}I'M'n'} \\ \times U_{J\mu\nu}(\gamma;I'M'n') + \Delta^{\dagger}_{\overline{\alpha}IMn,\overline{\gamma}I'M'n'} \\ \times V_{J\mu\nu}(\gamma;I'M'n').$$
(2.15)

Here

(A + 1)

$$\mathcal{E}_{J\nu} = -E_{J\nu} + \frac{1}{2} (E_0^{(A+1)} + E_0^{(A-1)}), \qquad (2.16)$$

$$\epsilon_{\alpha IMn,\,\gamma I'M'n'}^{\prime} = \delta_{\alpha\gamma}\delta_{II'}\delta_{MM'}\delta_{nn'}(h_a' - \lambda_A), \quad (2.17)$$

$$\lambda_A = \frac{1}{2} (E_0^{(A+1)} - E_0^{(A-1)}), \qquad (2.18)$$

$$\omega_{\alpha INn,\gamma I'M'n'}^{(A\pm1)} = \delta_{\alpha\gamma}\delta_{II'}\delta_{MM'}\delta_{nn'}(E_{In}^{(A\pm1)} - E_0^{(A\pm1)}),$$
(2.19)

$$\Gamma_{aIMn,\gamma I'M'n'}^{(A\pm1)} = \frac{1}{2} \sum_{LM_L} \sum_{bd} s_{\gamma} (j_a m_a j_c - m_c | LM_L) F_{acdb}(L)$$
$$\times \langle I'M'n'(A\pm1) | B_{LM_L}(db) | IMn(A\pm1) \rangle$$
(2.20)

$$\Delta_{\alpha IMn,\gamma I'M'n'} = \frac{1}{2} \sum_{LM_L} \sum_{bd} (j_a m_a j_c - m_c | LM_L) G_{acdb}(L)$$
$$\times \langle I'M'n'(A-1) | A_{LM_L}(db) |$$
$$\times IMn(A+1) \rangle.$$
(2.21)

Furthermore  $E_0^{(A \pm 1)}$  refer to the ground state energies of the neighboring even nuclei, the matrix elements of  $\Gamma^{\dagger}$  are derived from those of Eq. (2.20) simply by the replacement of the operator *B* by  $B^{\dagger}$ , and the matrix elements of  $\Delta^{\dagger}$  are similarly derived from those of  $\Delta$  by the replacement of *A* by  $A^{\dagger}$  together with the interchange  $A \pm 1 \rightarrow A \mp 1$ . Finally  $\epsilon_a''$  is obtained from  $\epsilon_a'$  by the replacement of  $h_a'$  by  $h_a''$ .

In order to specify a scale for the solutions, we take a suitable matrix element of the summed anticommutator,

$$\sum_{\alpha} \{a_{\alpha}, a_{\alpha}^{\dagger}\} = \Omega, \qquad (2.22)$$

$$\Omega = \sum_{j_a} (2j_a + 1).$$
 (2.23)

We thus find

$$\frac{1}{\Omega} \sum_{\alpha IMn} \left[ |U_{J\mu\nu}(\alpha; IMn)|^2 + |V_{J\mu\nu}(\alpha; IMn)|^2 = 1. \right]$$
(2.24)

All of the above equations are still exact and are not necessarily restricted to deformed nuclei. In order to do physics, however, we shall have to impose restrictions on the number and nature of the core states included in any application, as well as on the size of the single-particle space. An essential property of the formalism developed is that the restrictions just listed can be introduced in such a manner that the fundamental symmetries of the Hamiltonian, rotational invariance, and number conservation can be maintained. (If the interaction was translationally invariant, this property could also be guaranteed [11,12].) In fact the main stimulus for introduction of our method in the first place was to restore the broken symmetries of mean-field solutions of the manybody problem. Later it was realized that many other applications, such as the one studied in this paper, were possible.

With the inclusion of generalized pairing, we encounter a property of our equations that they share with the quasiparticle solutions of the Hartree-Fock-Bogoliubov theory [20], namely a doubling of solutions, such that only half describe physical states. In contrast to the well-known case, where the eigenvalues occur as oppositely signed pairs, and the positive energy solutions are the physical ones, in the general theory, because we are also describing excited states, the clean separation of solutions by the sign of the energy fails, and alternatives for identifying physical solutions must be formulated. One of the results in this paper will be a considerable simplification in the method used to make this separation.

### III. MATRIX ELEMENTS OF SINGLE-PARTICLE TRANSITION OPERATORS

We continue the exposition of the general Kerman-Klein formalism by deriving formulas for transition amplitudes of a general one-body operator. We choose this operator to be a tensor of rank L,  $T_{LM_I}$ , that we write in the form

$$T_{LM_L} = \sum_{\beta\gamma} t_{\beta\gamma} a^{\dagger}_{\beta} a_{\gamma}.$$
(3.1)

The notation is such that the quantities  $t_{\alpha\beta}$  include a product of matrix elements of single-particle operators and of associated coupling strengths (charges, gyromagnetic ratios, etc.). We wish to calculate the matrix element  $\langle J' \mu' \nu' | T_{LM_L} | J \mu \nu \rangle$ . To carry through the calculation, we substitute for the ket a formally exact expression in terms of the action of single-particle operators on the states of the core [21],

$$J\mu\nu\rangle = \frac{1}{\Omega} \sum_{\alpha,IMK} \left[ U_{J\mu\nu}(\alpha,IMK)a_{\alpha}^{\dagger} | \underline{IMK} \rangle + V_{J\mu\nu}(\alpha,IMK)a_{\alpha} | \overline{IMK} \rangle \right], \qquad (3.2)$$

where an underline identifies the lighter of the two cores and an overline the heavier one. By using the commutation relations and completeness, this leads to the following expression for the transition element:

$$\langle J'\mu'\nu'|T_{LM_{L}}|J\mu\nu\rangle = \frac{1}{\Omega} \sum_{\alpha,IMK,I'M'K'} \left[ U_{J'\mu'\nu'}(\alpha,I'M'K')U_{J\mu\nu}(\alpha,IMK)\langle \underline{I'M'K'}|T_{LM_{L}}|\underline{IMK}\rangle + V_{J'\mu'\nu'}(\alpha,I'M'K')V_{J\mu\nu}(\alpha,IMK)\langle \overline{I'M'K'}|T_{LM_{L}}|\overline{IMK}\rangle \right]$$

$$+ \frac{1}{\Omega} \sum_{\alpha,\gamma,IMK} t_{\alpha\gamma} \left[ U_{J'\mu'\nu'}(\overline{\alpha},IMK)U_{J\mu\nu}(\overline{\gamma},IMK) - V_{J\mu\nu}(\alpha,IMK)V_{J'\mu'\nu'}(\gamma,IMK) \right].$$
(3.3)

This is now evaluated by use of the Wigner-Eckart theorem with the following definitions of the reduced matrix elements:

$$\langle J'\mu'\nu'|T_{LM_{L}}|J\mu\nu\rangle = \frac{(-1)^{J-\mu}}{\sqrt{2L+1}} (J'\mu'J-\mu|LM_{L})\langle J'\nu'||T_{L}||J\nu\rangle,$$
(3.4)

$$\langle I'M'K'|T_{LM_{L}}|IMK\rangle = \frac{(-1)^{I-M}}{\sqrt{2L+1}}(I'M'I-M|LM_{L})\langle I'K'||T_{L}||IK\rangle,$$
(3.5)

$$t_{\alpha\gamma} = \frac{(-1)^{j_c - m_c}}{\sqrt{2L + 1}} (j_a m_a j_c - m_c | LM_L) t_{ac}, \qquad (3.6)$$

$$V_{J\mu\nu}(\alpha, IMK) = \frac{(-1)^{J-\mu}}{\sqrt{2j_a+1}} (IMJ - \mu | j_a m_a) v_{J\nu}(aIK),$$
(3.7)

$$U_{J\mu\nu}(\alpha, IMK) = \frac{(-1)^{J-\mu+j_a+m_a}}{\sqrt{2j_a+1}} (IMJ-\mu|j_am_a) u_{J\nu}(aIK).$$
(3.8)

With the help of these definitions, we obtain the formula for the reduced matrix element that is utilized in the KKDF model,

$$\langle J'\nu'||T_{L}||J\nu\rangle = \frac{1}{\Omega} \sum_{aIKI'K'} (-1)^{j_{a}+J'+I+L} \begin{cases} I & I' & L \\ J' & J & j_{a} \end{cases} [u_{J\nu}(aIK)u_{J'\nu'}(aI'K') \langle \underline{I'K'}||T_{L}||\underline{IK}\rangle + v_{J\nu}(aIK)v_{J'\nu'}(aI'K') \\ \times \langle \overline{I'K'}||T_{L}||\overline{IK}\rangle] + \frac{1}{\Omega} \sum_{acIK} t_{ac} [(-1)^{j_{a}+I+J+L} \begin{cases} j_{a} & j_{c} & L \\ J & J' & I \end{cases} u_{J'\nu'}(aIK)u_{J\nu}(cIK) \\ + (-1)^{j_{a}+I+J+1} \begin{cases} j_{a} & j_{c} & L \\ J' & J & I \end{cases} v_{J\nu}(aIK)v_{J'\nu'}(cIK) \end{bmatrix}.$$

$$(3.9)$$

This is, with some phase corrections, the formula that was derived in a previous work.

### IV. TRANSFORMATION TO INTRINSIC SYSTEM FOR AXIAL CASE

We have described previously [1-3] several applications of the formalism reviewed in the preceding sections to strongly deformed nuclei. Some of the results, together with some additional calculations, will be used as the basis for a numerical study of the relation of the method of this paper to the traditional strong coupling core-particle model. As will be explained in Sec. VI, this relation can be studied using the formalism already at hand (theory expressed in the "laboratory" system of coordinates); in fact it turned out to be economical for us to carry out all numerical work from this standpoint. Nevertheless, in the following two sections we shall undertake to develop the connection between our method and the way such calculations are normally presented in the intrinsic system. Our justification for this digression is that whenever we have presented a public account of our previous work in this field, one question invariably raised was precisely this connection.

In what follows, we shall answer the question raised in two steps. In the first, carried out in this section, we shall derive a form of our equations in the intrinsic coordinate system that is equivalent to the theory described above, except for two points. The first is that below we do not keep track of number conservation; this choice is just a matter of slight simplification of the notation and can be avoided. Second, we assume that the matrix elements of the multipole and pairing operators are approximated by their forms in the axial rotor limit. We have previously used this assumption in all our recent work for the special cases that arise when we consider the KKDF version of the theory (see below), when we found it necessary to extrapolate measured values; here, higher order corrections can be included in principle. In the second step, considered in the next section, we shall show that the conventional core-particle approach involves a further specialization of the general results derived in this section and examine this limiting case in some theoretical detail. Only at that point do we also introduce the simplifications that distinguish the KKDF model from the Kerman-Klein equations.

For illustrative purposes, we take a model of the even (core) nuclei that consists of the ground-state band  $|IMK=0\rangle = |IM\rangle$  and a finite number of positive parity excited bands  $|IMKn\rangle$ . For the remainder of this section the symbol *n* will be suppressed. We are thus assuming that the eigenstates of the even nuclei have axial symmetry and that their eigenstates can be assigned a definite value of *K*, the component of the angular momentum along the figure axis. This assumption is reasonable as long as the states of the same angular momentum belonging to different bands are well-separated in energy.

We first use rotational invariance to study the structure of the amplitudes *V* and *U* defined in Eqs. (2.11) and (2.12), respectively. For this purpose we introduce a complete set of states  $|R\rangle$  localized in the Euler angles,  $R = (\alpha \beta \gamma)$  and write

$$|IMK\rangle = \int dR|R\rangle \langle R|IMK\rangle$$
$$= \left(\frac{2I+1}{8\pi^2}\right)^{1/2} \int dR|R\rangle D_{MK}^{(I)}(R).$$
(4.1)

The identification of a scalar product of many-body states with the Wigner D function is part of the definition of the model. When Eq. (4.1) is substituted into the definition of V, and use is made of the definitions to follow, we are thereby led to the study of an amplitude such as

$$\langle J\mu\nu|a_{\alpha}|R\rangle = \langle J\mu\nu|U(R)U^{-1}(R)a_{\alpha}U(R)|0\rangle$$
$$= \sum_{\mu'\kappa_{a}} \langle J\mu\nu|U|J\mu'\nu\rangle\langle J\mu'\nu|U^{-1}a_{\alpha}U|0\rangle$$
$$= \sum_{\mu'\kappa_{a}} D^{(J)*}_{\mu\mu'}(R)D^{(j_{a})*}_{m_{a}\kappa_{a}}(R)$$
$$\times \chi_{J\mu'\nu}(j_{a}\kappa_{a})(-1)^{j_{a}+\kappa_{a}}, \qquad (4.2)$$

where U(R) is a unitary rotation operator defined by the value of R. The previous manipulations have utilized the following relations and definitions (of which the first two are standard):

$$\langle JK|U(R)|JM\rangle = D_{KM}^{(J)*}(R), \qquad (4.3)$$

$$U^{-1}(R)a_{jm}U(R) = \sum_{\kappa} a_{j\kappa} D_{m\kappa}^{(j)*}(R), \qquad (4.4)$$

$$\langle J\mu\nu | a_{jm} | 0 \rangle \equiv (-1)^{j+m} \chi_{J\mu\nu}(jm).$$
(4.5)

The introduction of the phase in Eq. (4.5) simplifies the structure of the transformed equations of motion given below.

With the help of the integral of a product of three D functions and the application of standard symmetry properties of CG coefficients, we find

$$V_{J\mu\nu}(\alpha; IMK) = \sum_{\kappa_a} \sqrt{8\pi^2/(2j_a+1)} (-1)^{J-\mu} (IMJ)$$
$$-\mu |j_a m_a) (JK - \kappa_a j_a \kappa_a | IK)$$
$$\times (-1)^{j_a + \kappa_a} \chi_{JK - \kappa_a \nu} (j_a \kappa_a). \tag{4.6}$$

A similar analysis carried out for the amplitude U yields the result

$$U_{J\mu\nu}(\alpha; IMK) = \sum_{\kappa_a} \sqrt{8\pi^{2/2j_a+1)}}$$
$$\times (-1)^{J-\mu+j_a-\kappa_a+j_a+m_a}(IMJ-\mu|j_am_a)$$
$$\times (JK-\kappa_a j_a\kappa_a|IK)\phi_{JK-\kappa_a\nu}(j_a\kappa_a), \quad (4.7)$$

$$\phi_{J\mu\nu}(j_a\kappa_a) = \langle J\mu\nu | a^{\dagger}_{j_a-\kappa_a} | 0 \rangle.$$
(4.8)

Starting from Eqs. (2.14) and (2.15) and utilizing the forms (4.6) and (4.7), we next derive equations satisfied by the amplitudes  $\chi$  and  $\phi$ . The technique is to eliminate the CG coefficients that occur in Eqs. (4.6) and (4.7) by multiplying by  $(IMJ - \mu|j_am_a)(JK - \kappa_a j_a \kappa_a|IK)$  and by the re-

ciprocal of the factors premultiplying these CG coefficients in the one or the other of these equations, summing over M,  $\mu$ , and I, and using standard formulas of angular momentum algebra. Some details are provided in Appendix A. In the equations to follow, the quantities that appear for the first time are defined by the equations

$$\mathcal{R}(m,K|j,J) = \sqrt{(j+m)(j-m+1)} \\ \times \sqrt{(J-K+m)(J+K-m+1)}, \quad (4.9) \\ \langle I'M'K'|B_{LM_{L}}^{\dagger}(db)|IMK\rangle = q_{K'K}^{(L,0)}(db)\sqrt{(2I+1)/(2I'+1)} \\ \times (IMLM_{L}|I'M') \\ \times (IKLK'-K|I'K'), \quad (4.10) \\ \langle I'M'K'|A_{LM_{L}}^{\dagger}(db)|IMK\rangle = \Delta_{K'K}^{(L,0)}(db)\sqrt{(2I+1)/(2I'+1)} \\ \times (IMLM_{L}|I'M') \\ \times (IKLK'-K|I'K'), \quad (4.11) \\ \end{pmatrix}$$

$$\omega_{IK}^{(A\pm1)} = E_K^{(A\pm1)} + \frac{1}{2\mathcal{I}_K^{(A\pm1)}} [I(I+1) - K^2]. \quad (4.12)$$

Of these equations, the quantity  $\mathcal{R}$  is recognized as arising from the matrix elements of the Coriolis coupling and the remaining equations are expressions valid for the axial rotor model for matrix elements of transition operators (see further below) and excitation energies. These expressions constitute definitions of the intrinsic multipole moments q, of the intrinsic pairing moments  $\Delta$ , of the bandhead energies  $E_K$ , and of the moments of inertia  $\mathcal{I}_K$ .

The resulting equations (with partial suppression of the index  $\nu$ ) are

$$\mathcal{E}_{J\nu\chi_{J,K-\kappa_{a}}(j_{a}\kappa_{a})} = \left\{ \epsilon_{a}' + E_{K}^{(A+1)} + \frac{1}{2\mathcal{I}_{K}^{(A+1)}} [J(J+1) - K^{2} + j_{a}(j_{a}+1) + 2\kappa_{a}(K-\kappa_{a})] \right\} \chi_{J,K-\kappa_{a}}(j_{a}\kappa_{a}) \\ + \frac{1}{2\mathcal{I}_{K}^{(A+1)}} \mathcal{R}(\kappa_{a},K|j_{a},J)\chi_{J,K-\kappa_{a}+1}(j_{a}\kappa_{a}-1) + \frac{1}{2\mathcal{I}_{K}^{(A+1)}} \mathcal{R}(-\kappa_{a},-K|j_{a},J)\chi_{J,K-\kappa_{a}-1}(j_{a}\kappa_{a}+1) \\ + \sum_{bcd\kappa_{c}K'L} \frac{1}{2}(-1)^{j_{c}+\kappa_{a}+L}F_{acdb}(L)q_{K'K}^{(L,0)}(db)(j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K')\chi_{J,K-\kappa_{a}}(j_{c}\kappa_{c}) \\ + \sum_{bcd\kappa_{c}K'L} \frac{1}{2}(-1)^{j_{c}+\kappa_{a}+L}G_{acdb}(L)\Delta_{K'K}^{(L,0)}(db)(j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K')\phi_{J,K-\kappa_{a}}(j_{c}\kappa_{c}),$$

$$(4.13)$$

$$\begin{split} \mathcal{E}_{J\nu}\phi_{J,K-\kappa_{a}}(j_{a}\kappa_{a}) = & \left\{ -\epsilon_{a}'' + E_{K}^{(A-1)} + \frac{1}{2\mathcal{I}_{K}^{(A-1)}} \big[ J(J+1) - K^{2} + j_{a}(j_{a}+1) + 2\kappa_{a}(K-\kappa_{a}) \big] \right\} \phi_{J,K-\kappa_{a}}(j_{a}\kappa_{a}) \\ & + \frac{1}{2\mathcal{I}_{K}^{(A-1)}} \mathcal{R}(\kappa_{a},K|j_{a},J) \phi_{J,K-\kappa_{a}+1}(j_{a}\kappa_{a}-1) + \frac{1}{2\mathcal{I}_{K}^{(A-1)}} \mathcal{R}(-\kappa_{a},-K|j_{a},J) \phi_{J,K-\kappa_{a}-1}(j_{a}\kappa_{a}+1) \end{split}$$

$$-\sum_{bcd\kappa_{c}K'L}\frac{1}{2}(-1)^{j_{c}+\kappa_{c}}F_{acdb}(L)q_{K'K}^{(L,0)}(db)(j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K')\phi_{J,K-\kappa_{a}}(j_{c}\kappa_{c})$$
  
+
$$\sum_{bcd\kappa_{c}K'L}\frac{1}{2}G_{acdb}(L)\Delta_{K'K}^{(L,0)}(db)(-)^{j_{c}+\kappa_{c}}(j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K')\chi_{J,K-\kappa_{a}}(j_{c}\kappa_{c}).$$
 (4.14)

In these expressions, we have deliberately chosen, for conciseness of expression, not to do the sum on  $\kappa_c$ , where the value  $\kappa_c = K' - K - \kappa_a$  is imposed by the resident CG coefficient.

We may characterize Eqs. (4.13) and (4.14) as the Kerman-Klein equations for an axially symmetric rotor in the intrinsic frame. These equations fully conserve angular momentum, but, as previously remarked, we have violated number conservation (by equating the multipole matrix elements of two neighboring even nuclei).

Relations (4.10) and (4.11), which have been used in all our previous applications, are approximate, and therefore require further discussion. For example, Eq. (4.10) follows as the value of the first term of the operator expression

$$B_{LM_{L}}^{\dagger}(db) = \sum_{\lambda_{1},\dots,\lambda_{p}} \sum P_{I'M'K'} q_{K'K}^{(L,\lambda)}(db)$$
$$\times \{D_{M_{L},K'-K+\lambda_{1}+\dots+\lambda_{p}}^{(L)}, I_{\lambda_{1}}'\dots I_{\lambda_{p}}'\} P_{IMK}.$$

$$(4.15)$$

Here the *P* are the projection operators for the specified band members,  $I'_{\lambda}$  is a spherical tensor component of the intrinsic angular momentum, and the braces imply a symmetrized expression. Assuming that the connected bands have the same parity, *p* is even for even electric multipoles and odd magnetic multipoles and odd for odd electric multipoles and even magnetic multipoles. If the connected bands have opposite parity, there is a corresponding relation. The form of Eq. (4.15) is a consequence of the assumption that *B* must be a tensor operator of appropriate rank in the Hilbert space of the axial rotor. The further assumption that we can limit ourselves to the first term is that for the states of interest the rotor is almost rigid, as is true for the low-lying states of strongly deformed nuclei. The corresponding expression for the pairing operator requires only the replacements

$$q_{K'K}^{(L,\lambda)} \rightarrow \Delta_{K'K}^{(L,\lambda)}, \qquad (4.16)$$

and the realization that the projection operators to the left and to the right refer to different cores.

The inclusion of odd multipole or pairing interactions requires that, minimally, we choose p=1. The evaluation of such a multipole term is carried out in Appendix B.

### V. CORE-PARTICLE COUPLING MODEL

### A. Spectra

For further development, we specialize the formulas of the previous section to the conventional monopole pairing plus quadrupole-quadrupole model. It is this assumption (and the way in which it is implemented) that reduces the previous theory to the KKDF model. We confine our attention initially to the special case that we include only the groundstate band of the neighboring even cores. (The general case will be considered subsequently.) We also assume that we are treating well-deformed nuclei and continue to ignore number conservation. For L=0 pairing we have in the limit of a constant pairing matrix element

$$-\sum_{b} G_{aabb} \Delta_{00}^{(0,0)}(bb) \equiv 2\Delta_a \sqrt{2j_a + 1} \cong 2\Delta \sqrt{2j_a + 1}.$$
(5.1)

For the quadrupole interaction, we write

$$F_{abcd}(2) = -\kappa_2 F_{ab} F_{dc}, \qquad (5.2)$$

$$\sum_{bd} F_{db} q_{00}^{(2,0)}(db) = Q_0.$$
(5.3)

Because we are dealing with a K=0 band, axial symmetry implies that  $\kappa_a = \kappa_c = \kappa$ , and the quadrupole potential becomes

$$\mathcal{V}_{ac}^{\kappa} = -\frac{1}{2} \kappa_2 F_{ac} Q_0 (-1)^{j_c + \kappa} (j_c - \kappa j_a \kappa | 20).$$
 (5.4)

The potential  $\mathcal{V}$  is symmetric provided we choose

$$F_{ca} = (-1)^{j_a + j_c + 1} F_{ac}, \qquad (5.5)$$

which is consistent with Eq. (2.5).

We next study the limit of our equations found by introducing the simplifications made above. We also begin by neglecting the core excitation energies, and by doing so lose rotational invariance. In fact the next development is a proof that the resulting equations can be reduced to the deformed BCS form. This is standard stuff and is included because of its importance as a step in connecting the KKDF model with the standard core-particle model.

Since in the limit of a collapsed rotational spectrum, the resulting equations do not depend on the total angular momentum, we can thus set (with  $\kappa_a = \kappa$ )

$$\chi_{J,-\kappa}(j_c\kappa) \to \chi_{\kappa c},$$
  
$$\phi_{J,-\kappa}(j_c\kappa) \to \phi_{\kappa c},$$
  
$$\mathcal{E}_{J\nu} \to \mathcal{E}_{\kappa\tau}.$$
 (5.6)

Evidently  $\kappa$  is the component of the quasiparticle angular momentum along the axis of symmetry, and  $\tau$  resolves de-



$$\mathcal{E}_{\kappa\tau}\chi_{\kappa a} = \epsilon_a \chi_{\kappa a} + \mathcal{V}_{ac}^{\kappa}\chi_{\kappa a} - \Delta\phi_{\kappa a}, \qquad (5.7)$$

$$\mathcal{E}_{\kappa\tau}\phi_{\kappa a} = -\epsilon_a\phi_{\kappa a} - \mathcal{V}^{\kappa}_{ac}\phi_{\kappa a} - \Delta\chi_{\kappa a}.$$
(5.8)

From now on we set  $\epsilon'_a = \epsilon''_a = \epsilon_a$ .

These equations are solved by introducing the unitary transformation that diagonalizes the single-particle Hamiltonian

$$\mathcal{H}_{ac}^{\kappa} = \boldsymbol{\epsilon}_a \delta_{ac} + \mathcal{V}_{ac}^{\kappa} \,, \tag{5.9}$$

namely,

$$\chi_{\kappa c} = \sum_{\tau} A_{c\tau}^{\kappa} v_{\kappa\tau},$$

$$v_{\kappa\tau} = \sum_{c} A_{c\tau}^{\kappa*} \chi_{\kappa c},$$
(5.10)

$$\sum_{\tau} A_{a\tau}^{\kappa*} A_{b\tau}^{\kappa} = \delta_{ab},$$

$$\sum_{a} A_{a\tau}^{\kappa*} A_{a\tau'}^{\kappa} = \delta_{\tau\tau'},$$

$$\sum_{ac} A_{a\tau}^{\kappa*} \mathcal{H}_{ac}^{\kappa} A_{c\tau'}^{\kappa} = e_{\kappa\tau} \delta \tau \tau'.$$
(5.11)

We thus obtain a standard set of BCS equations

$$\mathcal{E}_{\kappa\tau} v_{\kappa\tau} = e_{\kappa\tau} v_{\kappa\tau} - \Delta u_{\kappa\tau}, \qquad (5.12)$$

$$\mathcal{E}_{\kappa\tau}u_{\kappa\tau} = -e_{\kappa\tau}u_{\kappa\tau} - \Delta v_{\kappa\tau}, \qquad (5.13)$$

with the usual solutions

$$\mathcal{E}_{\kappa\tau} = \pm \sqrt{e_{\kappa\tau}^2 + \Delta^2}, \qquad (5.14)$$

where corresponding to the plus sign, we have the physical solutions

$$\psi_{\kappa\tau} = \begin{pmatrix} v_{\kappa\tau} \\ u_{\kappa\tau} \end{pmatrix}, \tag{5.15}$$

and to the minus sign the unphysical solutions

$$\overline{\psi}_{\kappa\tau} = \begin{pmatrix} -u_{\kappa\tau} \\ v_{\kappa\tau} \end{pmatrix}.$$
(5.16)

As stated above, we have reviewed this familiar material because of its importance in the definition of the standard core-particle model. The point is that the full set of solutions of the deformed BCS equations, physical and unphysical together, generate a complete set of vectors; the solutions of the full set of equations of the KKDF model will ultimately be expanded in this set, and the conventional core-particle model will be understood as an approximate form of this expansion. We have now laid the groundwork for the solution of the full equations of motion (4.13) and (4.14). For this general solution the notational change contained in Eq. (5.6) is generalized to

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$$\chi_{J,-\kappa}(J_c\kappa) \to \chi_{J\kappa c},$$
  
$$\phi_{J,-\kappa}(j_c\kappa) \to \phi_{J\kappa c}.$$
 (5.17)

The retention of the angular momentum quantum number J expresses the fact that the full problem has rotational symmetry. Introducing again the transformation that diagonalizes the single-particle Hamiltonian  $\mathcal{H}^{\kappa}$ ,

$$\chi_{J\kappa a} = \sum_{\tau} A^{\kappa}_{a\tau} \chi_{J\kappa\tau},$$
$$\chi_{J\kappa\tau} = \sum_{a} A^{\kappa*}_{a\tau} \chi_{J\kappa a}, \qquad (5.18)$$

with a corresponding transformation for  $\phi$ , the equations of motion become

$$\mathcal{E}_{J\nu}\chi_{J\kappa\tau} = e_{\kappa\tau}\chi_{J\kappa\tau} - \Delta\phi_{J\kappa\tau} + \sum_{\kappa'\tau'} U^{J}_{\kappa\tau,\kappa'\tau'}\chi_{J\kappa'\tau'},$$
(5.19)

$$\mathcal{E}_{J\nu}\phi_{J\kappa\tau} = -e_{\kappa\tau}\phi_{J\kappa\tau} - \Delta\chi_{J\kappa\tau} + \sum_{\kappa'\tau'} U^{J}_{\kappa\tau,\kappa'\tau'}\phi_{J\kappa'\tau'},$$
(5.20)

and the nonvanishing matrix elements of U that occur in these equations (that reinstate the angular momentum and include the Coriolis coupling) are

$$2\mathcal{I}U^{J}_{\kappa\tau,\kappa\tau'} = \sum_{a} A^{*}_{a\tau} [J(J+1) + j_{a}(j_{a}+1) - 2\kappa^{2}] A_{a\tau'},$$
  

$$2\mathcal{I}U^{J}_{\kappa\tau,\kappa-1\tau'} = \sum_{a} A^{*}_{a\tau} \mathcal{R}(\kappa,0|j_{a},J) A_{a\tau'},$$
  

$$2\mathcal{I}U^{J}_{\kappa\tau,\kappa+1\tau'} = \sum_{a} A^{*}_{a\tau} \mathcal{R}(-\kappa,0|j_{a},J) A_{a\tau'}.$$
 (5.21)

We recall that the quantities  $\mathcal{R}$  are defined in Eq. (4.9).

Before continuing, it may be helpful to consider the physical content of Eqs. (5.19) and (5.20). Let us recall the meaning of the notation. The triple of quantum numbers  $J, \kappa, \tau$  identifies the different angular momentum states of the axial band with K quantum number  $\kappa$  and additional labeling  $\tau$ . The "Coriolis" coupling represented by the matrix elements of U mixes states of the same J but different axial components, effectively destroying the axial symmetry. For further discussion, we introduce the amplitudes

$$\Psi_{J\kappa\tau} = \begin{pmatrix} \chi_{J\kappa\tau} \\ \phi_{J\kappa\tau} \end{pmatrix}.$$
 (5.22)

If we look once more at the limit in which U=0, we have two sets of solutions of Eqs. (5.19) and (5.20), namely, the physical and unphysical BCS solutions, respectively,



$$\overline{\Psi}_{J\kappa\tau} = \overline{C}_{J\kappa\tau} \overline{\psi}_{\kappa\tau}. \tag{5.24}$$

Under these assumptions, Eqs. (5.19) and (5.20) reduce to Eqs. (5.7) and (5.8). Furthermore the constants C and  $\overline{C}$  are not determined, expressing the collapse of the rotational spectrum and the loss of rotational invariance.

By contrast, the exact solution of Eqs. (5.19) and (5.20) has the form

$$\Psi_{J\nu} = \sum_{\kappa\tau} \left[ C_{J\kappa\tau} \psi_{\kappa\tau} + \overline{C}_{J\kappa\tau} \overline{\psi}_{\kappa\tau} \right], \qquad (5.25)$$

which is to be understood as the expansion of the solution of the full Hamiltonian in terms of solutions of the unperturbed problem.

In our actual applications, we have not used the expansion (5.25), and therefore we shall not pursue this line in full generality. Our only reason for exhibiting this equation is that it provides the basis for defining the conventional coreparticle model. In this model only the first term on the right-hand side of Eq. (5.25) is retained, under the assumption that the physical solution of the problem with rotational excitation restored can be approximated adequately in terms of the physical solutions without rotation. It is this assumption that we shall later check by comparison with the full solution.

As a consequence of the assumption just described, we obtain the equations of the standard core-particle model, which in the present notation read

$$\mathcal{E}_{J\nu}C_{J\kappa\tau} = \mathcal{E}_{\kappa\tau}C_{J\kappa\tau} + \sum_{\kappa'\tau'} W^{J}_{\kappa\tau,\kappa'\tau'}C_{J\kappa'\tau'}, \qquad (5.26)$$

$$W_{\kappa\tau,\kappa'\tau'} = \widetilde{\psi}_{\kappa\tau} U^J_{\kappa\tau,\kappa'\tau'} \psi_{\kappa'\tau'}.$$
(5.27)

This is a standard diagonalization problem with the "correct" number of solutions.

We consider next the general case defined in the theoretical formulation of the previous section, with multiple bands in the core nuclei, but with the maintenance of axial symmetry. Though not really necessary, it makes sound physical sense to proceed as follows: We lean on the fact that the interband quadrupole transitions are weak compared to intraband transitions. Thus we shall first ignore the terms associated with these transitions as well as the perturbation associated with finite excitation energy above the bandhead. What remains is a Hartree-Bogoliubov approximation for excited bands. Next we add the "Coriolis coupling" and thus obtain a series of bands in close analogy with our treatment of Coriolis coupling for the ground-state band. Finally, we introduce the coupling arising from interband transitions in the cores.

In fact, it is hardly necessary to give many details of the previous steps. All we need is an enhanced notation. Instead of the ground state band, we consider a band  $K\sigma$ , where 00 is the ground state band, 01 the beta band, 20 the gamma band, etc. Now to all the quantities defined above, such as  $\Delta$ ,  $Q_0$ ,  $\mathcal{V}_{ac}^{\kappa}$ ,  $\chi_{\kappa c}$ ,  $\phi_{\kappa c}$ , etc., we add a superscript ( $K\sigma$ ). Thus after transformation by the matrix  $A_{c\tau}^{\kappa,K\sigma}$  the excited state HB equations become

$$(\mathcal{E}_{\kappa\tau}^{K\sigma} - E^{K\sigma})v_{\kappa\tau}^{K\sigma} = e_{\kappa\tau}^{K\sigma}v_{\kappa\tau}^{K\sigma} - \Delta^{K\sigma}u_{\kappa\tau}^{K\sigma}, \qquad (5.28)$$

$$(\mathcal{E}^{K\sigma}_{\kappa\tau} - E^{K\sigma})u^{K\sigma}_{\kappa\tau} = -e^{K\sigma}_{\kappa\tau}u^{K\sigma}_{\kappa\tau} - \Delta^{K\sigma}v^{K\sigma}_{\kappa\tau}, \qquad (5.29)$$

with the solutions

$$\mathcal{E}_{\kappa\tau}^{K\sigma} = E^{K\sigma} \pm \sqrt{(e_{\kappa\tau}^{K\sigma})^2 + (\Delta^{K\sigma})^2}, \qquad (5.30)$$

where the first term on the right-hand side is clearly the bandhead energy. The remainder of the calculation also parallels that made for the case of the ground-state band. The only quantities requiring more than a notational change are the matrix elements of the operator U defined in Eq. (5.21). The necessary emendations can be read off directly from the core-particle equations (4.13) and (4.14).

Thus we have specified a procedure for deriving a set of state vectors  $\Psi_{J\nu}^{K\sigma}$  and associated energies  $\mathcal{E}_{J\nu}^{K\sigma}$ . We have taken account of all terms in the effective Hamiltonian except for the interband multipole fields. To finally include the latter, we write

$$\hat{\mathcal{V}} = \tau_3(\hat{\mathcal{V}}_d + \hat{\mathcal{V}}_{od}), \tag{5.31}$$

where  $\tau_3$  is the usual Pauli matrix, *d* refers to the intraband parts of the multipole field, and *od* to the interband parts. It remains to take into account only the latter piece. This is done by a final mixing

$$\Theta_{J\rho} = \sum_{\nu K\sigma} \mathcal{A}^{J}_{\rho,\nu K\sigma} \Psi^{K\sigma}_{J\nu}, \qquad (5.32)$$

where the mixing coefficients are determined by the conditions

$$\mathcal{E}_{J\rho}\mathcal{A}^{J}_{\rho,\nu K\sigma} = \mathcal{E}^{K\sigma}_{J\nu}\mathcal{A}^{J}_{\rho,\nu K\sigma} + \sum_{\nu' K'\sigma'} \mathcal{F}^{J}_{\nu K\sigma,\nu' K'\sigma'}\mathcal{A}^{J}_{\rho,\nu' K'\sigma'},$$
(5.33)

$$\mathcal{F}^{J}_{\nu K\sigma,\nu'K'\sigma'} = \widetilde{\Psi}^{K\sigma}_{J\nu} \tau_{3} \hat{\mathcal{V}}_{od} \Psi^{K'\sigma'}_{J\nu'}.$$
(5.34)

In the last two sections, we have derived the conventional form of the core-particle coupling theory from the KKDF formalism. In fact the equations derived in the first of these sections were exact, i.e., completely equivalent to those of KKDF, indeed only their form in the "intrinsic frame." The core-particle coupling model as customarily presented involves, as described after Eq. (5.25), an additional approximation in the solution of these equations. Indeed, the essence of the model lies in this approximation rather than in whether calculations are carried out in the intrinsic system as described above or in the laboratory system as is done in the full application of the KKDF method. In the next full section, we shall record the form of the core-particle approximation in the laboratory frame.

#### **B.** Core-particle coupling model: Transitions

Here we shall only indicate the step involving the exact transformation of Eq. (3.9) into an expression referring to the intrinsic system. Since we shall not utilize this version of the formalism, we leave the further transformation by the introduction of the approximate solutions developed in the pre-

ceding subsection as an exercise for the reader. This step is to introduce values for the reduced matrix elements on the right-hand side of Eq. (3.9) and to carry out the summations over *I* and *I'* in order to reach a formula appropriate to the core-particle coupling model. By comparing Eq. (3.4) with Eq. (4.10), Eq. (3.7) with Eq. (4.6), and Eq. (3.8) with Eq. (4.7), we can read off the formulas

$$\langle I'K' || T_L || IK \rangle = \sqrt{2I+1} q_{K'K}^{(L,0)} (IKLK' - K | I'K'),$$
(5.35)

$$v_{J\nu}(aIK) = \sum_{\kappa_a} \sqrt{8\pi^2} (-1)^{j_a + \kappa_a} (JK - \kappa_a j_a \kappa_a | IK)$$
$$\chi_{JK - \kappa_a}(j_a \kappa_a), \tag{5.36}$$

$$u_{J\nu}(aIK) = \sum_{\kappa_a} \sqrt{8\pi^2(-1)^{j_a - \kappa_a}} (JK - \kappa_a j_a \kappa_a | IK)$$
$$\times \phi_{JK - \kappa_a}(j_a \kappa_a). \tag{5.37}$$

Carrying out the summations over I and I', we are led to the equation

$$\langle J'\nu'||T_{L}||J\nu\rangle = \frac{8\pi^{2}}{\Omega} \sum_{a\kappa_{a}\kappa K'} \frac{1}{\sqrt{2J'+1}} (JK - \kappa_{a}LK' - K|J'K' - \kappa_{a}) [\phi_{JK-\kappa_{a}}(j_{a}\kappa_{a})\phi_{J'K'-\kappa_{a}}(j_{a}\kappa_{a}) + \chi_{JK-\kappa_{a}}(j_{a}\kappa_{a})\chi_{J'K'-\kappa_{a}}(j_{a}\kappa_{a})] + \frac{8\pi^{2}}{\Omega} \sum_{acK} t_{ac} [(-1)^{j_{c}+\kappa_{c}}(j_{a}-\kappa_{a}j_{c}\kappa_{c}|L\kappa_{c}-\kappa_{a})(JK-\kappa_{c}L\kappa_{c}-\kappa_{a}|J'K-\kappa_{a})] \times \frac{1}{\sqrt{(2L+1)(2J'+1)}} \phi_{J'K-\kappa_{a}}(j_{a}\kappa_{a})\phi_{JK-\kappa_{c}}(j_{c}\kappa_{c}) + (-1)^{j_{c}+\kappa_{c}+J+J'+L}(j_{a}-\kappa_{a}j_{c}\kappa_{c}|L\kappa_{c}-\kappa_{a}) \times (J'K-\kappa_{c}L\kappa_{c}-\kappa_{a}|JK-\kappa_{a}) \frac{1}{\sqrt{(2L+1)(2J+1)}} \chi_{JK-\kappa_{a}}(j_{a}\kappa_{a})\chi_{J'K-\kappa_{c}}(j_{c}\kappa_{c}).$$
(5.38)

### VI. CORE-PARTICLE COUPLING MODEL IN LABORATORY FRAME

We show here that the core-particle coupling model can be formulated just as conveniently in the laboratory frame of reference as in the intrinsic frame. We start with the fundamental matrix equations of motion, Eqs. (2.14) and (2.15), and reduce them by application of the Wigner-Eckart theorem. By means of Eqs. (3.7) and (3.8), Eqs. (4.10) and (4.11), and standard angular momentum algebra, we find the equations (assuming that K' - K and L are even, as is the case for the specific model considered in the body of this paper)

$$\mathcal{E}_{J\nu}v_{J\nu}(aIK) = (\epsilon_a + \omega_{IK})v_{J\nu}(aIK) + \sum_{cI'K'} \Gamma(aIK, cI'K')v_{J\nu}(cI'K') + \sum_{cI'K'} \Delta(aIK, cI'K')u_{J\nu}(cI'K'),$$
(6.1)

$$\mathcal{E}_{J\nu}u_{J\nu}(aIK) = (-\epsilon_a + \omega_{IK})u_{J\nu}(aIK)$$
$$-\sum_{cI'K'} \Gamma(aIK, cI'K')u_{J\nu}(cI'K')$$

$$+\sum_{cI'K'} \Delta(aIK, cI'K') v_{J\nu}(cI'K'),$$
(6.2)

$$\Gamma(aIK,cI'K') = \frac{1}{2}\sum_{Lbd} F_{acdb}(L)q_{K'K}^{(L,0)} \\ \times (db)\sqrt{(2L+1)(2I+1)} \\ \times (-1)^{j_a+I+J} \begin{cases} j_a & j_c & L \\ I' & I & J \end{cases} \\ \times (IKLK'-K|I'K'), \qquad (6.3) \end{cases}$$

$$\Delta(aIK,cI'K') = \frac{1}{2}\sum_{Lbd} G_{acdb}(L)\Delta^{(L,0)}_{K'K} \\ \times (db)\sqrt{(2L+1)(2I+1)} \\ \times (-1)^{j_a+I+J} \begin{cases} j_a & j_c & L \\ I' & I & J \end{cases} \\ \times (IKLK'-K|I'K').$$
(6.4)

In Eqs. (6.1) and (6.2) we have set  $\epsilon_a' = \epsilon_a'' = \epsilon_a$ .

We introduce a condensed notation for Eqs. (6.1) and (6.2), writing them in the operator form

$$\mathcal{E}_{J\nu}\Psi_{J\nu} = \hat{\mathcal{K}}\Psi_{J\nu} + \hat{\omega}\Psi_{J\nu}, \qquad (6.5)$$

$$\hat{\mathcal{K}} = \begin{pmatrix} \boldsymbol{\epsilon} + \boldsymbol{\Gamma} & \boldsymbol{\Delta} \\ \boldsymbol{\Delta} & -\boldsymbol{\epsilon} - \boldsymbol{\Gamma} \end{pmatrix}, \tag{6.6}$$

$$\hat{\omega} = \begin{pmatrix} \omega & 0\\ 0 & \omega \end{pmatrix}. \tag{6.7}$$

We solve these equations in the approximation that forms part of the definition of the core-particle model, as explained after Eq. (5.25). Again we consider first the simplest case where only the ground state band of the cores is included. The extension to excited bands and interband coupling can be dealt with in analogy to the treatment described for the intrinsic system. Let the physical solutions of Eq. (6.5) with  $\hat{\omega}=0$  be designated as  $\Psi_{J\nu}^{(0)}$ , with corresponding energies  $\mathcal{E}_{J\nu}^{(0)}$ . Here the symbol  $\nu$  abbreviates the set ( $\kappa\tau$ ). We approximate the solutions of the full equation by the expansion

$$\Psi_{J\nu} = \sum_{\nu'} \mathcal{C}^{J}_{\nu\nu'} \Psi^{(0)}_{J\nu'}.$$
(6.8)

The introduction of this expansion into Eq. (6.5) leads immediately to the standard eigenvalue problem

$$\mathcal{E}_{J\nu}\mathcal{C}^{J}_{\nu\nu'} = \mathcal{E}^{(0)}_{J\nu'}\mathcal{C}^{J}_{\nu\nu'} + \sum_{\nu''} \mathcal{U}^{J}_{\nu'\nu''}\mathcal{C}^{J}_{\nu\nu''}, \qquad (6.9)$$

$$\mathcal{U}_{\nu'\nu''}^{J} = \widetilde{\Psi}_{J\nu'}^{(0)} \hat{\omega} \Psi_{J\nu''}^{(0)}.$$
 (6.10)

This equation is to be compared with Eq. (5.26), to which it is equivalent as long as  $\hat{\omega}$  has the form assumed in the derivation of the latter. In fact, Eq. (6.9) has an advantage in the case that the excitation spectrum is not conveniently expressed in algebraic form, but its numerical values are known from experiment.

We can extend the theory to include multiple bands in the core nuclei. We use the labels  $K\sigma$  to distinguish the different bands and now take as a zeroth approximation the coupling of the odd particle to a single one of these bands. The theory is, to start with, the same as that described above except that we must distinguish the results for the various cores, and this is done by a superscript  $K\sigma$ . In so far as the multipole fields and pairing fields for the band  $K\sigma$  are almost equal to those for the ground band, the energies  $\mathcal{E}_{J\nu}^{K\sigma(0)}$  are almost independent of  $K\sigma$ . We prefer to lift this degeneracy by shifting each of these energies by  $E^{K\sigma}$ , the bandhead energy, and redefining  $\hat{\omega}$  to be the excitation energy above the bandhead in each case. The step that follows is to introduce the mixing due to the core excitations and again only the change in notation already specified is necessary to record the equations that generalize Eqs. (6.9) and (6.10).

The final step is to include the further mixing due to interband multipole fields (assuming that such mixing for the pairing fields can be neglected). For this purpose, we decompose  $\hat{\Gamma}$  into an intraband piece (subscript *d*) and an interband part (subscript *od*), the latter having so far been neglected, according to the equation

$$\hat{\Gamma} = \tau_3 (\hat{\Gamma}_d + \hat{\Gamma}_{od}), \qquad (6.11)$$

where  $\tau_3$  is the usual Pauli matrix. The perturbation previously neglected is dealt with by the expansion

$$\Theta_{J\rho} = \sum_{\nu K\sigma} \mathcal{D}^{J}_{\rho,\nu K\sigma} \Psi^{K\sigma}_{J\nu}, \qquad (6.12)$$

where the mixing coefficients are determined by the conditions

$$\mathcal{E}_{J\rho}\mathcal{D}^{J}_{\rho,\nu K\sigma} = \mathcal{E}^{K\sigma}_{J\nu}\mathcal{D}^{J}_{\rho,\nu K\sigma} + \sum_{\nu' K'\sigma'} \mathcal{G}^{J}_{\nu K\sigma,\nu' K'\sigma'}\mathcal{D}^{J}_{\rho,\nu' K'\sigma'},$$
(6.13)

$$\mathcal{G}^{J}_{\nu K\sigma,\nu'K'\sigma'} = \widetilde{\Psi}^{K\sigma}_{J\nu} \tau_3 \widehat{\Gamma}_{od} \Psi^{K'\sigma'}_{J\nu'}.$$
(6.14)

#### VII. IMPROVED ALGORITHM

The main source of difficulty perceived in the solution of the KKDF equations is that the set of solutions is overcomplete by a factor of 2. This is a consequence of the fact that the basis states form an overcomplete (and, consequently, nonorthogonal set). Thus half of the states found by solving the EOM are not physical and have to be identified and removed. The technique previously used to perform this task has now been understood to be unnecessarily complicated.

In the previous approach [1,7] the Hamiltonian is first decomposed into symmetric and antisymmetric parts with respect to particle-hole conjugation. If only the antisymmetric part is diagonalized, then for every positive energy eigenvalue there is a negative partner. From the BCS theory we know that the positive eigenvalues are the physical solutions and the negative eigenvalues the nonphysical ones. Then the symmetric part is turned on "slowly" and at every step the physical solutions are identified using a projection operator built from the wave functions of the previous step. Since the equations of motion have to be solved at each step, the time needed to perform the calculation is correspondingly longer than for a single diagonalization. (In most applications a typical number of steps is 5.)

A simpler and quicker approach has now been identified. Since the problem decomposes into subproblems involving states of a fixed angular momentum, we can invoke the nocrossing theorem. This means that the relative order in energy of the physical and of the nonphysical states does not change as we turn on the symmetric part of the Hamiltonian. If the lower half of the states (negative in particular) are the unphysical ones in the BCS limit, then at the physical limit where the full Hamiltonian is used, the lower half of the states are again the unphysical ones. Consequently, we need only to solve the equations of motion at the two limits, the BCS limit and the full Hamiltonian limit. These remarks about the technique of solution apply not only to the strong coupling examples studied in the next section, but also to less straightforward applications of the KKDF method.

#### VIII. APPLICATIONS

We illustrate the remarks of the previous sections with applications to a pair of well-deformed nuclei. The first application is to the nucleus  $^{157}$ Gd, which we have studied previously [1,2].  $^{157}$ Gd is a well deformed nucleus and thus





FIG. 1. Negative parity energy levels for <sup>157</sup>Gd. The circles correspond to the experimental values, the solid line to the KKDF model, and the dotted line to the core-particle coupling model.

suitable for application of the strong coupling core-particle model. To recall a few details, we used a large single-particle space (including all states from five major shells). The energies and matrix elements of these single-particle levels were calculated using the Woods-Saxon potential. The odd neutron is coupled to the cores <sup>156</sup>Gd and <sup>158</sup>Gd, which are represented not only by their ground bands, but also by several excited bands, as was found necessary to fit all the observed bands of <sup>157</sup>Gd. The core excitation energies,  $\omega_I$ , were given by phenomenological formulas tuned to experiment. In the same way as in the previous papers, the strength of the quadrupole field is treated as a free parameter and the values of the single-particle energies found from Woods-Saxon calculations are allowed to vary by  $\pm 5\%$ . First we solved the EOM problem of the full KKDF model and fixed the strength of the quadrupole force and the single-particle energies in order to achieve the best fit. Then we solved the EOM for the core-particle model as described in Sec. VI, using the same parameters. The results are shown in Fig. 1. We can see from the figure that the two models give very similar results. In Fig. 2 we show the result of the B(E2)calculations. Again it is clear that the two models give very similar results.

The second application was to the proton spectrum of  $^{157}$ Tb, with  $^{156}$ Gd and  $^{158}$ Dy cores. We used the same method as described above and the results are shown in Fig. 3. The conclusion is the same as in the previous application, namely that the two methods give very similar results. Observed B(E2) values are too few to allow a meaningful comparison.

To the extent that the examples chosen are typical, it is apparent that for well-deformed nuclei the strong coupling core-particle model gives almost as good results as the full KKDF model. We emphasize, however, the greater range of validity of the KKDF model, in particular to cases such as transitional nuclei [4,22], where none of the usual traditional versions of the core-particle model is applicable.

# IX. DISCUSSION AND CONCLUDING REMARKS

In this paper, we have studied a semimicroscopic coreparticle coupling theory, the KKDF theory, and particularly



FIG. 2. B(E2) transitions for <sup>157</sup>Gd. Comparison of the KKDF model and the core-particle coupling model. The points with error bars are the experimental data, the dashed lines result from the core-particle model, and the solid lines from the KKDF model.

its relationship to the traditional strong coupling core-particle model. The KKDF theory is formulated in the laboratory system of coordinates, and as such, can be applied both to the spherical vibrational (weak coupling) and deformed rotational (strong coupling) regimes, as well as to transitional cases. A significant portion of this paper has been devoted to transforming the KKDF equations from the laboratory to the intrinsic system of coordinates, the latter defined only for the well-deformed regime. We have pointed out the additional approximation necessary to reduce the KKDF equations to those of the usual core-particle limit. We have then applied both the full and the limiting model to a few illustrative nuclei and found only small differences in the numerical results. This justification is, for our purposes, less significant than it would have been in the past, since we have also formulated an improved algorithm that renders the KKDF equations essentially as simple to deal with as the defined approximation.



FIG. 3. Positive parity energy levels for <sup>157</sup>Tb. The circles correspond to the experimental values, the solid line to the KKDF model, and the dotted line to the core-particle coupling model.

The reason for the good agreement between the approximate and the complete theory obviously expresses the fact that there is little mixing between physical and unphysical states as we "turn on" the coupling that is initially suppressed in our approach. This means that they stay well separated in energy. We can expect this situation to change for applications where there are multiple avoided crossings.

### APPENDIX A: SOME DETAILS OF THE DERIVATION OF THE CORE-PARTICLE COUPLING MODEL

We provide some details of the derivations of Eqs. (4.13) and (4.14). The first terms that require special attention are those involving the excitation energy in the even nuclei. We immediately do the sum over  $M, \mu$ . Now consider Eq. (4.13), where we encounter the term

$$(\omega_{IK} - E_K)(J\mu' j_a \kappa_a | IK) = \left( j_a - \kappa_a J\mu' \left| \frac{1}{2\mathcal{I}_K} [(\mathbf{J} + \mathbf{j})^2 - K^2] \right| IK \right), \quad (A1)$$

(suppressing mass number). We can replace the combination  $(\mathbf{J}+\mathbf{j})^2$  by

$$J(J+1) + j_a(j_a+1) + 2(K-\kappa_a)\kappa_a + j_-J_+ + j_+J_-.$$
(A2)

Applying the standard algebra of the raising and lowering operators and shifting the variables  $\kappa_a$  as required for these terms, we thus obtain additional contributions of single-particle type as well as the Coriolis coupling.

We consider next the contributions of the multipole and pairing fields, a calculation that requires most of the modest labor involved in the derivation of Eqs. (4.13) and (4.14). As an example of what is involved, we compute the contribution of the even multipoles to the right-hand side of Eq. (4.14), which we label  $T(\Gamma^{\dagger}:JKj_a\kappa_a)$ . Utilizing Eqs. (4.7) and (4.10), we must evaluate the expression

$$T(\Gamma^{\dagger}: JKj_{a}\kappa_{a}) = \frac{1}{2}\sum_{k} (-1)^{j_{c}+m_{a}+\kappa_{c}-\kappa_{a}}\sqrt{(2j_{a}+1)(2I+1)/(2j_{c}+1)(2I'+1)}F_{acdb}(L)q_{K'K}^{(L,0)}(db)(j_{a}-m_{a}j_{c}m_{c}|LM_{L})$$

$$\times (IMLM_{L}|I'M')(I'M'Jm_{c}-M'|j_{c}m_{c})(IMJm_{a}-M|j_{a}m_{a})(JK-\kappa_{a}j_{a}\kappa_{a}|IK)(IKLK'_{K}|I'K')$$

$$\times (JK'-\kappa_{c}j_{c}\kappa_{c}|I'K')\phi_{J,K'-\kappa_{c}}(j_{c}\kappa_{c}).$$
(A3)

In this equation the sum is over all angular momentum variables not indicated explicitly on the left-hand side except for  $m_a$ , which disappears from the final result.

To evaluate this expression, we first study the partial sum

$$S = \sum_{m_c} (-1)^{j_c + m_a} \sqrt{(2j_a + 1)/(2j_c + 1)} (j_a - m_a j_c m_c | Lm_c - m_a) (IMLm_c - m_a | I'M') (I'M'Jm_c - M'|j_c m_c)$$
  
=  $(-1)^{j_a + I' + J} \sqrt{(2L+1)(2I'+1)} \begin{cases} j_a & j_c & L \\ I' & I & J \end{cases} (IMJm_a - M|j_a m_a),$  (A4)

which can be derived from Edmonds [23]. The sum over M then removes two more CG coefficients from Eq. (A3). The next step is to apply Edmonds (6.2.6) to evaluate the sum over I', leading to a final trivial sum over I. We thus find

$$S' = \sum_{II'} (-1)^{j_a + I' + J} \sqrt{(2L+1)(2I+1)} (JK - \kappa_a j_a \kappa_a | IK)$$

$$\times (IKLK' - K | I'K') (JK' - \kappa_c j_c \kappa_c | I'K') \begin{cases} j_a & j_c & L \\ I' & I & J \end{cases}$$

$$= (-1)^{\kappa_c - \kappa_a + j_c + \kappa_c} (j_c - \kappa_c j_a \kappa_a | LK' - K).$$
(A5)

Equations (A4) and (A5) are the essential results for the evaluation of Eq. (A3) leading to the appropriate term in Eq. (4.14). The pairing term in the same equation and the multipole and pairing terms in Eq. (4.13) can be shown (after straightforward transformations for the latter) to involve the same basic sums, up to phase factors.

#### APPENDIX B: CONTRIBUTION OF ODD MULTIPOLE OPERATORS

In the main text, we have included in the general core-particle equations (4.13) and (4.14) only contributions from even electric multipole-multipole interactions, assuming that the included bands are all of the same parity. If we wish to include odd electric multipole-multipole forces to lowest order, we must replace the matrix element Eq. (4.10) by the value of the matrix element

$$\langle I'M'K'|B_{LM_{L}}^{\dagger}(db)|IMK\rangle = q_{K'K}^{(L,1)}(db)\sum_{\lambda} \langle I'M'K'|\{D_{M_{L}K'-K+\lambda}^{L},I_{\lambda}'\}|IMK\rangle.$$
(B1)

Here  $I'_{\lambda}$ ,  $\lambda = \pm 1,3$  are the spherical tensor components of the angular momentum in the "intrinsic" system, expressed in terms of the Cartesian components (where they differ) by the equations

$$I'_{+1} = -\frac{1}{\sqrt{2}}(I'_{1} + iI'_{2}) = -\frac{1}{\sqrt{2}}I'_{+},$$
  

$$I'_{-1} = \frac{1}{\sqrt{2}}(I'_{1} - iI'_{2}) = \frac{1}{\sqrt{2}}I'_{-}.$$
(B2)

With the help of the well-known matrix elements of the intrinsic components, Eq. (B1) takes the value

$$\langle I'M'K'|B_{LM_{L}}^{\dagger}(db)|IMK\rangle = q_{K'K}^{(L,1)}(db)(IMLM_{L}|I'M') \left\{ -\frac{1}{\sqrt{2}} [(IK-1LK'-K+1|I'K')\sqrt{(I+K)(I-K+1)} + \sqrt{(I-K')(I'+K'+1)}(IKLK'-K+1|I'K'+1)] + \frac{1}{\sqrt{2}} [(IK+1LK'-K-1|I'K') + \sqrt{(I-K)(I+K+1)} + \sqrt{(I'+K')(I'-K'+1)}(IKLK'-K-1|I'K'-1)] + (K+K')(IKLK'-K|I'K') \right\}.$$

$$(B3)$$

With these values, we are now in a position to evaluate the contributions of an odd electric multipole force to our core-particle coupling equations. We first consider the contributions to Eq. (4.14). As an example, consider the first term of Eq. (B3). The calculation parallels that described in the previous appendix. The sum (A4) repeats itself in every case. The sum (A5) is replaced, in general, by different expressions. In the case of the first term of Eq. (B3), the sum S' is replaced by the sum

$$S_{1}' = \sum_{II'} (-1)^{j_{a}+I'+J} \sqrt{(2L+1)(2I+1)} (JK - \kappa_{a}j_{a}\kappa_{a}|IK) (IK - 1LK' - K + 1|I'K') (JK' - \kappa_{c}j_{c}\kappa_{c}|I'K') \times \begin{cases} j_{a} & j_{c} & L \\ I' & I & J \end{cases} \sqrt{(I+K)(I-K+1)}.$$
(B4)

For  $S'_1$ , the sum over I' can be carried out as before, but after this has been done, instead of a final normalization condition for CG coefficients, we encounter the sum

$$\sum_{I} (JK - \kappa_a j_a \kappa_a | IK) (JK - \kappa_a - 1 j_a \kappa_a | IK - 1) \sqrt{(I + K)(I - K + 1)} = \sqrt{(J - K + \kappa_a + 1)(J + K - \kappa)},$$
(B5)

which involves the same "trick" as used in the evaluation of the Coriolis coupling. Of the terms arising from Eq. (B3), the first and third require the procedure just described, the second and fourth a similar procedure in which we interchange the order of the sums on I and I', and the fifth the same calculation as in the previous appendix. We also find that the first two terms are equal, as are the third and fourth.

Altogether, we find for the contribution to Eq. (4.14), the expression

$$\sum_{bcd\kappa_{c}K'L} (-1)^{j_{c}+\kappa_{c}} F_{acdb}(L) q_{K'K}^{(L,1)}(db) \left[ \frac{1}{\sqrt{2}} \sqrt{(J-K+\kappa_{a}+1)(J+K-\kappa_{a})} (j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K'-1) \phi_{J,K-1-\kappa_{a}}(j_{c}\kappa_{c}) - \frac{1}{\sqrt{2}} \sqrt{(J+K-\kappa_{a}+1)(J-K+\kappa_{a})} (j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K'+1) \phi_{J,K+1-\kappa_{a}}(j_{c}\kappa_{c}) - \frac{1}{2} (K+K') (j_{c}-\kappa_{c}j_{a}\kappa_{a}|LK-K') \phi_{J,K-\kappa_{a}}(j_{c}\kappa_{c}) \right].$$
(B6)

For conciseness of expression, we have not done the sum over  $\kappa_c$ . In this form it can be shown that the corresponding contribution to Eq. (4.13) differs only by overall sign and by the replacement

$$(-1)^{j_c+\kappa_c} \rightarrow (-1)^{j_c+\kappa_a+L}.$$
(B7)

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