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

Pavlos Protopapas * and Abraham Klein †
Department of Physics, University of Pennsylvania, Philadelphia, PA 19104-6396
(August 10, 1996)

Abstract

We review briefly the fundamental equations of a semi-microscopic 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. $^{157}$Gd and $^{157}$Tb, the core-coupling method and the full theory give similar results.

PACS number(s): 21.60.-n, 21.60.Ev, 21.10.-k, 21.10.Re

I. INTRODUCTION

We have recently undertaken the task of revitalizing and extending a semi-microscopic 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 core-particle 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 between times, 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 Dönaü 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 excitation. 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 core-particle 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 core-particle 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

We start with a shell-model Hamiltonian of the form

\[ H = \sum_{\alpha} h_{a}a_{\alpha}^{\dagger}a_{\alpha} + \frac{1}{4} \sum_{abcd} \sum_{LM} F_{abcd}(L)B_{LM}^{\dagger}(ac)B_{LM}(db) + \frac{1}{4} \sum_{abcd} \sum_{ML} G_{abcd}(L)A_{LM}^{\dagger}(ab)A_{LM}(cd). \]  

(2.1)

Here \( h_{a} \) are the spherical single-particle energies referred to the nearest closed shell, \( \alpha \) refers to the standard set of single-particle quantum numbers, including in particular the pair \((j_{a}, m_{a})\) and \( a \) refers to the same set with \( m_{a} \) omitted. \( B_{LM}^{\dagger} \) is the particle-hole multipole operator,

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

(2.2)

and \( A_{LM}^{\dagger} \) is the particle-particle multipole operator,

\[ A_{LM}^{\dagger}(ab) \equiv \sum_{m_{a}m_{b}} (j_{a}m_{a}j_{b} - m_{b}|LM_{L})a_{\alpha}^{\dagger}a_{\beta}^{\dagger}, \]  

(2.3)

where \((j_{1}m_{1}j_{2}m_{2}|jm)\) 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,

\[ F_{abcd}(L) \equiv \sum_{m_{a}m_{b}} s_{\gamma}s_{\beta}(j_{a}m_{a}j_{c} - m_{c}|LM_{L})(j_{d}m_{d}j_{b} - m_{b}|LM_{L})V_{\alpha\beta\gamma\delta}, \]  

(2.4)

which satisfies the relation
and $G$ the particle-particle matrix elements

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

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 $|IMn\rangle$. The corresponding 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,

$$[a_\alpha, H] = h'_a a_\alpha$$

$$\quad + \frac{1}{2} \sum_{bd\gamma} \sum_{LM} s_\gamma (j_a m_a j_c - m_c|LM) F_{acdb}(L)a_\gamma B_{LM}(db)$$

$$\quad + \frac{1}{2} \sum_{bd\gamma} \sum_{LM} (j_a m_a j_c - m_c|LM) G_{acbd}(L)a_\gamma A_{LM}(bd),$$

$$[a_\alpha^\dagger, H] = -h'_a a_\alpha^\dagger$$

$$\quad - \frac{1}{2} \sum_{bd\gamma} \sum_{LM} s_\gamma (j_a - m_a j_c m_c|LM) F_{acdb}(L)B_{LM}^\dagger (db)a_\gamma^\dagger$$

$$\quad - \frac{1}{2} \sum_{bd\gamma} \sum_{LM} (j_a - m_a j_c m_c|LM) G_{acbd}(L)A_{LM}^\dagger (bd)a_\gamma.$$ (2.8)

Here

$$h'_a = h_a - \frac{1}{4} \sum_{Lj} F_{acac}(L) \frac{2L+1}{2j_a+1}$$

are modified single-particle energies.

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

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

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

\[
h_a'' = h_a' - \sum_{L_jc} \frac{2L + 1}{2j_a + 1} (G_{acac} + \frac{1}{2} F_{acac}).
\] (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

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

Here

\[
\mathcal{E}_{J\nu} = -E_{J\nu} + \frac{1}{2}(E_0^{(A+1)} + E_0^{(A-1)}),
\]
\[
\epsilon'_{\alpha IMn,\gamma I'M'n'} = \delta_{\alpha\gamma} \delta_{II'} \delta_{MM'} \delta_{nn'} (h_a' - \lambda_A),
\]
\[
\lambda_A = \frac{1}{2}(E_0^{(A+1)} - E_0^{(A-1)}),
\]
\[
\omega^{(A\pm 1)}_{\alpha IMn,\gamma I'M'n'} = \delta_{\alpha\gamma} \delta_{II'} \delta_{MM'} \delta_{nn'} (E_{I'n}^{(A\pm 1)} - E_{I'n}^{(A\pm 1)}),
\]
\[
\Gamma^{(A\pm 1)}_{\alpha IMn,\gamma I'M'n'} = \frac{1}{2} \sum_{L_M L_L} \sum_{bd} s_\gamma (j_a m_a j_c - m_c) [LM_L] F_{acdb}(L),
\]
\[
\langle I'M'n'(A \pm 1)|B_{LM_L}(db)|IMn(A \pm 1)\rangle
\]
\[
\Delta_{\alpha IMn,\gamma I'M'n'} = \frac{1}{2} \sum_{L_M L_L} \sum_{bd} (j_a m_a j_c - m_c) [LM_L] G_{acdb}(L)
\]
\[
\langle I'M'n'(A - 1)|A_{LM_L}(db)|IMn(A + 1)\rangle.
\] (2.20)

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 (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,

\[
\sum_\alpha \{ a_\alpha, a_\alpha^\dagger \} = \Omega,
\]
\[
\Omega = \sum_{j_a} (2j_a + 1).
\] (2.22)

We thus find

\[
5
\]
\[
\frac{1}{\Omega} \sum_{\alpha IMn} |U_{J\mu\nu}(\alpha; IMn)|^2 + |V_{J\mu\nu}(\alpha; IMn)|^2 = 1.
\] (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.

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

We next apply the formalism to the computation of matrix elements of single-particle tensor operators, \(T_{LM_L}\), that we write in the form

\[
T_{LM_L} = \sum_{\beta\gamma} t_{\beta\gamma} a_{\beta}^\dagger a_{\gamma}.
\] (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,

\[
|J\mu\nu\rangle = \frac{1}{\Omega} \sum_{\alpha,IMK} [U_{J\mu\nu}(\alpha, IMK)a_{\alpha}^\dagger|IMK\rangle + V_{J\mu\nu}(\alpha, IMK)a_{\alpha}|IMK\rangle],
\] (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:

\[
\langle J'\mu'\nu'|T_{LM_L}|J\mu\nu\rangle = \frac{1}{\Omega} \sum_{\alpha,IMK}\sum_{\alpha',IMK'} [U_{J'\mu'\nu'}(\alpha, IM'K')U_{J\mu\nu}(\alpha, IMK)
\times\langle IM'K'|T_{LM_L}|IMK\rangle + [V_{J'\mu'\nu'}(\alpha, IM'K')V_{J\mu\nu}(\alpha, IMK)\langle IM'K'|T_{LM_L}|IMK\rangle
+ \frac{1}{\Omega} \sum_{\alpha,\gamma,IMK} t_{\alpha\gamma} [U_{J'\mu'\nu'}(\bar{\alpha}, IMK)U_{J\mu\nu}(\bar{\gamma}, IMK)
- V_{J'\mu\nu}(\alpha, IMK)V_{J\mu\nu}(\gamma, IMK)]].
\] (3.3)

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

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

\[
\langle IM'K'|T_{LM_L}|IMK\rangle = \frac{(-1)^{I'-M}}{\sqrt{2L+1}} \langle I'M'I - M|LM_L\rangle
\times \langle IK'|T_L||IK\rangle,
\] (3.5)

\[
t_{\alpha\gamma} = \frac{(-1)^{J_c-M_c}}{\sqrt{2L+1}} (j_am_a j_c - m_c|LM_L) t_{ac},
\] (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)

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

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

\[
\langle J'\nu'||T_L||J\nu \rangle = \frac{1}{\Omega} \sum_{acIK} t_{ac} \left[ (-1)^{j_a+I+L} \left\{ \begin{array}{ccc}
J' & L \\
j_a & J & J_a \\
\end{array} \right\} u_{J\nu}(cIK) v_{J\nu}(aIK) + (-1)^{j_a+I+1+L} \left\{ \begin{array}{ccc}
J' & L \\
j_a & J & J_a \\
\end{array} \right\} v_{J\nu}(aIK) u_{J\nu}(cIK) \right]
\]
(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, we shall derive a form of our equations in the intrinsic coordinate system that is fully equivalent to the theory described above. Second we shall show that the conventional core-particle approach involves a further specialization of this general result and examine this limiting case in some theoretical detail.

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 \( |IM Kn \rangle \). 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

$$|IMK\rangle = \int dR |R\rangle \langle R|IMK\rangle$$

$$= \left(\frac{2I + 1}{8\pi^2}\right)^{\frac{1}{2}} \int dR |R\rangle D^{(j)}_{MK}(R)$$

The identification of a scalar product of many-body states with the Wigner $D$ function is part of the definition of the model. When (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

$$\langle J_{\mu\nu}|a_\alpha|R\rangle = \langle J_{\mu\nu}|U(R)U^{-1}(R)a_\alpha U(R)|0\rangle$$

$$= \sum_{\mu'\kappa_a} \langle J_{\mu\nu}|U|J_{\mu'\nu}\rangle \langle J_{\mu'\nu}|U^{-1}a_\alpha U|0\rangle$$

$$= \sum_{\mu'\kappa_a} D^{(j)_\ast}_{\mu\mu'}(R) D^{(j'\ast)}_{m_a\kappa_a}(R) \chi_{J_{\mu'\nu}}(j_a\kappa_a)(-1)^{j_{a'\kappa_a}},$$

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):

$$\langle JK|U(R)|JM\rangle = D^{(j)_\ast}_{KM}(R),$$

$$U^{-1}(R)a_{jm} U(R) = \sum_{\kappa} a_{j\kappa} D^{(j)}_{m\kappa}(R),$$

$$\langle J_{\mu\nu}|a_{jm}|0\rangle \equiv (-1)^{j_{a'\kappa_a}} \chi_{J_{\mu\nu}}(jm).$$

The introduction of the phase in (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

$$V_{j_{\mu\nu}}(\alpha;IMK) = \sum_{\kappa_a} \sqrt{\frac{8\pi^2}{2j_{a}+1}} (-1)^{j_{a'}-\mu} (IMJ - \mu|j_{a}m_a)$$

$$\times \langle JK - \kappa_a j_a\kappa_a |IK\rangle (-1)^{j_{a'\kappa_a}} \chi_{JK - \kappa_a\nu}(j_a\kappa_a).$$

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

$$U_{j_{\mu\nu}}(\alpha;IMK) = \sum_{\kappa_a} \sqrt{\frac{8\pi^2}{2j_{a}+1}} (-1)^{j_{a'}-\kappa_a} (IMJ - \mu|j_{a}m_a)$$

$$\times \langle JK - \kappa_a j_a\kappa_a |IK\rangle \phi_{JK - \kappa_a\nu}(j_a\kappa_a),$$

$$\phi_{j_{\mu\nu}}(j_a\kappa_a) = \langle J_{\mu\nu}|a_{jm}^\dagger|0\rangle.$$
coefficients that occur in (4.6) and (4.7) by multiplying by \((IMJ - \mu|ja_m|)(JK - \kappa_{JaK_a}|IK')\)
and by the reciprocal of the factors pre-multiplying these CG coefficients in the one or the
other of these equations, summing over \(M, \mu\) and \(J\), 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

\[
\mathcal{R}(m, K|j, J) = \sqrt{(j + m)(j - m + 1)} \\
\times (J - K + m)(J + K - m + 1), \tag{4.9}
\]

\[
\langle I'M'K'|B_{LML}^\dagger(db)|IMK\rangle = q^{(L, 0)}_{K'K}(db) \sqrt{\frac{2I + 1}{2I' + 1}} \\
\times (IMLM_L|I'M'(IKLK' - K|I'K')), \tag{4.10}
\]

\[
\langle I'M'K'|A_{LML}^\dagger(db)|IMK\rangle = \Delta^{(L, 0)}_{K'K}(db) \sqrt{\frac{2I + 1}{2I' + 1}} \\
\times (IMLM_L|I'M'(IKLK' - K|I'K')), \tag{4.11}
\]

\[
\omega^{(A \pm 1)}_{J, K'} = E^{(A \pm 1)}_K + \frac{1}{2T^{(A \pm 1)}_K} |I(I + 1) - K^2|. \tag{4.12}
\]

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 band-head energies \(E_K\), and of the moments of inertia \(T_K\).

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

\[
\mathcal{E}_{J, \nu, \chi, J, K - \kappa_a(ja\kappa_a)} = \{\epsilon'_a + E^{(A+1)}_K + \frac{1}{2T^{(A+1)}_K}[J(J + 1) - K^2] \\
+ ja(j_a + 1) + 2\kappa_a(K - \kappa_a)]\} \chi_{J, K - \kappa_a(ja\kappa_a)} \\
+ \frac{1}{2T^{(A+1)}_K} \mathcal{R}(\kappa_a, K|ja, J) \chi_{J, K - \kappa_a+1(ja\kappa_a - 1)} \\
+ \frac{1}{2T^{(A+1)}_K} \mathcal{R}(-\kappa_a, -K|ja, J) \chi_{J, K - \kappa_a-1(ja\kappa_a + 1)} \\
+ \sum_{bcdeK'KL} \frac{1}{2}(-1)^{j_c + \kappa_a + L} F_{abcd}(L) q^{(L, 0)}_{K'K}(db) \\
\times (j_c - \kappa_c ja\kappa_a|LK - K') \chi_{J, K - \kappa_c(jc\kappa_c)} \\
+ \sum_{bcdeK'KL} \frac{1}{2}(-1)^{j_c + \kappa_a + L} G_{abcd}(L) \Delta^{(L, 0)}_{K'K}(db) \\
\times (j_c - \kappa_c ja\kappa_a|LK - K') \phi_{J, K - \kappa_a(jc\kappa_c)}, \tag{4.13}
\]

\[
\mathcal{E}_{J, \nu, \phi, J, K - \kappa_a(ja\kappa_a)} = \{-\epsilon''_a + E^{(A-1)}_K + \frac{1}{2T^{(A-1)}_K}[J(J + 1) - K^2] \\
+ ja(j_a + 1) + 2\kappa_a(K - \kappa_a)]\} \phi_{J, K - \kappa_a(ja\kappa_a)} \\
+ \frac{1}{2T^{(A-1)}_K} \mathcal{R}(\kappa_a, K|ja, J) \phi_{J, K - \kappa_a+1(ja\kappa_a - 1)}
\]
\[ + \frac{1}{2I_K^{(A-1)}} \mathcal{R}(-\kappa_a, -K|j_a, J) \phi_{J,K-\kappa_a-1}(j_a\kappa_a + 1) \]
\[ - \sum_{bcd\kappa,K'} \frac{1}{2}(-1)^{j_c+\kappa_e} F_{acdb}(L) q_{K'K}^{(L,0)}(db) \]
\[ \times (j_c - \kappa_c j_a \kappa_a |LK - K') \phi_{J,K-\kappa_a}(j_c\kappa_c) \]
\[ + \sum_{bcd\kappa,K'} \frac{1}{2} G_{acdb}(L) \Delta_{K'K}^{(L,0)}(db)(-)^{j_c+\kappa_c} \]
\[ \times (j_c - \kappa_c j_a \kappa_a |LK - K') \chi_{J,K-\kappa_a}(j_c\kappa_c). \] (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.

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

\[ B_{LM}^\dagger(db) = \sum_{\lambda_1,\ldots,\lambda_p} \sum_{P,I'} \phi_{KL}^{(L,\lambda)}(db) \]
\[ \times \left\{ D_{ML,K'-K+\lambda_1+\ldots+\lambda_p}^{(L)} I'_1 \cdots I'_{\lambda_p} \right\} P_{IMK}. \] (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 (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

\[ q_{K'K}^{(L,\lambda)} \rightarrow \Delta_{K'K}^{(L,\lambda)}, \] (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 and confine our attention initially to the special case that we include only the ground-state band of the neighboring even cores. (The general case will be considered subsequently.) We also assume that we are
treating well-deformed nuclei and ignore number conservation. For $L = 0$ pairing we have
in the limit of a constant pairing matrix element
\[
- \sum_b G_{aabb} \Delta_{00}^{(0,0)} \equiv 2\Delta_a \sqrt{2j_a + 1} \approx 2\Delta \sqrt{2j_a + 1}. \tag{5.1}
\]

For the quadrupole interaction, we write
\[
F_{abcd}^{(2)} = -\kappa_2 F_{ab} F_{dc}, \tag{5.2}
\]
\[
\sum_{bd} F_{db}^{(2,0)} \equiv Q_0. \tag{5.3}
\]

Because we are dealing with a $K = 0$ band, axial symmetry implies that $\kappa_a = \kappa_c = \kappa$, and
the quadrupole potential becomes
\[
V_{ac}^\kappa = -\frac{1}{2} \kappa_2 F_{ac} Q_0 (-1)^{j_c + \kappa} (j_c - \kappa j_a |20). \tag{5.4}
\]

The potential $V$ is symmetric provided we choose
\[
F_{ca} = (-1)^{j_a + j_c + 1} F_{ac}, \tag{5.5}
\]
which is consistent with (2.5).

We next study the limit of our equations found by introducing the simplifications made
above and also neglecting the core excitation energies. The resulting equations do not depend
on the total angular momentum, and we thus set (with $\kappa_a = \kappa$)
\[
\chi_{J,-\kappa}(j_c \kappa) \rightarrow \chi_{\kappa c},
\]
\[
\phi_{J,-\kappa}(j_c \kappa) \rightarrow \phi_{\kappa c},
\]
\[
E_{J\nu} \rightarrow E_{\kappa \tau}. \tag{5.6}
\]

Evidently $\kappa$ is the component of the quasi-particle angular momentum along the axis of symmetry, and $\tau$ resolves degeneracies in the values of $\kappa$. In the limit considered our equations
thus reduce to a Hartree-Bogoliubov set
\[
E_{\kappa \tau} \chi_{\kappa a} = \epsilon_a \chi_{\kappa a} + V_{ac}^\kappa \chi_{\kappa a} - \Delta \phi_{\kappa a}, \tag{5.7}
\]
\[
E_{\kappa \tau} \phi_{\kappa a} = -\epsilon_a \phi_{\kappa a} - V_{ac}^\kappa \phi_{\kappa a} - \Delta \chi_{\kappa a}. \tag{5.8}
\]

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
\[
H_{ac}^\kappa = \epsilon_a \delta_{ac} + V_{ac}^\kappa, \tag{5.9}
\]

namely,
\[ \chi_{\kappa c} = \sum_{\tau} A_{\kappa \tau}^c \psi_{\kappa \tau}, \]
\[ \psi_{\kappa \tau} = \sum_{c} A_{\kappa \tau}^{c*} \chi_{\kappa c}, \] (5.10)

\[ \sum_{\tau} A_{\kappa \tau}^{c*} A_{\kappa \tau}^c = \delta_{ab}, \]
\[ \sum_{\tau} A_{\kappa \tau}^{c*} A_{\kappa \tau}^{c'} = \delta_{\tau \tau'}, \]
\[ \sum_{ac} A_{\kappa \tau}^{c*} H_{ac}^\kappa A_{\kappa \tau}^c = e_{\kappa \tau} \delta_{\tau \tau'}. \] (5.11)

We thus obtain a standard set of BCS equations

\[ \mathcal{E}_{\kappa \tau} \psi_{\kappa \tau} = e_{\kappa \tau} \psi_{\kappa \tau} - \Delta u_{\kappa \tau}, \] (5.12)
\[ \mathcal{E}_{\kappa \tau} \psi_{\kappa \tau} = -e_{\kappa \tau} \psi_{\kappa \tau} - \Delta u_{\kappa \tau}, \] (5.13)

with the usual solutions

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

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

\[ \psi_{\kappa \tau} = \begin{pmatrix} v_{\kappa \tau} \\ u_{\kappa \tau} \end{pmatrix}, \] (5.15)

and to the minus sign the unphysical solutions

\[ \tilde{\psi}_{\kappa \tau} = \begin{pmatrix} -u_{\kappa \tau} \\ v_{\kappa \tau} \end{pmatrix}. \] (5.16)

We have reviewed this familiar material because of its importance in the definition of the standard core-particle model.

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 (5.6) is generalized to

\[ \chi_{J,-\kappa}(J_{c\kappa}) \rightarrow \chi_{J_{c\kappa}}, \]
\[ \phi_{J,-\kappa}(J_{c\kappa}) \rightarrow \phi_{J_{c\kappa}}, \]
\[ \mathcal{E}_{J\nu} \rightarrow \mathcal{E}_{J_{\kappa\tau}}. \] (5.17)

Introducing again the transformation that diagonalizes the single-particle Hamiltonian \( H^\kappa \),

\[ \chi_{J_{c\kappa}} = \sum_{\tau} A_{c\tau}^\kappa \chi_{J_{\kappa\tau}}, \]
\[ \chi_{J_{c\kappa}} = \sum_{a} A_{a\tau}^{c*} \chi_{J_{c\kappa}}, \] (5.18)

with a corresponding transformation for \( \phi \), the equations of motion become
and the non-vanishing matrix elements of $U$ that occur in these equations (that reinstate the angular momentum and include the Coriolis coupling) are

\[2IU_{J_\kappa \kappa_\tau, J_\kappa_\tau'} = \sum_A A^*_{a_\tau} \left( J(J + 1) + j_a(j_a + 1) - 2\kappa^2 \right) A_{a_\tau'}, \]

\[2IU_{J_\kappa \kappa - 1, J_\kappa_\tau'} = \sum_A A^*_{a_\tau} \mathcal{R}(\kappa, 0|j_a, J) A_{a_\tau'}, \]

\[2IU_{J_\kappa \kappa + 1, J_\kappa_\tau'} = \sum_A A^*_{a_\tau} \mathcal{R}(-\kappa, 0|j_a, J) A_{a_\tau'}.\] (5.21)

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

At this point we introduce the defining approximation for the core-particle coupling model, first defining

\[\Psi_{J_\kappa} = \begin{pmatrix} \chi_{J_\kappa} \\ \phi_{J_\kappa} \end{pmatrix},\] (5.22)

and then assuming that $\Psi$ can be expanded in terms of the physical solutions of Eqs. (5.7) and (5.8), namely,

\[\Psi_{J_\kappa} \simeq C_{J_\kappa} \psi_{\kappa}.\] (5.23)

By contrast, the exact expression must be the sum of a physical and an unphysical solution. If we include the latter, we have, in fact, returned to the KKDF model and to its basic technical problem of selecting physical solutions. Although, as we shall see later, we have found a simplified method to handle this problem, compared to the approach used in earlier work, it remains of interest to know when the traditional core-particle model is valid.

With the help of (5.23), Eqs. (5.19) and (5.20) can be reduced to a form of the core-particle coupling equations ready for final numerical study, namely,

\[E_{J_\kappa} C_{J_\kappa} = E_{\kappa} C_{J_\kappa} + \sum_{J_\kappa_\tau'} W_{J_\kappa \kappa_\tau'} C_{J_\kappa_\tau'},\] (5.24)

\[W_{\kappa, \kappa_\tau'} = \tilde{\psi}_{\tau} U_{\kappa, \kappa_\tau'} \psi_{\kappa_\tau'}.\] (5.25)

This is a standard diagonalization problem with the “correct” number of solutions. These solutions will be compared with the exact solution of the corresponding KKDF equations.

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 band-head. 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 $\Delta$, $Q_0$, $V_{\alpha\ell}$, $\chi_{\kappa\ell}$, $\phi_{\kappa\ell}$, etc., we add a superscript $(K\sigma)$. Thus after transformation by the matrix $A_{\kappa,K\sigma}^{\kappa,K_{\sigma}}$, the excited state HB equations become

$$
\begin{align}
(E_{\kappa\tau}^{K\sigma} - E_{\kappa\tau}^{K\sigma})v_{\kappa\tau}^{K\sigma} &= \varepsilon_{\kappa\tau}^{K\sigma}v_{\kappa\tau}^{K\sigma} - \Delta_{\kappa\tau}^{K\sigma}u_{\kappa\tau}^{K\sigma}, \\
(E_{\kappa\tau}^{K\sigma} - E_{\kappa\tau}^{K\sigma})u_{\kappa\tau}^{K\sigma} &= -\varepsilon_{\kappa\tau}^{K\sigma}u_{\kappa\tau}^{K\sigma} - \Delta_{\kappa\tau}^{K\sigma}v_{\kappa\tau}^{K\sigma},
\end{align}
$$

with the solutions

$$
E_{\kappa\tau}^{K\sigma} = E^{K\sigma} \pm \sqrt{ (\varepsilon_{\kappa\tau}^{K\sigma})^2 + (\Delta_{\kappa\tau}^{K\sigma})^2 },
$$

where the first term on the right hand side is clearly the band-head 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 form 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 $\mathcal{E}_{K\sigma}$, where we have amalgamated the pair of quantum numbers $\kappa\tau$ into the symbol $\nu$. We have taken account of all terms in the effective Hamiltonian except for the interband multipole fields. To finally include the latter, we write

$$
\hat{\nu} = \tau_3(\hat{\nu}_d + \hat{\nu}_{od}),
$$

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

$$
\Theta_{J\rho} = \sum_{\nu K\sigma} A_{J,\rho,\nu K\sigma} \Psi_{J\nu}^{K\sigma},
$$

where the mixing coefficients are determined by the conditions

$$
\begin{align}
\mathcal{E}_{J\rho}A_{J,\rho,\nu K\sigma}^{J,\rho,\nu K\sigma} &= \mathcal{E}_{J\nu}^{K\sigma}A_{J,\rho,\nu K\sigma}^{J,\rho,\nu K\sigma} \\
&+ \sum_{\nu' K'\sigma'} \mathcal{F}_{J,\nu K\sigma,\nu' K'\sigma'}^{J,\rho,\nu K\sigma} A_{J,\rho,\nu' K'\sigma'}^{J,\rho,\nu' K'\sigma'};
\end{align}
$$

$$
\mathcal{F}_{J,\nu K\sigma,\nu' K'\sigma'}^{J,\rho,\nu K\sigma} = \tilde{\Psi}_{J\nu}^{K\sigma} \tau_3 \hat{\nu}_{od} \Psi_{J\nu'}^{K'\sigma'}.
$$

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, 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 intrinsic system. coupling theory in the laboratory frame.

B. Core-particle coupling model: transitions

Here we shall only indicate the step involving the exact transformation of (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 preceding subsection as an exercise for the reader. This step is to introduce values for the reduced matrix elements on the right hand side of (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 (3.4) with (4.10), (3.7) with (4.6), and (3.8) with (4.7), we can read off the formulas

\[
\langle I'K'||T_L||IK \rangle = \sqrt{2I + 1} q^{(L,0)}_{K,K'} (IKL - K'I'K'), \tag{5.33}
\]

\[
v_{J\nu}(aIK) = \sum_{\kappa_a} \sqrt{8\pi^2} (-1)^{J_a + \kappa_a} (JK - \kappa_a j_a \kappa_a |IK) \times \chi_{JK - \kappa_a}(j_a \kappa_a), \tag{5.34}
\]

\[
u_{J\nu}(aIK) = \sum_{\kappa_a} \sqrt{8\pi^2} (-1)^{J_a - \kappa_a} (JK - \kappa_a j_a \kappa_a |IK) \times \phi_{JK - \kappa_a}(j_a \kappa_a). \tag{5.35}
\]

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

\[
\langle J'\nu'||T_L||J\nu \rangle = \frac{8\pi^2}{\Omega} \sum_{a\kappa_a K K'} \frac{1}{\sqrt{2J' + 1}} (JK - \kappa_a LK' - K|J'K' - \kappa_a)
\times [\phi_{JK - \kappa_a}(j_a \kappa_a) \phi_{J'K' - \kappa_a}(j_a \kappa_a) + \chi_{JK - \kappa_a}(j_a \kappa_a) \chi_{J'K' - \kappa_a}(j_a \kappa_a)]
+ \frac{8\pi^2}{\Omega} \sum_{acK} t_{ac}((-1)^{J_c + \kappa_c}(J_a - \kappa_a j_c \kappa_c |L \kappa_c - \kappa_a)(JK - \kappa_c L \kappa_c - \kappa_a |J'K - \kappa_a)
\times \frac{1}{\sqrt{(2L + 1)(2J' + 1)}} \phi_{JK - \kappa_e}(j_c \kappa_c)
+ (-1)^{J_c + \kappa_c + J + J'}(J_a - \kappa_a j_c \kappa_c |L \kappa_c - \kappa_a)(J'K - \kappa_c L \kappa_c - \kappa_a |JK - \kappa_a)
\times \frac{1}{\sqrt{(2L + 1)(2J + 1)}} \chi_{JK - \kappa_a}(j_a \kappa_a) \chi_{J'K - \kappa_c}(j_c \kappa_c). \tag{5.36}
\]

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),

\[
E_{J\nu}v_{J\nu}(aIK) = (\epsilon_a + \omega_{IK})v_{J\nu}(aIK)
+ \sum_{cI'K'} \Gamma(aIK, cI'K')v_{J\nu}(cI'K')
+ \sum_{cI'K'} \Delta(aIK, cI'K')u_{J\nu}(cI'K'),
\]

(6.1)

\[
E_{J\nu}u_{J\nu}(aIK) = (-\epsilon_a + \omega_{IK})u_{J\nu}(aIK)
- \sum_{cI'K'} \Gamma(aIK, cI'K')u_{J\nu}(cI'K')
+ \sum_{cI'K'} \Delta(aIK, cI'K')v_{J\nu}(cI'K'),
\]

(6.2)

\[
\Gamma(aIK, cI'K') = \frac{1}{2} \sum_{Lbd} F_{acdb}(L)q_{IK, K'}^{(L, 0)}(db) \sqrt{(2L + 1)(2I + 1)}
\times (-1)^{j_a + I + J} \left\{ \begin{array}{c} j_a \ j_c \\ I' \ I \ J \end{array} \right\} (IKLK' - K|I'K'),
\]

(6.3)

\[
\Delta(aIK, cI'K') = \frac{1}{2} \sum_{Lbd} G_{acdb}(L)\Delta_{IK, K'}^{(L, 0)}(db) \sqrt{(2L + 1)(2I + 1)}
\times (-1)^{j_a + I + J} \left\{ \begin{array}{c} j_a \ j_c \\ I' \ I \ J \end{array} \right\} (IKLK' - K|I'K').
\]

(6.4)

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

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

\[
E_{J\nu} \Psi_{J\nu} = \hat{K} \Psi_{J\nu} + \hat{\omega} \Psi_{J\nu},
\]

(6.5)

\[
\hat{K} = \begin{pmatrix} \epsilon + \Gamma & \Delta \\ \Delta & -\epsilon - \Gamma \end{pmatrix},
\]

(6.6)

\[
\hat{\omega} = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix}.
\]

(6.7)

We solve these equations in the approximation that forms part of the definition of the core-particle model. 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 (6.5) with \( \hat{\omega} = 0 \) be designated as \( \Psi_{J\nu}^{(0)} \), with corresponding energies \( E_{J\nu}^{(0)} \). Here the symbol \( \nu \) abbreviates the set \( (\kappa \tau) \). We approximate the solutions of the full equation by the expansion

\[
\Psi_{J\nu} = \sum_{J\nu'} C_{J\nu'}^{J\nu} \Psi_{J\nu'}^{(0)}.
\]

(6.8)

The introduction of this expansion into (6.5) leads immediately to the standard eigenvalue problem
\[ \mathcal{E}_{j\nu} c_{j\nu'} = \mathcal{E}^{(0)}_{j\nu} c_{j\nu'} + \sum_{\nu''} u_{j\nu'\nu''} c_{j\nu''}, \]  
(6.9)  
\[ \mathcal{U}_{j\nu'\nu''} = \tilde{\Psi}_{j\nu'} \hat{\omega} \tilde{\Psi}_{j\nu''}. \]  
(6.10)

This equation is to be compared with Eq. (5.24), to which it is equivalent as long as \( \hat{\omega} \) has the form assumed in the derivation of the latter. In fact, (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 \( \mathcal{E}^{K\sigma(0)}_{j\nu} \) are almost independent of \( K\sigma \). We prefer to lift this degeneracy by shifting each of these energies by \( E^{K\sigma} \), the band head energy, and redefining \( \hat{\omega} \) to be the excitation energy above the band head 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 (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

\[ \hat{\Gamma} = \tau_3 (\hat{\Gamma}_d + \hat{\Gamma}_{od}), \]  
(6.11)  
where \( \tau_3 \) is the usual Pauli matrix. The perturbation previously neglected is dealt with by the expansion

\[ \Theta_{J\rho} = \sum_{\nu K\sigma} D^J_{\rho,\nu K\sigma} \Psi^K_{J\nu}, \]  
(6.12)

where the mixing coefficients are determined by the conditions

\[ \mathcal{E}_{J\rho} D^J_{\rho,\nu K\sigma} = \mathcal{E}^{K\sigma}_{j\nu} D^J_{\rho,\nu K\sigma} \]  
(6.13)  
\[ + \sum_{\nu' K'\sigma'} G^J_{\nu K\sigma,\nu' K'\sigma'} D^J_{\rho,\nu' K'\sigma'}, \]  
\[ G^J_{\nu K\sigma,\nu' K'\sigma'} = \tilde{\Psi}_{j\nu} \tau_3 \hat{\Gamma}_{od} \tilde{\Psi}_{j\nu'}. \]  
(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 over-complete by a factor of two. This is a consequence of the fact that the basis states form an over-complete (and, consequently, non-orthogonal 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 anti-symmetric parts with respect to particle-hole conjugation. If only the anti-symmetric 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 non-physical 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 wavefunctions 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 no-crossing theorem. This means that the relative order in energy of the physical and of the non-physical 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 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 5 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 $^{156}$Gd and $^{158}$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 $^{157}$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 ±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 show in Fig. (1). We can see from the figure that the two models give very similar results. In Fig. (3) 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. (2).
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 \([4,18]\), 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 semi-microscopic core-particle coupling theory, the KKDF theory, and particularly 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.

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

\[
(\omega_{IK} - E_K)(J \mu' j a \kappa_a |IK) = (j_a - \kappa_a J \mu' |1/2^I_K[(J + j)^2 - K^2]|IK),
\]

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

\[
J(J + 1) + j_a(j_a + 1) + 2(K - \kappa_a)\kappa_a + j_- J_+ + j_+ J_-.
\]

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 (4.14), which we label $T\left(\Gamma^\dagger : J K_j a \kappa_a\right)$. Utilizing Eqs. (4.7) and (4.10), we must evaluate the expression

$$
T\left(\Gamma^\dagger : J K_j a \kappa_a\right) = \frac{1}{2} \sum (-1)^{j_c + m_a + \kappa_c - \kappa_a} \sqrt{\frac{(2j_a + 1)(2I + 1)}{(2j_c + 1)(2I' + 1)}} \times
$$

$$
F_{a c d b}(L) q^{(L, 0)}_{K' K}(d b) \times (j_a - m_a j_c m_c | L m_c - m_a)(I M L M | I' M')(I' M' J m_c - M' | j_c m_c) \times (I M J m_a - M | j_a m_a)(J K - \kappa_a j_a \kappa_a | I K) \times (I K L K' | I' K')(J K' - \kappa_c j_c \kappa_c | I' K') \phi_{I, K', -\kappa_c}(j_c \kappa_c). \quad (A.3)
$$

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

$$
S = \sum_{m_c} (-1)^{j_c + m_a} \frac{2j_a + 1}{2j_c + 1} \times (j_a - m_a j_c m_c | L m_c - m_a)(I M L m_c - m_a | I' M')(I' M' J m_c - M' | j_c m_c) = (-1)^{j_a + I' + J} \sqrt{(2L + 1)(2I' + 1)} \times \left\{ \begin{array}{c}
    j_a \ j_c \ L \\
    I' \ I \ J
\end{array} \right\} (I M J m_a - M | j_a m_a), \quad (A.4)
$$

which can be derived from Edmonds (6.2.7). The sum over $M$ then removes two more CG coefficients from (A.3) 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

$$
S' = \sum_{II'} (-1)^{j_a + I' + J} \sqrt{(2L + 1)(2I + 1)}(J K - \kappa_a j_a \kappa_a | I K) \times (I K L K' - K | I' K')(J K' - \kappa_c j_c \kappa_c | I' K') \left\{ \begin{array}{c}
    j_o \ j_c \ L \\
    I' \ I \ J
\end{array} \right\} = (-1)^{\kappa_c - \kappa_a + j_c + \kappa_c} (j_c - \kappa_c j_a \kappa_a | L K' - K). \quad (A.5)
$$

Equations (A.4) and (A.5) are the essential results for the evaluation of (A.3) leading to the appropriate term in (4.14). The pairing term in the same equation and the multipole and pairing terms in (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

\[
\langle I'M'K'|B_{LM_L}^\dagger(db)|IMK \rangle = q_{IK'}^{(L_1)}(db) \sum_{\lambda} \langle I'M'K'|D_{LM,L'}\rangle_{-K-\lambda} I'_\lambda |IMK\rangle.
\]

\( B_{LM_L} \) is replaced, in general, by different expressions. In the case of the first term of (B.3), the calculation parallels that described in the previous appendix. The sum (A.4) repeats itself in every case. The sum (A.5) is replaced, in general, by different expressions. In the case of the first term of (B.3), the sum \( S' \) is replaced by the sum

\[
S'_1 = \sum_{I'J} (-1)^{j_a+I'+J} \sqrt{(2L+1)(2I+1)} (JK - \kappa_a j_a \kappa_a |IK \rangle
\]

\[
\times (IK - 1LK'-K+1|I'K') (JK' - \kappa_a j_a \kappa_a |I'K') \times \left\{ \begin{array}{c} j_a \hfill \\
I' \hfill \\
I \hfill \\
J \hfill \end{array} \right\} \sqrt{(I+K)(I-K+1)}.
\]

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 (4.14). As an example, consider the first term of (B.3). The calculation parallels that described in the previous appendix. The sum (A.4) repeats itself in every case. The sum (A.5) is replaced, in general, by different expressions. In the case of the first term of (B.3), the sum \( S' \) is replaced by the sum

\[
S'_1 = \sum_I (JK - \kappa_a j_a \kappa_a |IK \rangle (JK - \kappa_a j_a \kappa_a |IK - 1) \sqrt{(I+K)(I-K+1)}
\]

\[
= \sqrt{(J-K+\kappa_a+1)(J+K-\kappa)}, \quad \text{(B.5)}
\]
which involves the same “trick” as used in the evaluation of the Coriolis coupling. Of the
terms arising from (B.3), 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

\[
\sum_{bcd\kappa cK'L} (-1)^{j_{c}+\kappa_{c}} F_{abcd}(L) q_{K'K}^{(L,1)}(db) \\
\times \left[ \frac{1}{\sqrt{2}} \sqrt{(J - K + \kappa_{a} + 1)(J + K - \kappa_{a})(j_{c} - \kappa_{c}j_{a}\kappa_{a}|LK - K' - 1)} \phi_{J,K-1-\kappa_{a}}(j_{c}\kappa_{c}) \\
- \frac{1}{\sqrt{2}} \sqrt{(J + K - \kappa_{a} + 1)(J - K + \kappa_{a})(j_{c} - \kappa_{c}j_{a}\kappa_{a}|LK - K' + 1)} \phi_{J,K+1-\kappa_{a}}(j_{c}\kappa_{c}) \\
- \frac{1}{2} (K + K')(j_{c} - \kappa_{c}j_{a}\kappa_{a}|LK - K') \phi_{J,K-\kappa_{a}}(j_{c}\kappa_{c}). \right] \tag{B.6}
\]

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

\[
(-1)^{j_{c}+\kappa_{c}} \rightarrow (-1)^{j_{c}+\kappa_{a}+L}. \tag{B.7}
\]
REFERENCES

[19] This expression was first called to the attention of one of the authors (AK) in 1965 by G. Do Dang and was later used by him in his unpublished lectures on nuclear theory. It reappears in the work of Dönau and Frauendorf [7,8].
FIG. 1. Negative parity energy levels for $^{157}$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.

FIG. 2. Positive parity energy levels for $^{157}$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.
FIG. 3. B(E2) transitions for $^{157}$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.