Foundations of self-consistent particle-rotor models and of self-consistent cranking models

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The Kerman-Klein formulation of the equations of motion for a nuclear shell model and its associated variational principle are reviewed briefly. It is then applied to the derivation of the self-consistent particle-rotor model and of the self-consistent cranking model, for both axially symmetric and triaxial nuclei. Two derivations of the particle-rotor model are given. One of these is of a form that lends itself to an expansion of the result in powers of the ratio of single-particle angular momentum to collective angular momentum, which is essential to reach the cranking limit. The derivation of the latter also requires a distinct, angular-momentum violating step. The structure of the result implies the possibility of tilted-axis cranking for the axial case and full three-dimensional cranking for the triaxial one. The final equations remain number conserving.

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I. INTRODUCTION

The aims of this paper are to study anew the foundations of the particle-rotor model [1,2] and of the cranking model [2]. The basic procedure is to apply the Kerman-Klein (KK) method [3–5] in a suitably defined strong-coupling limit to a standard microscopic shell model. Before entering into a discussion of this subject matter, it may be useful to the reader to begin with a brief history of a method that was introduced almost four decades ago. Such a summary serves several purposes. First of all, despite the fact that the KK method provides a fundamental theoretical formulation for the study of collective motion, its practical impact on the field of nuclear structure has been minor. It may be important to point out why this has so far been the case. We also explain the timing of the current formal paper by its relationship to recent successful applications. Finally, we observe that in its role as a general method of applying Heisenberg matrix mechanics, the KK techniques have been applied successfully outside the nuclear many-body problem, to particle quantum mechanics and to relativistic quantum field theories.

The KK method was introduced into the nuclear many-body problem as a method of restoring the broken symmetry of mean-field theory [3]. The earliest papers [4,5] were devoted to the derivation, starting from a formulation that respected all the relevant symmetries, of the standard approximations for the study of vibrational and rotational nuclei and the suggestion of ways of going beyond those approximations. There followed more than a decade of development of applications, mostly, though not exclusively, by the writer and associates, work that has been reviewed at length [6] and more briefly [7]. Our applications were mainly to the study of nuclear vibrations, but at the same time there was further development of the theory. During the same period, the theory was reinvented by Belyaev and Zelevinsky [8–10] and applied by them to the study of deformed nuclei, using perturbative expansions about the deformed mean-field limit. A suitably chosen subset of our papers and their papers may be regarded as permanent contributions to the subject of nuclear collective motion. With regard to our efforts to go beyond standard approximations with the new method, there were some partial successes, as detailed in the cited review, but viewed in retrospect, the attempt to apply our method fully microscopically was premature: the shell model spaces underlying the calculations were too small, and our early algorithms had serious weaknesses. In any event, mainly because our attention was diverted elsewhere, no attempts to carry out applications were made between 1978 and 1993, though we did produce the cited review during this period, as well as a paper devoted to a reexamination and extension of the theoretical foundations [11].

In 1993, we undertook a program of applications [12–17], currently in hiatus, more limited in scope than our early work, but, as outlined below, more successful in its results. This program was inspired by and represents a further development of the earlier work of Dönau and Frauendorf (DF) [18,19], who suggested that the KK approach be coupled with some phenomenological input and thus be implemented as a semimicroscopic core-particle coupling model, more general than any of the existing ones, but still not too difficult to apply. The practical success of our recent efforts is tied to the fact that we are able to deal with large shell model spaces (essentially all bound single-particle levels) and the availability of the necessary phenomenological input either from experiment or from standard models. We have studied some strong-coupling spectra [12,13], some backbending cases [14], and examined the relation of our results to those obtainable with the standard particle-rotor model [15]. More importantly, we have proposed a solution to the Coriolis attenuation problem [16], and we have taken a step in the direction of fully microscopic calculations [17] by showing for a selected strong-coupling case, that the results of the semimicroscopic calculations satisfy certain sum rules that play an essential role in such (future) calculations. From a survey of the work done, it is clear that we have hardly scratched the surface covering the possible applications of this theory. (As one example the KK method can also deal with transitional nuclei [19,20].) The purpose of the present formal paper is both to provide some theoretical closure to our recent work and some stimulus for further applications.

The KK method has also had some impact, though not a

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decisive one, on our work on large amplitude collective motion. For details we direct the reader to a recent review [21].

Finally, we sketch the systematic applications of the KK method to problems outside nuclear physics. We have had a continuing interest, for example, in the application to bound-state problems in quantum mechanics, both to provide alternative exact solutions to known solvable problems, as well as to provide accurate numerical solutions in other cases [22–24]. We have also shown that our method provides a powerful approach to the study of quantum mechanics in the semiclassical limit, both for separable and for nonseparable systems (in the nonchaotic regime) [25–27]. In another series of papers, we have addressed the problem of restoring the broken symmetry in early examples of relativistic field theories with soliton solutions [28–32] and, more recently, in the Skyrmion model [33].

We turn now to the actual subject matter of this paper. The particle-rotor model (PRM) was introduced as an angular momentum-conserving phenomenological description of odd deformed nuclei. Because of its relative ease of application and, on the whole, quite remarkable success, it has been applied even up to the present (for instance, Ref. [34]), with various alterations of detail, to a myriad of applications, over a lifetime of more than four and a half decades. Among the extensions, we mention in particular that to the description of triaxial nuclei [35–37], the original model having been formulated for axially symmetric nuclei.

In one of the textbooks [2], p. 109, we find, after a glowing appraisal of the success of the model, the following statement: ''However, until now a clear-cut microscopic derivation has been missing.'' In fact, a microscopic derivation had been given earlier [38], based on the (KK) method. The microscopic foundation of the axially symmetric PRM was studied more recently in Ref. [15], starting from a semimicroscopic version of the KK approach, and compared in accuracy, for several examples of well-deformed nuclei, both with its more accurate progenitor and with the inherently less accurate cranking approximation. The first aim of the present paper is to provide a more comprehensive study of the foundations of the PRM than has hitherto been available in the literature.

The cranking model was originally introduced into nuclear physics [39], within the framework of a prescribed single-particle model, to deal with the enigma presented by the first values encountered for the moments of inertia of deformed nuclei. An extended version [40], the one considered in most applications until recent years, was based on the self-consistent mean-field theory of a deformed rotating object. This early work was designed primarily to provide formulas for the moment of inertia.

The full range of applicability of the self-consistent cranking model, as well as its limitations, was realized in the so-called cranked shell model (CSM) [41], that has been widely applied to the analysis of band crossing and other high-spin phenomena. (For a current list of references, especially reviews, see Ref. [42].) The formulations under discussion, which apply to axially symmetric nuclei, assume that collective rotation occurs about a principal axis perpendicular to the symmetry axis. Such a formulation is referred to currently as principal-axis cranking (PAC) as opposed to a recent generalization, called tilted-axis cranking (TAC) [42–46]. In the latter, even in the axial case, the system may rotate about an axis in a principal plane of the assumed (quadrupole) intrinsic shape, and for the triaxial case about an arbitrary (dynamically determined) direction with respect to the principal axes.

A second aim of the present paper is to establish the relationship of the cranking models, including the recent generalized versions, to a microscopic theory. The previous literature on this subject is modest in extent. The standard references are Refs. [47] ad [48], the major results of which are reproduced and discussed in Ref. [2]. Briefly, starting from a formulation of the microscopic theory by means of generator coordinates, the energy is evaluated approximately as a power series in the angular momentum by a method due to Kamlah [49], valid for large deformations. When the variational method is applied to the lowest nontrivial approximation of this procedure, it can be shown that the cranking theory is a solution of the resulting equations. This is summarized by stating that cranking is a solution, involving a semiclassical approximation, of the method of variation *after* projection as opposed to the exact procedure of variation *before* projection.

To our knowledge, the only other studies of this subject are those based on the KK method, a brief treatment of the case of rotation in a plane [50] that predates the above-cited work and two studies that postdated them, one again on the problem of rotation in a plane [51] and the second a restricted study of the triaxial case [52,53]. (Some discussion of the cranking limit, also based on a variant of the KK method, can be found in Ref. [54].) Up to now we have never presented a full account of the three-dimensional treatment either for axial or for triaxial nuclei, an approach that differs from anything found in the standard literature [2]. Stimulation for the present undertaking has come both form its relation to our recent work and from the renewed interest in generalized cranking models [42–46].

The foundations of the study are presented in Sec. II. We utilize a shell model Hamiltonian, widely employed for medium and heavy nuclei, with two-particle interactions in which the latter are separated into two parts clearly distinguished as multipole and pairing forces, respectively. The advantage of such a model is that the (*c*-number) equations of motion that can be derived from it by the KK method are completely rigorous. It is a simplifying feature for the further study to recognize that these equations can be derived from a variational principle that we called the trace variational principle, suggested in our earliest paper [4] and developed more fully in [54]. This variational principle has several noteworthy features: (i) It is formulated for the many-body problem in the language of second quantization. (ii) The quantities varied are not wave functions, but rather a suitably chosen set of matrix elements, in our case coefficients of fractional parentage (to be discussed at the appropriate point of Sec. II). (iii) Rather than involving the Rayleigh-Ritz principle for one state at a time, the functional to be varied is the trace of

energy expectation values over a prescribed space of states.[1]

The theory is elaborated in Sec. II only as far as is required for the remaining body of the text. Further development is presented in the Appendix. We turn to applications in Sec. III, where we derive the self-consistent PRM from the variational principle associated with the KK equations. (With one possible exception [60], we are unaware of any recent work, other than our own, that has examined the foundations of the PRM.)

The formalism presented in Sec. III does not lend itself naturally to a derivation of the self-consistent cranking theory, which should be a limit of the self-consistent PRM. In Sec. IV we describe an alternative derivation of the PRM, following ideas first advanced briefly in Ref. [50], that does lead directly to the cranking limit. The considerations of Secs. III and IV apply to axially symmetric nuclei. Both treatments are extended to the case of triaxial nuclei in Sec. V. Further discussion of results and conclusions are given in Sec. VI.

II. EQUATIONS OF MOTION AND VARIATIONAL PRINCIPLE

We choose a shell-model Hamiltonian in the form

$$H=h_a a^\dagger_\alpha a_\alpha+\frac{1}{2}F_{\alpha\gamma\delta\beta}a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\beta a_\delta+\frac{1}{2}G_{\alpha\gamma\beta\delta}a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta . \tag{2.1}$$

In this standard model, the $a_\alpha, a^\dagger_\alpha$ are the destruction, creation operators for fermions in the shell-model mode $\alpha=(nljm\tau)$ (τ distinguishing neutrons from protons); $F_{\alpha\gamma\delta\beta}$ describes multipole forces and $G_{\alpha\gamma\delta\beta}$ pairing forces. In this version, all multipolarities allowed by angular momentum conservation are included, though in practice we limit ourselves to the lowest few multipoles of each type. We shall also consistently use the summation convention, except when we wish to highlight some set of indices. With the help of the definitions

$$F_{\alpha\gamma\delta\beta}=s_\gamma(j_a m_a j_c -m_c|LM_L)\times s_\beta(j_d m_d j_b -m_b|LM_L)F_{acdb}(L), \tag{2.2}$$

$$G_{\alpha\gamma\delta\beta}=(j_a m_a j_c m_c|LM_L)(j_d m_d j_b m_b|LM_L)G_{acdb}(L), \tag{2.3}$$

$$s_\gamma=(-1)^{j_c-m_c}=\sqrt{2j_c+1}(j_c m_c j_c -m_c|00), \tag{2.4}$$

where $(jmj'm'|LM)$ is a Clebsch-Gordon (CG) coefficient, the operator equations of motion can be obtained in the form

$$[a_\alpha,H]=h'_a a_\alpha+F_{\alpha\alpha'\beta'\beta}a_{\alpha'}a^\dagger_\beta a_{\beta'}+G_{\alpha\alpha'\beta\beta'}a^\dagger_{\alpha'}a_{\beta'}a_\beta , \tag{2.5}$$

$$h'_a=h_a-\frac{1}{2}F_{abab}\frac{2L+1}{2j_a+1}, \tag{2.6}$$

$$[a^\dagger_{\bar\alpha},H]=-h''_a a^\dagger_{\bar\alpha}-F_{\beta\beta'\alpha'\bar\alpha}\bar a^\dagger_{\beta'}a_\beta a^\dagger_{\alpha'}-G_{\beta\bar\beta'\alpha'\bar\alpha}\bar a_{\alpha'}a^\dagger_\beta a^\dagger_{\bar\beta'}, \tag{2.7}$$

$$h''_a=h'_a+2\frac{2L+1}{2j_a+1}G_{abab}(L). \tag{2.8}$$

Here, for example, $\bar\alpha=(j_a,-m_a)$.

To develop a dynamical scheme, we turn to the problem of obtaining equations for the matrix elements of Eqs. (2.5) and (2.7). We designate a state of interest of an odd nucleus as $|JM\nu\rangle$, where J is the total angular momentum, M is its z component, and ν are the remaining quantum numbers necessary for unique specification of the state. Neighboring even nuclei are specified, correspondingly, as $|\overline{IMn}\rangle$, referring to a heavier neighbor, and $|\underline{IMn}\rangle$, referring to a lighter neighbor. Below we shall then derive equations for the matrix elements, referred to as CFP (coefficients of fractional parentage),

$$\langle JM\nu|a_\alpha|\overline{IM_I n}\rangle=V_{JM\nu}(\alpha IM_I n), \tag{2.9}$$

$$\langle JM\nu|a^\dagger_{\bar\alpha}|\underline{IM_I n}\rangle=U_{JM\nu}(\alpha IM_I n). \tag{2.10}$$

We shall require the full notation when we turn to applications in the next section. For the formal developments of this section, however, we utilize a compressed notation, with

$$JM\nu\to i, \quad IM_I n\to n. \tag{2.11}$$

With new symbols defined and discussed below, we thus obtain the equations

$$\mathcal{E}_i V_i(\alpha n)=(\epsilon'_a-E^*_{\bar n})V_i(\alpha n)+F_{\alpha\alpha'\beta'\beta}[V^*_{i'}(\beta n')V_{i'}(\beta' n)]V_i(\alpha' n')+G_{\alpha\bar\alpha'\beta\bar\beta'}[U^*_{i'}(\beta' n')V_{i'}(\beta n)]U_i(\alpha' n'), \tag{2.12}$$

[1] It turns out that not all aspects of our formulation are novel. Thus an incomplete version of the trace variational principle is to be found in one of the initial series of papers on matrix mechanics [55], in which the variational parameters are matrix elements of the coordinates and momenta. This application to particle quantum mechanics was discovered and developed independently by us in several accounts of which the most recent is Ref. [27]. A version of the trace variational principle can, furthermore, be found is in a classic text in mathematical physics [56]. Here the formulation is close to standard Rayleigh-Ritz, in that the quantities varied are wave function. This formulation has found its way into the theory of density functionals [57,58]. Most recently the trace variational principle for fields has appeared in a quaternion generalization of quantum mechanics [59].

$$\mathcal{E}_i U_i(\alpha n) = (-\epsilon''_a - E^*_{\underline{n}}) U_i(\alpha n) - F_{\overline{\beta\beta'}\,\overline{\alpha'}\,\overline{\alpha}}[U^*_{i'}(\beta n') U_{i'}(\alpha' n)] U_i(\beta' n') + G_{\overline{\alpha\alpha'}\,\overline{\beta'}\,\beta}[V^*_{i'}(\beta n') U_{i'}(\beta' n)] V_i(\alpha' n'). \tag{2.13}$$

In the definitions, to be given below, of the various energies that appear in these equations, we understand that E_i is the energy of the state $|i\rangle$ and that $E_{\overline{n}}$ and $E_{\underline{n}}$ are, correspondingly the energies of the neighboring even states, with the subscript 0 standing either for the ground state, or for the lowest energy state considered, which for conciseness we shall continue to refer to as the ground state. We thus encounter the quantities

$$\mathcal{E}_i = -E_i + \frac{1}{2}(E_{\overline{0}} + E_{\underline{0}}), \tag{2.14}$$

$$\epsilon'_a = h'_a - \lambda, \tag{2.15}$$

$$\lambda = \frac{1}{2}(E_{\overline{0}} - E_{\underline{0}}), \tag{2.16}$$

$$E^*_n = E_n - E_0. \tag{2.17}$$

The physical significance of the quantities defined in Eqs. (2.14)–(2.17) is evident. $\mathcal{E}_i$ are the negatives of the energies of the odd nucleus relative to the ground-state energies of its even neighbors, ϵ_a, variously primed, are single-particle energies measured relative to the chemical potential λ, and E^*_n are excitation energies of the appropriate even nuclei. Finally in achieving the form of Eq. (2.13), we have assumed that F and G are real. Given the Hamiltonian (2.1), Eqs. (2.12) and (2.13) are an exact set of consequences that define a nonlinear eigenvalue problem with eigenvalue $\mathcal{E}_i$. The elements on the right-hand sides of these equations define an effective Hamiltonian that will be discussed in considerable further detail in the course of this work.

We display next a functional, $\mathcal{F}$, whose vanishing first variations yield the equations of motion, namely,

$$\begin{aligned}\mathcal{F} = {} & \epsilon'_a |V_i(\alpha n)|^2 - \epsilon''_a |U_i(\alpha n)|^2 \\ & + \frac{1}{2} F_{\alpha\alpha'\beta'\beta}[V^*_{i'}(\beta n') V_{i'}(\beta' n)][V^*_i(\alpha n) V_i(\alpha' n')] \\ & + G_{\alpha\overline{\alpha'}\,\beta'\overline{\beta}}[U^*_{i'}(\beta n') V_{i'}(\beta' n)][V^*_i(\alpha n) U_i(\alpha' n')] \\ & - \frac{1}{2} F_{\overline{\beta\alpha'}\,\overline{\beta'}\,\alpha}[U^*_{i'}(\beta n') U_{i'}(\beta' n)][U^*_i(\alpha n) U_i(\alpha' n')] \\ & - \mathcal{E}_i[|V_i(\alpha n)|^2 + U_i(\alpha n)|^2] - E^*_{\underline{n}} |V_i(\alpha n)|^2 \\ & - E^*_{\underline{n}} |U_i(\alpha n)|^2 \end{aligned} \tag{2.18}$$

$$\equiv \mathcal{G} - \mathcal{E}_i[|V_i(\alpha n)|^2 + |U_i(\alpha n)|^2]. \tag{2.19}$$

One verifies that the equations of motion (2.12) and (2.13) emerge, respectively, from the requirements

$$\frac{\delta \mathcal{F}}{\delta V^*_i(\alpha n)} = \frac{\delta \mathcal{F}}{\delta U^*_i(\alpha n)} = 0. \tag{2.20}$$

It is natural to inquire at this point if the functional $\mathcal{F}$ has any simple physical significance, in particular, if it is related to a Rayleigh-Ritz principle. To answer this question, we evaluate the sum

$$\mathrm{Tr}(\overline{H} + \underline{H}) = \sum_n [\langle \overline{n}|H|\overline{n}\rangle + \langle \underline{n}|H|\underline{n}\rangle]. \tag{2.21}$$

The evaluation of this sum with the aim of eventually recognizing the relevant pieces of $\mathcal{F}$ requires, in addition to the standard tool of completeness, some algebraic rearrangement of the trace involving the lighter system, just as was necessary in the equations of motion. We then find that the interaction terms match exactly those in Eq. (2.18), but that the single particle terms do not. Instead we find

$$h'_a \to h_a \equiv \overline{h_a}, \tag{2.22}$$

$$h'''_a \to h_a + 2\frac{2L+1}{2j_a+1} G_{acac}(L) + \sqrt{\frac{2j_b+1}{2j_a+1}} F_{aabb}(0) \equiv \underline{h_a}. \tag{2.23}$$

We are thus tempted to replace the functional $\mathcal{F}$, as basis for the theory, by a functional that contains the new single-particle energies. We do not make this change because it destroys the simple physical significance of the Lagrange multiplier terms in Eq. (2.18) to which we next turn our attention. (In practice, these extra single-particle terms are often ignored anyway.)

We consider then the Lagrange-multiplier terms that appear in Eq. (2.18). The relevant question concerns the constraints that have been imposed on the variations. Since

$$\sum_{i\alpha} |V_i(\alpha n)|^2 = \sum_\alpha \langle \overline{n}|a^\dagger_\alpha a_\alpha|\overline{n}\rangle = \langle \overline{n}|\hat{N}|\overline{n}\rangle, \tag{2.24}$$

where $\hat{N}$ is the number operator, we see that the excitation energies $E^*_{\overline{n}}$ enter as Lagrange multipliers for the conservation of nucleons in the heavier even nucleus. Similarly the term involving the sum over the $|U_i(\alpha n)|^2$ expresses (to an additive constant) the conservation of nucleons in the lighter system. Finally, we show that the eigenvalue $\mathcal{E}_i$ is (no surprise here) a Lagrange multiplier for an appropriate normalization condition. To see this we take the matrix element in the state $|i\rangle$ of the summed anticommutator,

$$\sum_\alpha \{a_\alpha, a^\dagger_\alpha\} = \Omega, \Omega = \sum_{j_a} (2j_a+1) = \sum_a \Omega_a, \tag{2.25}$$

and thus find

$$\frac{1}{\Omega}\sum_{\alpha n}\left[|V_i(\alpha n)|^2+|U_i(\alpha n)|^2\right]=1. \tag{2.26}$$

Orthogonality constraints on the solutions need not be imposed, since they follow directly from the equations of motion.

There is more to the story, however. We must note that Eq. (2.26) is only a sum of required normalization conditions. From the summed anticommutator for each level,

$$\sum_{m_a}\{a_\alpha, a_\alpha^\dagger\}=\Omega_a, \tag{2.27}$$

we have

$$\frac{1}{\Omega_a}\sum_{m_a n}\left[|V_i(\alpha n)|^2+U_i(\alpha n)|^2\right]=1. \tag{2.28}$$

If Eqs. (2.12) and (2.13) described a linear eigenvalue problem, it would be impossible to impose the additional normalization conditions represented by Eq. (2.28). For the general nonlinear problem, there is no *a priori* inconsistency; the satisfaction of these conditions will be a part of any fully satisfactory algorithm. The form of the normalization condition (2.28) suggests, furthermore, that it may be both useful and natural to rescale the CFP,

$$V_i(\alpha n)=\sqrt{2j_a+1}v_i(\alpha n), \tag{2.29}$$

$$U_i(\alpha n)=\sqrt{2j_a+1}u_i(\alpha n). \tag{2.30}$$

There is considerably more to the formal theory than what has been presented thus far. However, we have all the tools needed for the further development in the text and thus relegate the additional theoretical considerations to the Appendix.

III. DERIVATION OF PARTICLE-ROTOR MODEL: AXIALLY SYMMETRIC CASE

As a first illustration of the formalism presented in the previous section, we assume that the even (core) nuclei are in a single axially symmetric band $|IM_IK\rangle$, where K is the component of the angular momentum along the figure axis. There are at least two cases where it makes some physical sense to isolate a single K value, where it is the ground-state band with $K=0$, or where the band has a large K value and we are dealing with an isomeric state.

Our first task is to express the CFP V and U in terms of the amplitudes that occur in the PRM. This is done by introducing deformed intrinsic basis states and applying standard properties of the rotation group, leading to Eqs. (3.7) and (3.8) below. These equations underlie the further considerations of this section, and variants of them play a similar role in Secs. IV and V. We first use rotational invariance to study the structure of the amplitudes V and U defined in Eqs. (2.9) and (2.10), respectively. We thus introduce a complete set of states $|R\rangle$ localized in the Euler angles, $R=(\alpha\beta\gamma)$, where α,β are the usual polar and azimuthal angles, respectively, and write

$$|IM_IK\rangle=\int dR\,|R\rangle\langle R|IM_IK\rangle$$
$$=\left(\frac{2I+1}{8\pi^2}\right)^{1/2}\int dR\,|R\rangle D^{(I)}_{M_IK}(R). \tag{3.1}$$

The identification of a scalar product of *many-body states* with the Wigner D function is not a trivial statement, but is rather an essential element in the definition of the model to be studied. In fact, the designation $|R\rangle$ for the many-body state is insufficiently detailed and is made more explicit by the statement

$$|R\rangle=U(R)|\hat{0}K\rangle, \tag{3.2}$$

where $|\hat{0}K\rangle$ is an axially symmetric intrinsic state spinning with angular momentum K about its symmetry axis, and $U(R)$ is the unitary rotation operator in the many-body space defined by the Euler angles that specify the rotation R. For such a state, we thus note the relation, with $(\alpha\beta\gamma)=(\hat{n}\gamma)$,

$$U(\hat{n}\gamma)|\hat{0}K\rangle\exp(-iK\gamma)=U(\hat{n}0)|0K\rangle. \tag{3.3}$$

The introduction of strictly localized states is, of course, an idealization that ignores the reality of band termination, but it is a standard approximation for well-deformed nuclei.[2]

When Eq. (3.1) is substituted into the definitions (2.9) of V and (2.10) of U, and use is made of completeness, standard properties of the rotation group, and of the definitions

$$(-1)^{j+m}\chi_{JM\nu}(jm,K)=\langle JM\nu|a_{jm}|\hat{0}K\rangle, \tag{3.5}$$

$$\phi_{JM\nu}(jm,K)=\langle JM\nu|a^\dagger_{j-m}|\hat{0}K\rangle, \tag{3.6}$$

we obtain the formulas

$$V_{JM\nu}(\alpha IM_IK)=\sum_{\kappa_a}\sqrt{\frac{8\pi^2}{2j_a+1}}(-1)^{J-M}$$
$$\times(IM_IJ-M|j_am_a)(JK-\kappa_aj_a\kappa_a|IK)$$
$$\times(-1)^{j_a+\kappa_a}\chi_{JK-\kappa_a\nu}(j_a\kappa_a,K), \tag{3.7}$$

[2]The previous discussion and that which follows does not take into account $\mathcal{R}$ invariance, the invariance of the quadrupole shape under a rotation of π about a principal axis. To include this symmetry in the discussion, we replace the state $|IM_IK\rangle$ by an eigenfunction of $\mathcal{R}$,

$$|IM_IK]=\tfrac{1}{2}\{|IM_IK\rangle+(-1)^{I+K}|IM_I-K\rangle\}. \tag{3.4}$$

We then imitate the arguments starting on p. 8 of Ref. [1]. The task is to sort and collect the extra terms that appear both in the equations of motion and in formulas for one- and two-particle observables.

$$U_{JM\nu}(\alpha IM_I K)=\sum_{\kappa_a}\sqrt{\frac{8\pi^2}{2j_a+1}}\times(-1)^{J-M+j_a-\kappa_a+j_a+m_a}\times(IM_IJ-M|j_am_a)\times(JK-\kappa_aj_a\kappa_a|IK)\phi_{JK-\kappa_a\nu}(j_a\kappa_a,K), \tag{3.8}$$

At this point we have a choice whether to transform the equation of motion (EOM) or the variational principle to the intrinsic system. It is most succinct to base further discussion on the variational principle (2.18). We evaluate this expression when the core collective states are restricted to the members of a single band of an axial rotor, and the states of the odd nucleus are any states that can arise from the coupling. Returning to a full nomenclature, this calls for the identifications

$$\overline{n}\to\overline{IM_IK},\quad \underline{n}\to\underline{IM_IK},\quad i\to JM\nu. \tag{3.9}$$

We are assuming here that there are corresponding bands in the two even nuclei that couple to the given odd nucleus. In the following we shall also suppress the bar and underline in the CFP, understanding them from context, but continue to emphasize this distinction in the energies.

The calculation that now follows is mainly an uninteresting exercise in angular momentum algebra. We choose to immediately display the final result, following that with the necessary definitions and a few relevant details. [Note that there is also a condensation in the notation with $(j_a\kappa_a,K)\to(a)$, $(j_a\kappa_a\pm1,\ K)\to(a\pm1)$.] We thus find

$$\begin{aligned}
\mathcal{F}=&\sum_{J\nu j_a\kappa_a}(\epsilon'_a-\overline{\varepsilon}_{J\nu})|\chi_{JK-\kappa_a\nu}(a)|^2-\sum_{J\nu j_a\kappa_a}(\epsilon''_a+\underline{\varepsilon}_{J\nu})|\phi_{JK-\kappa_a\nu}(a)|^2-\frac{1}{2}\sum_{J\nu j_a\kappa_a}\chi^*_{JK-\kappa_a\nu}(a)\overline{f}(JK)\\
&\times[\sqrt{(J+K-\kappa_a)(J-K+\kappa_a+1)}\sqrt{(j_a-\kappa_a)(j_a+\kappa_a+1)}\chi_{JK-\kappa_a-1\nu}(a+1)\\
&+\sqrt{(J-K+\kappa_a)(J+K-\kappa_a+1)}\sqrt{(j_a+\kappa_a)(j_a-\kappa_a+1)}\chi_{JK-\kappa_a+1\nu}(a-1)+2(K-\kappa_a)\kappa_a\chi_{JK-\kappa_aj_a\kappa_a}(a)]\\
&+\frac{1}{2}\sum_{J\nu j_a\kappa_a}\phi^*_{JK-\kappa_a\nu}(a)\underline{f}(JK)[\sqrt{(J+K-\kappa_a)(J-K+\kappa_a+1)}\sqrt{(j_a-\kappa_a)(j_a+\kappa_a+1)}\phi_{JK-\kappa_a-1\nu}(a+1)\\
&+\sqrt{(J-K+\kappa_a)(J+K-\kappa_a+1)}\sqrt{(j_a+\kappa_a)(j_a-\kappa_a+1)}\phi_{JK-\kappa_a+1\nu}(a-1)+2(K-\kappa_a)\kappa_a\phi_{JK-\kappa_a\nu}(a)].\\
&+\sum_{I''JJ'\nu\nu'j_a\ldots\kappa_a\ldots}\Bigg[\frac{1}{2}F_{aa'b'b}(L)\chi_{JK-\kappa_b'\nu}(b')\chi^*_{JK-\kappa_b\nu}(b)\chi_{J'K-\kappa_a'\nu'}(a')\chi^*_{J'K-\kappa_a\nu'}(a)\\
&-\frac{1}{2}F_{ba'b'a}(L)\phi_{JK-\kappa_b'\nu}(b')\phi^*_{JK-\kappa_b\nu}(b)\phi_{J'K-\kappa_a'\nu'}(a')\phi^*_{J'K-\kappa_a\nu'}(a)\\
&+G_{aa'b'b}\chi_{JK-\kappa_b'\nu}(b')\phi^*_{JK-\kappa_b\nu}(b)\phi_{J'K-\kappa_a'\nu'}(a')\chi^*_{J'K-\kappa_a\nu'}(a)\Bigg](-1)^{\kappa_b+\kappa_b'-1+j_a'+j_b+L+I''}\\
&\times\frac{(2L+1)}{(2J'+1)}\begin{Bmatrix}j_{a'} & j_a & L\\ j_{b'} & j_b & I''\end{Bmatrix}(j_a-\kappa_aj_b'\kappa_b'|I''\kappa_b'-\kappa_a)(j_a'-\kappa_a'j_b\kappa_b|I''\kappa_b-\kappa_a')(I''\kappa_b'-\kappa_aJK-\kappa_b'|J'K-\kappa_a)(I''\kappa_b\\
&-\kappa_a'JK-\kappa_b|J'K-\kappa_a').
\end{aligned}\tag{3.10}$$

Note also that the factors involving $\sqrt{8\pi^2}$ in Eqs. (3.7) and (3.8) have been absorbed in a rescaling of the intrinsic amplitudes χ and ϕ.

The only undefined quantities in this equation are $\overline{\varepsilon}_{J\nu}$, $\overline{f}(JK)$ and the corresponding underline quantities. These arise as follows: As part of the definition of an axial rotor, we assume that, equally for the barred and underlined quantities,

$$E^*(IK)\rightarrow E^*(\vec{I}^2-K^2)=E^*(\hat{I}_1^2+\hat{I}_2^2+\hat{I}_3^2-K^2), \tag{3.11}$$

where we have introduced intrinsic components of the angular momentum. The arrow indicates the replacement of an eigenvalue by a vector operator. This is done by making use of the appropriate one of the CG coefficients, namely,

$$E^*(IK)(JK-\kappa_a j_a \kappa_a|IK) = [JK-\kappa_a j_a \kappa_a|E^*(\vec{I}^2-K^2)|IK]. \tag{3.12}$$

Further, we see from Eq. (3.12) that we may replace $\vec{I}$ by $\vec{J}+\vec{j}_a$ and write (with $j_a\rightarrow j$),

$$\overline{E}^*(\vec{I}^2-K^2)=\overline{E}^*[(\vec{J}+\vec{j})^2-K^2] = \overline{E}^*(\vec{J}^2-K^2)+\frac{\partial \overline{E}^*}{\partial \hat{J}_i}\hat{j}_i+\cdots. \tag{3.13}$$

It is not necessary for these considerations that $E(IK)$ have the simple form of a rotor spectrum, only that it be a function as indicated. The first term of Eq. (3.13) may be replaced by an eigenvalue $\overline{E}^*[J(J+1)-K^2)]$, and the second term leads to the Coriolis coupling.

With the aid of the previous considerations, we can finally provide the required definitions,

$$\overline{\varepsilon}_{J\nu}=\mathcal{E}_{J\nu}-\overline{E}^*[J(J+1)-K^2], \tag{3.14}$$

$$\frac{\partial \overline{E}^*}{\partial J_i}=\overline{f}(\vec{J}^2-K^2)J_i, \tag{3.15}$$

where in the simplest case $\overline{f}$ is just the reciprocal of the moment of inertia. There are corresponding definitions for the underline quantities. These observations account for the form and origin of the first four terms of Eq. (3.10), which constitute single-particle, normalization (eigenvalue), and Coriolis coupling terms. To reach the final form of the interaction term requires that one sum over all magnetic quantum numbers in the laboratory system and over the core angular momenta. This involves basically the defining equations for $6-j$, symbols, Eqs. (6.2.6) and (6.2.7) of Ref. [61] and the sum rule (6.2.12) of the same reference.

By varying in turn with respect to $\chi^*_{JK-\kappa_a\nu}(a)$ and $\phi^*_{JK-\kappa_a\nu}(a)$, we obtain the equations of motion

$$\begin{aligned}
\overline{\varepsilon}_{J\nu}\chi_{JK-\kappa_a\nu}(a) &= \epsilon'_a\chi_{JK-\kappa_a\nu}(a)-\frac{1}{2}\overline{f}(JK)\sqrt{(J+K-\kappa_a)(J-K+\kappa_a+1)}\sqrt{(j_a-\kappa_a)(j_a+\kappa_a+1)}\chi_{JK-\kappa_a-1\nu}(a)\\
&-\sqrt{(J-K+\kappa_a)(J+K-\kappa_a+1)}\sqrt{(j_a+\kappa_a)(j_a-\kappa_a+1)}\chi_{JK-\kappa_a+1\nu}(a)-2(K-\kappa_a)\kappa_a\chi_{JK-\kappa_a\nu}(a)\\
&+[F_{aa'b'b}(L)\chi_{J'K-\kappa_{b'}\nu'}(b')\chi^*_{J'K-\kappa_b\nu'}(b)\chi_{JK-\kappa_{a'}\nu}(a')\\
&+G_{aa'b'b}(L)\chi_{J'K-\kappa_{b'}\nu'}(b')\phi^*_{J'K-\kappa_b\nu'}(b)\phi_{JK-\kappa_{a'}\nu}(a')]\frac{2L+1}{2J+1}\begin{Bmatrix} j_{a'} & j_a & L\\ j_{b'} & j_b & I\end{Bmatrix}\\
&\times(j_a-\kappa_a j_{b'}\kappa_{b'}|I\kappa_{b'}-\kappa_a)(j_{a'}-\kappa_{a'}j_b\kappa_b|I\kappa_b-\kappa_{a'})\\
&\times(I\kappa_{b'}-\kappa_a J'K-\kappa_{b'}|JK-\kappa_a)(I\kappa_b-\kappa_{a'}J'K-\kappa_b|JK-\kappa_{a'}),
\end{aligned} \tag{3.16}$$

$$\begin{aligned}
\underline{\varepsilon}_{J\nu}\phi_{JK-\kappa_a\nu}(a) &= -\epsilon''_a\phi_{JK-\kappa_a\nu}(a)+\frac{1}{2}\underline{f}(JK)\sqrt{(J+K-\kappa_a)(J-K+\kappa_a+1)}\sqrt{(j_a-\kappa_a)(j_a+\kappa_a+1)}\phi_{JK-\kappa_a-1\nu}(a)\\
&+\sqrt{(J-K+\kappa_a)(J+K-\kappa_a+1)}\sqrt{(j_a+\kappa_a)(j_a-\kappa_a+1)}\phi_{JK-\kappa_a+1\nu}(a)+2(K-\kappa_a)\kappa_a\phi_{JK-\kappa_a\nu}(a)\\
&-[F_{ba'b'a}(L)\phi_{J'K-\kappa_{b'}\nu'}(b')\phi^*_{J'K-\kappa_b\nu'}(b)\phi_{JK-\kappa_{a'}\nu}(a')\\
&+G_{aa'b'b}(L)\phi_{J'K-\kappa_{b'}\nu'}(b')\chi^*_{J'K-\kappa_b\nu'}(b)\chi_{JK-\kappa_{a'}\nu}(a')]\frac{2L+1}{2J+1}\begin{Bmatrix} j_{a'} & j_a & L\\ j_{b'} & j_b & I\end{Bmatrix}\\
&\times(j_a-\kappa_a j_{b'}\kappa_{b'}|I\kappa_{b'}-\kappa_a)(j_{a'}-\kappa_{a'}j_b\kappa_b|I\kappa_b-\kappa_{a'})\\
&\times(I\kappa_{b'}-\kappa_a J'K-\kappa_{b'}|JK-\kappa_a)(I\kappa_b-\kappa_{a'}J'K-\kappa_b|JK-\kappa_{a'}).
\end{aligned} \tag{3.17}$$

We add the normalization conditions for the particle-rotor model that follow from Eq. (2.28). We find

$$\sum_{\kappa_a} [|\chi_{JK-\kappa_a\nu}(a)|^2+|\phi_{JK-\kappa_a\nu}(a)|^2]=2j_a+1. \tag{3.18}$$

What we have derived is actually a generalized form of the PRM in that it conserves both angular momentum, as does the usual model, and particle number. In contrast the usual model, it is also fully microscopic. The relation to the usual PRM has been elucidated in a previous work [15].

IV. ALTERNATIVE DERIVATION AND ITS CRANKING LIMIT: AXIAL CASE

In addition to the PRM, self-consistent or otherwise, we are interested in the cranking theory, valid in the limit in which a single-particle angular momentum j_a may be neglected compared to the collective angular momentum. In principle, we should be able to derive this limit from the form of the theory developed in Sec. III. There is no problem with the single-particle, eigenvalue, or Coriolis coupling terms, as we shall see below. However, the interaction terms, as derived, do not provide a natural pathway to the limit sought. Therefore we start anew in this section, but concentrate on deriving an approximate version of the PRM in which an expansion in $(\langle j\rangle/J)$ has been made, the main difference compared to the previous calculation residing in the treatment of the interaction terms. We derive an approximate version of the PRM and then introduce the additional approximations necessary to reach the cranking limit.

For present purposes it is convenient to work in coordinate-spin-isospin space, designated by x. We work with amplitudes that we refer to as coordinate coefficients of fractional parentage (CCFP),

$$V_{JM\nu}(xIM_IK)=\langle JM\nu|\hat{\psi}(x)|\overline{IM_IK}\rangle, \tag{4.1}$$

$$U_{JM\nu}(xIM_IK)=\langle JM\nu|\hat{\psi}^\dagger(x)|\underline{IM_IK}\rangle, \tag{4.2}$$

where $\hat{\psi}(x)$ is the nucleon destruction operator at the space-spin-isospin point x. In terms of these amplitudes, we rewrite the variational functional $\mathcal{F}$ of Eq. (2.19) as

$$\begin{aligned}\mathcal{F}=&[\epsilon(xx')-\mathcal{E}_{J\nu}\delta(x-x')-\overline{E}^*(IK)\delta(x-x')]V_{JM\nu}(x'IM_IK)V^*_{JM\nu}(xIM_IK)\\&-[\epsilon(xx')+\mathcal{E}_{J\nu}\delta(x-x')+\underline{E}^*(IK)\delta(x-x')]U_{JM\nu}(xIM_IK)U^*_{JM\nu}(x'IM_IK)\\&+\frac{1}{2}F(xx'x''x''')V_{J'M'\nu'}(x''IM_IK)V^*_{J'M'\nu'}(x'''I'M_{I'}K)V_{JM\nu}(x'I'M_{I'}K)V^*_{JM\nu}(xIM_IK)\\&+G(xx'x''x''')V_{J'M'\nu'}(x''IM_IK)U^*_{J'M'\nu'}(x'''I'M_{I'}K)U_{JM\nu}(x'I'M_{I'}K)V^*_{JM\nu}(xIM_IK)\\&-\frac{1}{2}F(x'''x'x''x)U_{J'M'\nu'}(x''IM_IK)U^*_{J'M'\nu'}(x'''I'M_{I'}K)U_{JM\nu}(x'I'M_{I'}K)U^*_{JM\nu}(xIM_IK).\end{aligned} \tag{4.3}$$

We have set $\epsilon'=\epsilon''=\epsilon$ and shall adhere to this simplification for the remainder of our presentation. To carry out the transformation to Eq. (4.3), we have made use of the basis in which $\epsilon(xx')$ is diagonal,

$$a_\alpha=\varphi^*_\alpha(x)\hat{\psi}(x), \tag{4.4}$$

$$\epsilon_a\varphi_\alpha(x)=\epsilon(xx')\varphi_\alpha(x'), \tag{4.5}$$

$$F(xx'x''x''')=F_{\alpha\gamma\delta\beta}\varphi^*_\alpha(x)\varphi_\gamma(x')\varphi^*_\delta(x'')\varphi_\beta(x'''), \tag{4.6}$$

$$G(xx'x''x''')=G_{\alpha\gamma\beta\delta}\varphi^*_\delta(x''')\varphi^*_\beta(x')\varphi_\gamma(x')\varphi_\alpha(x). \tag{4.7}$$

The major device of the present derivation is the transformation from angular momentum eigenfunctions to eigenfunctions localized in angle space, a technique that has already been exploited in Sec. III. We base the developments on expressions for the CCFP that are derived by the same initial transformations that led to Eqs. (3.7) and (3.8), namely

$$\begin{pmatrix}V_{JM\nu}(xM_IK)\\U_{JM\nu}(xM_IK)\end{pmatrix}=\int dRD^{(J)*}_{MM'}(R)\begin{pmatrix}\chi_{JM'\nu}(Rx,K)\\\phi_{JM'\nu}(Rx,K)\end{pmatrix}\sqrt{\frac{2I+1}{8\pi^2}}D^{(I)}_{M_IK}(R), \tag{4.8}$$

$$\chi_{JM\nu}(Rx,K)=\langle JM\nu|\hat{\psi}(Rx)|\hat{0}K\rangle, \tag{4.9}$$

$$\phi_{JM\nu}(Rx,K)=\langle JM\nu|\hat{\psi}^\dagger(Rx)|\hat{0}K\rangle, \tag{4.10}$$

$$\hat{\psi}(Rx)=U^{-1}(R)\hat{\psi}(x)U(R). \tag{4.11}$$

We now substitute Eq. (4.8) into Eq. (4.3), and using the restricted completeness relation

$$\sum_{IM} D^{(I)}_{MK}(R) D^{(I)*}_{MK}(R') \frac{2I+1}{8\pi^2} = \delta(\hat{n}-\hat{n}') \exp[-iK(\gamma-\gamma')] \frac{1}{2\pi} \quad (4.12)$$

and the relation (3.3), we can eliminate the core angular momenta. The further evaluation also requires elementary properties of the D function and the rotational invariance of the Hamiltonian, as expressed by such relations as

$$\epsilon(RxRx') = \epsilon(xx'), \quad (4.13)$$

$$F(RxRx'Rx''Rx''') = F(xx'x''x'''). \quad (4.14)$$

Again we first quote the final result of the evaluation, including the expansion in $(\langle j\rangle/J)$ of the interaction term and subsequently provide such details as are essential. We find

$$\mathcal{F} = \mathcal{F}_1 + \mathcal{F}_2,$$

$$\begin{aligned}\mathcal{F}_1 = {} & [\epsilon(xx') - \bar{\varepsilon}_{J\nu}\delta(x-x')]\chi_{JM\nu}(x')\chi^*_{JM\nu}(x) - [\epsilon(xx') + \underline{\varepsilon}_{J\nu}\delta(x-x')]\phi_{JM\nu}(x)\phi^*_{JM\nu}(x') + \sum_{JM\nu} \bar{f}(JK) \\ & \times \left[\frac{1}{2}\sqrt{(J-M)(J+M+1)}\, j_+ \chi_{JM+1\nu}(x) + \frac{1}{2}\sqrt{(J+M)(J-M+1)}\, j_- \chi_{JM-1\nu}(x) + M j_3 \chi_{JM\nu}(x)\right]\chi^*_{JM\nu}(x) \\ & - \sum_{JM\nu} \underline{f}(JK)\left[\frac{1}{2}\sqrt{(J-M)(J+M+1)}\, j_+ \phi_{JM+1\nu}(x) + \frac{1}{2}\sqrt{(J+M)(J-M+1)}\, j_- \phi_{JM-1\nu}(x) + M j_3 \phi_{JM\nu}(x)\right]\phi^*_{JM\nu}(x),\end{aligned} \quad (4.15)$$

$$\begin{aligned}\mathcal{F}_2 = {} & \sum_{JMM'\nu\nu'} \frac{1}{2J+1}\left[\frac{1}{2}F(xx'x''x''')\chi_{JM\nu'}(x'')\chi^*_{JM'\nu'}(x''')\chi_{JM'\nu}(x')\chi^*_{JM\nu}(x)\right. \\ & \left. + G(xx'x''x''')\chi_{JM\nu'}(x'')\phi^*_{JM'\nu'}(x''')\phi_{JM'\nu}(x')\chi^*_{JM\nu}(x) - \frac{1}{2}F(x'''x'x''x)\phi_{JM\nu'}(x'')\phi^*_{JM'\nu'}(x''')\phi_{JM'\nu}(x')\phi^*_{JM\nu}(x)\right].\end{aligned} \quad (4.16)$$

We shall not comment further on the derivation of the Coriolis coupling terms of $\mathcal{F}_1$ both because the result is completely equivalent to the corresponding terms of Eq. (3.10), and because such details as might be of interest are a special case of those given in the next section on triaxial nuclei. We concentrate therefore on the origin of the interaction terms $\mathcal{F}_2$. We consider the first term of the interaction at the stage that the sums over IM and $I'M'$ have been carried out,

$$\frac{1}{2}\int dR dR' F(xx'x''x''') D^{(J)}_{M'M''}(R^{-1}R') D^{(J')*}_{M^{iv}M'''}(R^{-1}R')\chi_{JM'\nu}(Ry')\chi^*_{JM''\nu}(R'y)\chi_{J'M'''\nu'}(R'x')\chi^*_{J'\nu^{iv}\nu'}(Rx). \quad (4.17)$$

Introducing the definition

$$R^{-1}R' = \mathcal{R}, \quad (4.18)$$

and replacing the integral over R' by an integral $\mathcal{R}$, we could do the integrals exactly by decomposing the amplitudes χ into irreducible tensors. We resist the temptation to do this, since a full calculation was carried out in Sec. III. It is more useful for our purposes to proceed approximately by expanding $\mathcal{R}$ about the unit matrix wherever it appears as the argument of a χ function. This brings in at each order angular momentum operators acting on single-particle wave functions and therefore dimensionally is the source of the expansion in $(\langle j\rangle/J)$. For the interaction term the cranking limit will arise from the leading term of this expansion. With the help of the rotational invariance of the interaction and the orthonormality relations of the D functions, we reach the result

$$\frac{1}{2}\sum_{JMM'\nu\nu'} \frac{1}{2J+1} F(xx'x''x''')\chi_{JM\nu'}(x'')\chi^*_{JM'\nu'}(x''')\chi_{JM'\nu}(x')\chi^*_{JM\nu}(x), \quad (4.19)$$

which is the first term of $\mathcal{F}_2$.

We are finally ready to discuss the cranking limit. The essential observation is that once the expansion to leading order in $(\langle j\rangle/J)$ has been made both in the Coriolis coupling and in the interaction terms, the resulting approximate functional $\mathcal{F}$ presents itself as a single sum over J. However,

angular momentum is still conserved at this juncture. We lose angular momentum conservation by assuming that consistent with the condition $(\langle j\rangle/J)\ll 1$ we may identify M and K, i.e., we may neglect the angular momentum transferred to or from the particle, and write, furthermore (ω defined below),

$$\chi_{JK\nu}(x)\rightarrow\sqrt{2J(\omega)+1}\chi_{\omega\nu}(x), \tag{4.20}$$

$$\chi_{JK\pm1\nu}(x)\rightarrow\sqrt{2J(\omega)+1}C_{\mp}\chi_{\omega\nu}(x), \tag{4.21}$$

i.e., the amplitudes differing in K from the ''central value'' by a unit are assumed proportional to the central amplitude (which is defined as the cranking amplitude) up to scale factors $C_{\mp}$ discussed below. Similar definitions hold for the ϕ amplitudes. The factor $\sqrt{2J+1}$ is inserted for convenience, as will be evident from Eq. (4.24) given below.

These assumptions suggest the following definitions of the components of the angular frequency (overline and underline understood):

$$\omega_{\mp}(K)=f(JK)C_{\mp}\sqrt{(J\mp K+1)(J\pm K)}, \tag{4.22}$$

$$\omega_3=f(JK)K. \tag{4.23}$$

The introduction of the factors $C_{\mp}$ may appear gratuitous at first sight, but it is needed, as will become especially evident when we treat the triaxial case, to guarantee that in the cranking limit the theorem that the angular velocity is proportional to the angular momentum is valid in this limit [62].

Remembering the definition (3.14) and reinstating Cartesian intrinsic coordinates for the Coriolis coupling terms, we obtain the cranking variational expression

$$\begin{aligned}[\mathcal{F}/(2J(\omega)+1)]=&\epsilon(xx')\chi_{\omega\nu}(x')\chi^*_{\omega\nu}(x)-\epsilon(xx')\phi_{\omega\nu}(x)\phi^*_{\omega\nu}(x')+[\overline{\omega}_i j_i\chi_{\omega\nu}(x)]\chi^*_{\omega\nu}(x)\\&+[\underline{\omega}_i j_i\phi_{\omega\nu}(x)]\phi^*_{\omega\nu}(x)+\frac{1}{2}F(xx'x''x''')\chi_{\omega\nu'}(x'')\chi^*_{\omega\nu'}(x''')\chi_{\omega\nu}(x')\chi^*_{\omega\nu}(x)\\&+G(xx'x''x''')\chi_{\omega\nu'}(x'')\phi^*_{\omega\nu'}(x''')\chi_{\omega\nu}(x')\phi^*_{\omega\nu}(x)-\frac{1}{2}F(x'''x'x''x)\phi_{\omega\nu'}(x'')\phi^*_{\omega\nu'}(x''')\phi_{\omega\nu}(x')\phi^*_{\omega\nu}(x)\\&-\overline{\varepsilon}_{\omega\nu}\chi_{\omega\nu}(x)\chi^*_{\omega\nu}(x)-\underline{\varepsilon}_{\omega\nu}\phi_{\omega\nu}(x)\phi^*_{\omega\nu}(x).\end{aligned} \tag{4.24}$$

The equations of motion that follow are number conserving, and according to the definitions (4.22) and (4.23) allow solutions with principal axis cranking.

V. TRIAXIAL ROTOR: CORE-PARTICLE COUPLING MODEL AND CRANKING LIMIT

In this section, we assume that states of interest of neighboring even nuclei can be described phenomenologically by a Hamiltonian

$$\mathcal{H}_c=\frac{1}{2}a_i I_i^2+\frac{1}{4}a_{ij}\{I_i^2,I_j^2\}+\cdots. \tag{5.1}$$

In the calculations to be described below, we shall retain only the first term of $\mathcal{H}_c$. The underlying model arises as follows: We assume that we can identify states of the appropriate even nucleus as $|IM_I n\sigma\rangle$, which we read as the nth state of angular momentum I belonging to a triaxial intrinsic structure σ. We also define a rotated intrinsic state

$$|R\sigma\rangle=U(R)|\hat{0}\sigma\rangle. \tag{5.2}$$

It is part of the definition of the model that the scalar product

$$\langle R\sigma|IM_I n\sigma\rangle\equiv F^{(I)}_{M_I n}(R) \tag{5.3}$$

satisfies the eigenvalue equation

$$\mathcal{H}_c F^{(I)}_{M_I n}=E^*(In)F^{(I)}_{M_I n}. \tag{5.4}$$

Further useful equations satisfied by or defining the model include

$$|IM_I n\sigma\rangle=|IM_I K\sigma\rangle c^{(I\sigma)}_{Kn}, \tag{5.5}$$

$$\delta_{nn'}=\sum_K c^{(I\sigma)*}_{Kn}c^{(I\sigma)}_{Kn'}, \tag{5.6}$$

$$\delta_{KK'}=\sum_n c^{(I\sigma)*}_{Kn}c^{(I\sigma)}_{K'n}, \tag{5.7}$$

$$\langle R\sigma|IMK\sigma\rangle=\sqrt{\frac{2I+1}{8\pi^2}}D^{(I)}_{MK}(R). \tag{5.8}$$

We turn to the evaluation of the terms in the variational functional $\mathcal{F}$. We shall follow the methods of both Secs. III and IV, depending on the aim of a particular fragment of the calculation. Starting from the representation

$$\begin{aligned}V_{JM\nu}(\alpha IM_I n\sigma)&=\langle JM\nu|a_\alpha|R\sigma\rangle F^{(I)}_{M_I n}(R)\\&=\langle JM\nu|a_\alpha|R\sigma\rangle D^{(I)}_{M_I K}(R)c^{(I\sigma)}_{Kn},\end{aligned} \tag{5.9}$$

we can derive a formula for the current version of the CFP V that is analogous to Eq. (3.7), namely

$$V_{JM\nu}(\alpha;IM_In\sigma)=\sum_{K\kappa_a}\sqrt{\frac{8\pi^2}{2j_a+1}}(-1)^{J-M}\times(IM_IJ-M|j_am_a)(JKj_a\kappa_a|IK+\kappa_a)\times(-1)^{j_a+\kappa_a}\chi_{JK\nu}(j_a\kappa_a\sigma)c^{(I\sigma)}_{K+\kappa_an}, \tag{5.10}$$

$$(-1)^{j+m}\chi_{JK\nu}(jm\sigma)=\langle JK\nu|a_{jm}|\hat{0}\sigma\rangle. \tag{5.11}$$

The corresponding formula for the CFP U is

$$U_{JM\nu}(\alpha IM_In\sigma)=\sum_{K\kappa_a}\sqrt{\frac{8\pi^2}{2j_a+1}}(-1)^{J-M+j_a-\kappa_a+j_a+m_a}\times(IM_IJ-M|j_am_a)(JKj_a\kappa_a|IK+\kappa_a)\times\phi_{JK\nu}(j_a\kappa_a\sigma)c^{(I\sigma)}_{K+\kappa_an}, \tag{5.12}$$

$$\phi_{JM\nu}(j_a\kappa_a\sigma)=\langle JM\nu|a^{\dagger}_{j_a-\kappa_a}|\hat{0}\sigma\rangle. \tag{5.13}$$

With these formulas, we find the contributions of the simplest single-particle terms to take the form, in the shell-model or mode representation,

$$\sum_{JK\nu j_a\kappa_a}[(\epsilon_a-\mathcal{E}_{J\nu})|\chi_{JK\nu}(a)|^2-(\epsilon_a+\mathcal{E}_{J\nu}|\phi_{JK\nu}(a)|^2]. \tag{5.14}$$

We study next the term involving the Lagrange multiplier $\bar{E}^*(In)$. With the help of the defining Eq. (5.4) and a subsequent integration by parts, we have first of all

$$\bar{E}^*(In)V_{JM\nu}(IM_In\sigma)=\int dR[\mathcal{H}_c(\hat{I}_i)\times\langle JM\nu|a_\alpha|R\sigma\rangle]F^{(I\sigma)}_{M_In}(R). \tag{5.15}$$

With the help of the completeness relation

$$\sum_{IM_In}F^{(I\sigma)}_{M_In}(R)F^{(I\sigma)*}_{IM_In}(R')=\delta(R-R'), \tag{5.16}$$

we thus find for the total term

$$\bar{E}^*(In\sigma)|V_{JM\nu}(\alpha IM_In\sigma)|^2=\int dR[\mathcal{H}_c(\hat{I}_i)\langle JM\nu|a_\alpha|R\sigma\rangle]\times\langle JM\nu|a_\alpha|R\sigma\rangle^*. \tag{5.17}$$

The square bracket may be reexpressed as

$$\mathcal{H}_c(\hat{I}_i)\langle JM\nu|a_\alpha|R\sigma\rangle=[\mathcal{H}_c(\hat{I}_i)D^{(J)*}_{MK}(R)D^{(j_a)*}_{m_a\kappa_a}(R)]\times\langle JK\nu|a_{j_a\kappa_a}|\hat{0}\sigma\rangle. \tag{5.18}$$

As far as the application of $\mathcal{H}_c$ in Eq. (5.18) is concerned, we then write

$$\mathcal{H}_c(\hat{I}_i)\to\mathcal{H}_c(\hat{J}_i+\hat{j}_i)=\mathcal{H}_c(\hat{J}_i)+\frac{\partial\mathcal{H}_c}{\partial\hat{J}_i}\hat{j}_i+\cdots, \tag{5.19}$$

and work only to the order indicated explicitly.

At the same time it is convenient to rewrite

$$\mathcal{H}_c(\hat{I}_i)=\frac{1}{4}b_1(I_+I_-+I_-I_+)+\frac{1}{4}b_2(I_+^2+I_-^2)+\frac{1}{2}b_3I_3^2 \tag{5.20}$$

$$a_1=b_1+b_2,\quad a_2=b_1-b_2,\quad a_3=b_3. \tag{5.21}$$

It is now straightforward to calculate the contributions arising from the two terms of Eq. (5.19). For the first term we find

$$-8\pi^2\left\{\left[\frac{1}{2}b_1[J(J+1)-K^2]+\frac{1}{2}b_3K^2\right]|\chi_{JK\nu}(a)|^2\frac{1}{4}b_2\sqrt{(J-K+2)(J-K+1)(J+K-1)(J+K)}\chi_{JK-2\nu}(a)\chi^*_{JK\nu}(a)+\frac{1}{4}b_2\sqrt{(J+K+2)(J+K+1)(J-K-1)(J-K)}\chi_{JK+2\nu}(a)\chi^*_{JK\nu}(a)\right\}, \tag{5.22}$$

and for the second term,

$$-8\pi^2\left[\frac{1}{2}b_1\sqrt{(J-K+1)(J+K)(j_a+\kappa_a+1)(j_a-\kappa_a)}\chi_{JK-1\nu}(a+1)+\frac{1}{2}b_1\sqrt{(J+K+1)(J-K)(j_a-\kappa_a+1)(j_a+\kappa_a)}\times\chi_{JK+1\nu}(a-1)+\frac{1}{2}b_2\sqrt{(J-K+1)(J+K)(j_a-\kappa_a+1)(j_a+\kappa_a)}\chi_{JK-1\nu}(a-1)+\frac{1}{2}b_2\sqrt{(J+K+1)(J-K)(j_a+\kappa_a+1)(j_a-\kappa_a)}\chi_{JK+1\nu}(a+1)+b_3K\kappa_a\chi_{JK\nu}(j_a\kappa_a\sigma)\right]\chi^*_{JK\nu}(a). \tag{5.23}$$

Both of these terms can be identified as familiar structures. By means of this identification we shall have achieved both a simpler form for the particle-rotor formalism and for its limiting case, the cranking formalism. First consider Eq. (5.22). Note that the content of Eqs. (5.4) and (5.5) can be rewritten as

$$\mathcal{H}_c D^{(I)}_{M_I K} = D^{(I)}_{M_I K'} (\mathcal{H}_c)_{K'K}, \tag{5.24}$$

$$(\mathcal{H})_{KK'} c^{(I\sigma)}_{K'n} = E^*(In) c^{(I\sigma)}_{Kn}. \tag{5.25}$$

This eigenvalue equation was associated with even nuclei and thus with integer values of the angular momentum. By analytic continuation, we can define a corresponding eigenvalue equation for odd nuclei as follows:

$$[\mathcal{H}_c(\hat{J}_i)]_{KK'} c^{(J)}_{K'\tau} = E^*(J\tau) c^{(J)}_{K\tau}, \tag{5.26}$$

where J,K are now half integral. We then see that if we introduce a new set of particle amplitudes $\chi_{J\tau\nu}$ by means of the equation

$$\chi_{JK\nu}(j\kappa) = c^{(J)}_{K\tau} \chi_{J\tau\nu}(j\kappa), \tag{5.27}$$

we can transform Eq. (5.22) into the form

$$-E^*(J\tau)|\chi_{J\tau\nu}(a)|^2. \tag{5.28}$$

Finally, as we did for the axial case, we can combine energy terms by means of a definition

$$\varepsilon_{J\nu} = \mathcal{E}_{J\nu} + E^*(J\tau). \tag{5.29}$$

We turn our attention next to Eq. (5.23). We note first that this expression is an expanded version of

$$-[a_i \hat{J}_i \hat{j}_i \chi_{JK\nu}(a)] \chi^*_{JK\nu}(a), \tag{5.30}$$

where $\hat{J}_i$ acts on the value of K and $\hat{j}_i$ acts on the value of κ_a. Transforming to the new amplitudes $\chi_{J\tau\nu}$, expression (5.30) becomes

$$-[a_i \hat{J}_i \hat{j}_i \chi_{J\tau\nu}(a)] \chi^*_{J\tau\nu}(a), \tag{5.31}$$

where now

$$\hat{J}_i \chi_{J\tau\nu} = \chi_{J\tau'\nu}(J\tau'|J_i|J\tau), \tag{5.32}$$

$$(J\tau'|\hat{J}_i|J\tau) = c^{(J)}_{K'\tau'}(JK'|J_i|JK) c^{(J)*}_{K\tau}. \tag{5.33}$$

For the purpose of taking the cranking limit and comparing the forms derived in Sec. IV, we rewrite the results found so far and the corresponding terms involving ϕ amplitudes in coordinate space. For this we require only Eqs. (5.27), the corresponding equations

$$\chi_{JK\nu}(x) = \langle JK\nu|\hat{\psi}(x)|\hat{0}\sigma\rangle \tag{5.34}$$

$$= c^{(J)}_{K\tau} \chi_{J\tau\nu}(x), \tag{5.35}$$

and the similar equations for the terms involving ϕ. We thus find the contributions

$$\begin{aligned} &-\bar{\varepsilon}_{J\nu}|\chi_{J\tau\nu}(x)|^2 + \epsilon(xx')\chi_{J\tau\nu}(x')\chi^*_{J\tau\nu}(x) \\ &\quad + \bar{a}_i[J_i j_i(x)\chi_{J\tau\nu}(x)]\chi^*_{J\tau\nu}(x), \\ &-\underline{\varepsilon}_{J\nu}|\phi_{J\tau\nu}(x)|^2 + \epsilon(xx')\phi_{J\tau\nu}(x')\phi^*_{J\tau\nu}(x) \\ &\quad + \underline{a}_i[J_i j_i(x)\phi_{J\tau\nu}(x)]\phi^*_{J\tau\nu}(x). \end{aligned} \tag{5.36}$$

The cranking limit of these terms may now be taken by means of the replacements that generalize Eqs. (4.21) and (4.20),

$$\chi_{J\tau'\nu}(x) \to \sqrt{2J+1} C_\tau(\tau') \chi_{\omega\nu}(x), \tag{5.37}$$

and τ' refers to τ or any of the values coupled to τ by the matrices of $\hat{J}_i$, with $C_\tau(\tau) = 1$. This is the essential blurring of angular momentum conservation that takes us from the conserving particle-rotor approximation to the cranking approximation. It allows us as well to define the components of the angular velocity in generalization of Eq. (4.20),

$$\bar{\omega}_i(\tau) = \bar{a}_i \sum_{\tau'} C_\tau(\tau')(J\tau'|J_i|J\tau), \tag{5.38}$$

$$\tau' = \tau'(\tau). \tag{5.39}$$

As usual, there are corresponding equations for the amplitudes ϕ.

We may thus replace Eq. (5.36) by its cranking limit

$$\begin{aligned} &(2J+1)[-\bar{\varepsilon}_{\omega\nu}|\chi_{\omega\nu}(x)|^2 + \epsilon(xx')\chi_{\omega\nu}(x')\chi^*_{\omega\nu}(x) \\ &\quad + \bar{\omega}_i j_i(x)\chi_{\omega\nu}(x)]\chi^*_{\omega\nu}(x)(2J+1)[-\underline{\varepsilon}_{\omega\nu}|\phi_{\omega\nu}(x)|^2 \\ &\quad + \epsilon(xx')\phi_{\omega\nu}(x')\phi^*_{\omega\nu}(x) + \underline{\omega}_i j_i(x)\phi_{\omega\nu}(x)]\phi^*_{\omega\nu}(x), \end{aligned} \tag{5.40}$$

which is indistinguishable in form from the corresponding terms of Eq. (4.24).

It remains for us to compute the contributions of the interaction terms. We consider first an exact calculation analogous to that carried out in Sec. III, starting from the representations (5.10) and (5.12) for the CFP in the triaxial case. It is straightforward to generalize the corresponding calculations of Sec. III, as soon as one utilizes the orthonormality relations involving the coefficients $c^{(I)}_{Kn}$ at the first step. The final result for the interaction terms is

$$\sum_{I''JJ'KK'\nu\nu' j_a \ldots \kappa_a \ldots} \Bigg[\frac{1}{2} F_{aa'b'b}(L) \chi_{JK-\kappa_{b'}\nu}(b') \chi^*_{JK'-\kappa_b\nu}(b) \chi_{J'K'-\kappa_{a'}\nu'}(a') \chi^*_{J'K-\kappa_a\nu'}(a)$$

$$- \frac{1}{2} F_{ba'b'a}(L) \phi_{JK-\kappa_{b'}\nu}(b') \phi^*_{JK'-\kappa_b\nu}(b) \phi_{J'K'-\kappa_{a'}\nu'}(a') \phi^*_{J'K-\kappa_a\nu'}(a)$$

$$+ G_{aa'b'b} \chi_{JK-\kappa_{b'}\nu}(b') \phi^*_{JK'-\kappa_b\nu}(b) \phi_{J'K'-\kappa_{a'}\nu'}(a') \chi^*_{J'K-\kappa_a\nu'}(a) \Bigg]$$

$$\times (-1)^{\kappa_b+\kappa_{b'}-1+j_{a'}+j_b+L+I''} \frac{(2L+1)}{(2J'+1)} \begin{Bmatrix} j_{a'} & j_a & L \\ j_{b'} & j_b & I'' \end{Bmatrix} (j_a - \kappa_a j_{b'} \kappa_{b'} | I'' \kappa_{b'} - \kappa_a)(j_{a'} - \kappa_{a'} j_b \kappa_b | I'' \kappa_b - \kappa_{a'})$$

$$\times (I'' \kappa_{b'} - \kappa_a JK - \kappa_{b'} | J'K - \kappa_a)(I'' \kappa_b - \kappa_{a'} JK' - \kappa_b | J'K' - \kappa_{a'}). \tag{5.41}$$

Superficially, the change compared to Eq. (3.10) is that instead of a fixed value of K, we have a double sum over K and K'. The same expression holds for a finite number of interacting K bands provided the sums are restricted correspondingly.

Finally, we consider the calculation of the interaction term by the method of Sec. IV, needed to obtain the cranking limit. Here, in place of Eqs. (4.8)–(4.10), we utilize the forms

$$\begin{pmatrix} V_{JM\nu}(xM_In) \\ U_{JM\nu}(xM_In) \end{pmatrix} = \int dR D^{(J)*}_{MM'}(R) \begin{pmatrix} \chi_{JM'\nu}(Rx,\sigma) \\ \phi_{JM'\nu}(Rx,\sigma) \end{pmatrix} \sqrt{\frac{2I+1}{8\pi^2}} F^{(I)}_{M_In}(R), \tag{5.42}$$

$$\chi_{JM\nu}(Rx,\sigma) = \langle JM\nu | \hat{\psi}(Rx) | \hat{0}\sigma \rangle, \tag{5.43}$$

$$\phi_{JM\nu}(Rx,\sigma) = \langle JM\nu | \hat{\psi}^\dagger(Rx) | \hat{0}\sigma \rangle. \tag{5.44}$$

Once the full completeness relation (5.16) is utilized instead of the restricted completeness relation (4.12), the calculation mimics the one carried out in Sec. IV. In terms of the amplitudes $\chi_{J\tau\nu}$ and $\phi_{J\tau\nu}$, the result is

$$\sum_{J\tau\tau'\nu\nu'} \frac{1}{2J+1} \Bigg\{ \frac{1}{2} F(xx'x''x''') \chi_{J\tau\nu'}(x'') \chi^*_{J\tau'\nu'}(x''') \chi_{J\tau'\nu}(x') \chi^*_{J\tau\nu}(x)$$

$$+ G(xx'x''x''') \chi_{J\tau\nu'}(x'') \phi^*_{J\tau'\nu'}(x''') \phi_{J\tau'\nu}(x') \chi^*_{J\tau\nu}(x) - \frac{1}{2} F(x'''x'x''x) \phi_{J\tau\nu'}(x) \phi^*_{J\tau'\nu'}(x') \phi_{J\tau'\nu}(x''') \phi^*_{J\tau\nu}(x'') \Bigg\}. \tag{5.45}$$

The cranking limit of this expression is indistinguishable from the corresponding terms of Eq. (4.24) just as was the case for the single-particle terms (5.40). Thus the *form* of the cranking variational principle for the triaxial case is indistinguishable from that for the axial case and need not be written again. It is understood, however, that we are dealing with full three-dimensional cranking, and that the single-particle wave functions have suitably modified symmetry.

VI. SUMMARY AND DISCUSSION

We have studied the microscopic foundations of the particle-rotor model and of the cranking model for both axial and triaxial nuclei. The microscopic model was chosen in a form in which the interaction is given at the outset as a sum of multipole and pairing forces. We carried out the study from the point of view of the Kerman-Klein method based on the equations of motion for single fermion operators, and this choice of interaction has the advantage that the *c*-number equations of motion for the CFP are formally exact. These equations of motion and an associated variational principle, worked out in Sec. II, form the basis for the remaining considerations.[3]

As the first application, we derived in Sec. III a self-

[3]In the earliest papers on the KK approach [4,5], a more general shell-model interaction was used in the derivation of *c*-number equations. An essential part of the derivation involved the introduction of the physical arguments needed to separate this interaction into multipole and pairing contributions. As a consequence of the limitations of this procedure, the equations of motion found from it are not exact. Nevertheless, the final equations are formally equivalent to those utilized in this paper. The explanation for this concordance is that in the approach in this paper, the ''error'' involved in the separation has already been built into the starting Hamiltonian, as a further compromise, widely accepted, in the definition of the microscopic theory.

consistent particle-rotor model for axially symmetric nuclei. The derivation was carried out using basic ideas developed in Ref. [15], where, starting from a semimicroscopic version of the theory, we derived the standard non-self-consistent version of the particle-rotor model. The present discussion complements the previous one in the sense that it starts from a microscopic theory and carries the reasoning up to the edge of the semimicroscopic form.

We began this work with the prejudice that, as apposed to previous treatments, a natural path to the cranking model involved passing through the particle-rotor model. Though we were ultimately able to confirm this prejudice, the version of the particle-rotor model derived in Sec. III, though a useful one for applications [15], does not appear to be useful in the further transition to cranking. For this purpose we must be able to expand all contributions in powers of $(\langle j\rangle/J)$, the ratio of a characteristic single-particle angular momentum to the collective angular momentum. We have not discovered such an expansion for the interaction forms derived in this first treatment. Therefore in Sec. IV we start anew, utilizing an approach already described briefly for two-dimensional rotations in an early publication [50]. Rather than pushing through to a formally exact result, we stop the calculation at the leading order of the small parameter, and thus obtain an approximate version of the particle-rotor model that still conserves angular momentum, but is only a step away from the cranking limit. This further step violates angular momentum conservation by the way in which an angular velocity is introduced to replace the collective angular momentum. In Sec. V the considerations of both previous sections are generalized to the triaxial case.

Several special features of our treatment should be highlighted. For the axial case, as soon as the neighboring even nuclei are represented by bands with nonvanishing K values, we have tilted cranking in its simplest form. *A fortiori*, in the triaxial case we derive the possibility of full three-dimensional cranking. Within our mode of analysis, these statements may be taken to have the status of theorems. Another feature of our derivations of cranking models is that number conservation is maintained.

Nevertheless, in the light of recent developments associated with tilted cranking [42–46], possible limitations on our work have to be addressed. Superficially, our results apply to one quasiparticle spectra of odd nuclei, whereas the current focus of interest is on at least two quasiparticle spectra of even nuclei, and even more on multiquasiparticle states. In principle, however, these examples are covered by our considerations. Thus the two quasiparticle case is readily derived from the formalism developed in the Appendix. The multiple quasiparticle case is covered if one replaces the reference ground states of the even nuclei by suitably chosen band heads of two quasiparticle bands. Details of such calculations are best addressed within the framework of specific applications.

APPENDIX: FURTHER FORMAL DEVELOPMENT OF THE THEORY

The theory developed in Sec. II was sufficient for the purposes of the remainder of the body of this work, a study of the strong-coupling limit. However, for the formulation of useful algorithms applicable to obtaining solutions of the fully microscopic theory, it is also convenient to have a formulation in terms of a generalized density matrix.

To begin the extended development, it is helpful to introduce a more concise representation of the equations of motion (2.12) and (2.13) for the CFP by defining the vector

$$\Psi_i(\alpha n)=\begin{pmatrix} V_i(\alpha n)\\ U_i(\alpha n)\end{pmatrix}. \tag{A1}$$

The equations of motion can then be written

$$\mathcal{E}_i\Psi_i(\alpha n)=\mathcal{H}(\alpha n,\beta n')\Psi_i(\beta n'), \tag{A2}$$

where $\mathcal{H}(\alpha n,\beta n')$ is the Hermitian matrix

$$\mathcal{H}(\alpha n,\beta n')=\begin{pmatrix} (\epsilon'_a-E^*_n)\delta_{nn'}\delta_{\alpha\beta}+\overline{\Gamma}(\alpha n,\beta n') & \Delta(\alpha n,\beta n')\\ \Delta^*(\beta n',\alpha n) & (-\epsilon''_a-E^*_n)\delta_{nn'}\delta_{\alpha\beta}+\underline{\Gamma}(\alpha n,\beta n')\end{pmatrix}, \tag{A3}$$

and the potentials are defined as

$$\begin{aligned}\overline{\Gamma}(\alpha n,\gamma n')&=F_{\alpha\gamma\delta\beta}[V_i^*(\beta n')V_i(\delta n)]\\ &=F_{\alpha\gamma\delta\beta}\mathcal{R}_{11}(\delta n,\beta n'),\end{aligned} \tag{A4}$$

$$\begin{aligned}\underline{\Gamma}(\alpha n,\gamma n')&=F_{\overline{\delta\beta\alpha\gamma}}[U_i^*(\beta n')U_i(\delta n)]\\ &=F_{\overline{\delta\beta\alpha\gamma}}\,\mathrm{tr}\,\frac{1}{2}(1-\tau_3)\mathcal{R}_{22}(\delta n,\beta n'),\end{aligned} \tag{A5}$$

$$\begin{aligned}\Delta(\alpha n,\gamma n')&=G_{\alpha\gamma\overline{\beta\delta}}[U_i^*(\delta n')V_i(\beta n)]\\ &=G_{\alpha\gamma\overline{\beta\delta}}\mathcal{R}_{12}(\beta n,\delta n').\end{aligned} \tag{A6}$$

Here we have utilized a generalized density matrix $\mathcal{R}(\alpha n,\beta n')$, defined as

$$\mathcal{R}(\alpha n,\beta n')=\Psi_i(\alpha n)\Psi_i^*(\beta n')=\begin{pmatrix}\mathcal{R}_{11} & \mathcal{R}_{12}\\ \mathcal{R}_{21} & \mathcal{R}_{22}\end{pmatrix}, \tag{A7}$$

satisfying the idempotent condition

$$\mathcal{R}^2 = \Omega \mathcal{R}. \tag{A8}$$

The remainder of this discussion is devoted to the formulation of the theory in terms of the matrix $\mathcal{R}$. The first step is to combine the equations of motion (A2) with their complex conjugate equations so as to eliminate the eigenvalues $\mathcal{E}_i$. We thereby obtain the following equations for the generalized density matrix $\mathcal{R}$:

$$0 = \mathcal{R}(\alpha n, \gamma n'')\mathcal{H}(\gamma n'', \beta n') - \mathcal{H}(\alpha n, \gamma n'')\mathcal{R}(\gamma n'', \beta n'), \tag{A9}$$

i.e., we find the vanishing of the commutator, $[\mathcal{R}, \mathcal{H}] = 0$.

We exhibit next an alternative derivation of Eq. (A9) utilizing a variant of the variational principle (2.18), (2.19), a formulation that contains, as we shall see, more information than just Eq. (A9). Consider the functional

$$\mathcal{D} = \mathcal{G} - \Theta(\alpha n, \beta n')[\mathcal{R}^2(\beta n', \alpha n) - \Omega \mathcal{R}(\beta n', \alpha n)], \tag{A10}$$

where the ''new'' constraint with Lagrange multiplier matrix Θ is for normalization in the density matrix form. Since

$$\frac{\delta \mathcal{G}}{\delta \mathcal{R}(\beta n', \alpha n)} = \mathcal{H}(\alpha n, \beta n'), \tag{A11}$$

it follows that the variational condition applied to Eq. (A10) yields the equation

$$\mathcal{H} - \Theta \mathcal{R} - \mathcal{R}\Theta + \Theta\Omega = 0. \tag{A12}$$

From this condition, Eq. (A9) is readily derived by forming the appropriate commutator.

However, Eq. (A9) does not exhaust the content of Eq. (A12). Starting from the latter, we can derive the pair

$$\mathcal{R}\mathcal{H} = \mathcal{R}\Theta\mathcal{R} = \mathcal{H}\mathcal{R}, \tag{A13}$$

which implies that

$$\mathcal{H} = \Theta\Omega. \tag{A14}$$

Substituting this result back into Eq. (A12), we obtain

$$\mathcal{H} - \frac{1}{\Omega}\{\mathcal{R}, \mathcal{H}\} = 0. \tag{A15}$$

Equations (A9) and (A15) taken together provide a powerful approach to the construction of algorithms for the solution of the KK equations. Further discussion at this point would be severely premature.

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