Application of the Kerman-Klein Method to the Solution of a Spherical Shell Model for a Deformed Rare-Earth Nucleus

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Put forward more than three decades ago as an alternative to conventional shell-model calculations, the Kerman-Klein method has proved feasible previously only when applied to unrealistically small configuration spaces or when phenomenological simplifications have been superposed. Starting from a spherical shell-model Hamiltonian, we describe a fully microscopic calculation, free of the above limitations, of the properties of the ground-state band of a typical deformed rare-earth nucleus, ^{158}Gd. [S0031-9007(97)03251-1]

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The phenomenological shell model remains the bedrock of nuclear structure physics [1,2]. In its standard form, we accept the empirically established notions of closed shell or magic nuclei and of single particle or single hole excitations with respect to these special cores (below, for brevity, we speak only of particles). To study the properties of nuclei which are removed from these stable cores by two or more nucleons, one adds residual two-particle forces. To understand low energy behavior of low and medium mass nuclei, one restricts the allowed single-particle excitations and residual interactions to the valence shell. The solution of the resulting matrix diagonalization problem, which is straightforward in principle, has been achieved only up to mass number $N = 48$ [3] because of the rapid growth of the dimensionality of the Hamiltonian matrices. Beyond that there are several possibilities: One can study somewhat heavier nuclei with Monte Carlo calculations [4] that utilize the entire valence shell-model space. One can also reduce the dimensionality of the Hamiltonian matrices to tractable sizes in several ways, either by utilizing only the lowest irreducible representations of relevant approximate symmetries [5,6] or by applying the variational method to a trial space suggested by the deformed shell model [7,8]. Except for the first example cited [5], these latter methods allow one to break the bounds of the valence shell restriction.

More than three decades ago, Kerman and Klein proposed an alternative to the standard linear approach to the shell model. Originally designed as a method for restoring the broken symmetry of mean field solutions [9], it soon became clear that it was a general formulation of quantum mechanics [10] that could also be used to study the shell-model problem. It was argued that, especially in cases of well-developed collective motion, one could replace the linear methods that use a large basis of states by a nonlinear method involving a tractable set of states. Early attempts to apply this method to semimagic nuclei [11,12] were at best only modestly successful and were not followed up.

Our aim in this Letter is to reactivate the original program by reporting a successful application to a deformed nucleus in the rare earth region, ^{158}Gd. For such a nucleus not only is it technically impossible to apply the valence shell model based on spherical single-particle excitations, but the restriction to the valence shell itself fails badly [1,6–8]. Starting from a spherical shell model expanded to include all orbits bound in a realistic (Wood-Saxon) single-particle potential and a standard Hamiltonian widely applied for heavy nuclei, we describe a fully microscopic derivation of some of the properties of the ground state rotational band including energies, charge and mass quadrupole matrix elements, and pairing matrix elements. This work utilizes results obtained from a semimicroscopic description, referred to as CPC, of the low energy properties of *odd* deformed nuclei. The role played by odd nuclei in determining the properties of a neighboring even core will be clarified below. The results reported for ^{158}Gd are almost certainly not special to this nucleus, nor is the method necessarily confined to the ground-state band.

Model and method.—As a Hamiltonian we choose the form

$$H = \sum_{\alpha i} h_{ai} a^{\dagger}_{\alpha i} a_{\alpha i} - \frac{1}{2} \sum_{ij} \sum_{LM_L} \kappa_{ij;L} Q^{i\dagger}_{LM_L} Q^{j}_{LM_L} - \frac{1}{2} \sum_{i} \sum_{LM_L} g_{i;L} \Delta^{i\dagger}_{LM_L} \Delta^{i}_{LM_L} . \quad (1)$$

In the first term a and $a^{\dagger}$ are the spherical shell model annihilation and creation operators, α labels the principal and angular momentum quantum numbers of states in a spherical Wood-Saxon potential with spin-orbit coupling, the subscript a the same set minus the magnetic quantum number, i distinguishes neutron from proton, and h_{ai} are the eigenvalues in the respective wells. The second term is a sum of products of mass multipole moments with strengths $\kappa_{ij;L}$; in the following we shall retain only the most important terms, those with $L = 2$, though in a more refined treatment, we should include $L = 4$ [13]. The last term is a sum of pairing interactions with strengths

$g_{i;L}$, of which we include only the dominant monopole, though here the $L = 2$ term can also be considered to be well established [7]. The adequacy of the Hamiltonian (1) as a representation for those properties of a more realistic interaction that lead to collective behavior has been carefully documented in a recent investigation [14].

To explore the consequences of (1), we calculate the commutator of a and of $a^\dagger$ with the Hamiltonian and take the matrix elements between states $|J\mu\nu\rangle$ of a chosen odd nucleus of mass number N, with angular momentum quantum numbers J, μ and all other labels indicated by ν and the corresponding states of the relevant even neighbors, $|IMn(N \pm 1)\rangle$. Suppressing charge quantum numbers, we encounter in the single-particle terms the coefficients of fractional parentage (CFP)

$$V_{J\mu\nu}(\alpha; IMn\rangle = \langle J\mu\nu|a_\alpha|IMn(N + 1)\rangle, \quad (2)$$

$$U_{J\mu\nu}(\alpha; IMn) = \langle J\mu\nu|a_\alpha^\dagger|IMn(N - 1)\rangle. \quad (3)$$

For the evaluation of a typical interaction term, consider, in an abbreviated notation,

$$\langle J|aQ_2|I(N + 1)\rangle = \sum_{I'} V_J(I')\langle I'(N + 1|Q_2|I(N + 1)\rangle, \quad (4)$$

which involves on the completeness relation. By this means the nonlinear terms are expressed as sums of products of terms in which one factor, the CFP, depends on the odd nucleus, whereas the other depends on the properties of the even cores. With a corresponding treatment of the pairing interaction, we obtain equations with characteristics and properties that we now describe.

In addition to the CFP, which are coupled by the pairing interactions, there occur in these equations matrix elements of the mass quadrupole moments for two different, neighboring, even nuclei and matrix elements of the pairing interaction between the two neighbors. Together we refer to these as the core matrix elements. The structure of these equations, which is given in all detail in [15] and will not be reproduced here, bears a striking resemblance to those of the Hartree-Bogoliubov mean-field theory, but in contrast to the latter our equations are formally exact, conserving both angular momentum and particle number. Since the core matrix elements (see below) can be expressed as bilinear functions of the CFP, for a fully microscopic (self-consistent) solution, we must solve a nonlinear problem.

If we assume that the core matrix elements are known, however, the resulting equations are linear and define an Hermitian eigenvalue problem for the energies of the odd nucleus relative to the average ground ground state energy of the neighboring cores. In this interpretation, the chemical potential of the odd nucleus and the excitation spectra of the even neighbors are added to the list of quantities assumed to be known. The possibilities inherent in such a generalized semimicroscopic theory, first noted in [16], was developed and applied by Dönau and Frauendorf [17,18]. Recently further development and applications have been carried out by the authors in a series of papers of which the latest are [13,15]. In these applications the source of the core information is either experiment (in the present example) or phenomenology.

We recall the approximations that are necessary in order to make even the linear scheme workable. The most important can be understood by examination of (4). If the starting state of the core, $|In\rangle$, belongs to a given low-lying rotational band, then we know that intraband transitions are by far the dominant ones, though a few neighboring bands provide some residual strength, and these are included in the calculations in order to satisfy the sum rule. Once the choice of core bands has been made, there remains a vital question associated with the space of the single odd nucleon. For all the examples done, we find that results for the observables of interest have essentially converged when three major shells are included. For the purposes of the new results reported in this Letter, we have nevertheless done calculations that include all bound orbitals. The reason for this will be explained below.

Self-consistency: particle number.—We now take the additional step that transforms the semi-microscopic theory into a fully microscopic solution of the shell-model Hamiltonian. This will be the case provided the expressions for the core matrix elements, evaluated below in terms of the CFP (sum rules), reproduce the experimental values. By showing that this happens to a reasonable accuracy for all the observables associated with the ground-state band, we open the door to a viable alternative to other methods of studying low energy nuclear structure.

From the list of core properties, we first consider the conservation of particles. The operator for the total particle number,

$$\hat{N} = \sum_{\alpha,i} a_{\alpha i}^\dagger a_{\alpha i}, \quad (5)$$

can be separated into a sum of four terms

$$\hat{N} = \hat{N}_{p,+} + \hat{N}_{p,-} + \hat{N}_{n,+} + \hat{N}_{n,-}, \quad (6)$$

where the subscripts distinguish charge of the nucleons and parity of the single-particle orbitals. Because we include in the Hamiltonian (1) only multipoles of even parity, each of these quantities is conserved. The even nucleus chosen for study plays the role of the heavier of the two cores in a calculation [19] carried out for ^{157}Gd, an axially deformed nucleus with states $|IMK(N + 1)\rangle$, where K is the angular momentum of the bandhead. Further discussion will be confined to the ground-state band with $K = 0$, and this quantum number will be suppressed. We thus need the four sets of eigenvalues

$$N_{i,\pm} = \sum_{\alpha\pm}\langle IM(N + 1)|a_{\alpha i\pm}^\dagger a_{\alpha i\pm}|IM(N + 1)\rangle = \sum_{\alpha\pm,J\mu\nu} V_{J\mu\nu}^{i\star}(\alpha; IM)V_{J\mu\nu}^i(\alpha; IM), \quad (7)$$

each of which should be independent of I, as it is automatically independent of M. To evaluate these sum rules, one needs the CFP for the neutron levels of ^{157}Gd of both parities, which had been obtained earlier [19] and the proton levels of ^{157}Eu, which were obtained for present use. The results are shown below in Table I. It has been verified that the sums in (7) depend on I only in the third decimal place.

We consider the results given in the table to be strongly encouraging. In this regard, two points must be noted. The first concerns the problem of the normalization of the CFP. Though we failed to emphasize the point in our previous work, transition matrix elements calculated in CPC are independent of an overall rescaling of the normalization, provided it is the same for all states $|J\mu\nu\rangle$. In our work we assumed unit normalization, as in the strong coupling core-particle model, but this choice cannot be exact, as we know from our early work on spherical nuclei [11]. To make the appropriate corrections requires incorporating into our algorithm a set of sum rules derived from the Fermion anticommutation relations. This has not yet been done. Second, to achieve a result so close to the exact one, we must include (numerically significant) contributions from a large number of solutions of the eigenvalue problem, including high-lying ones that play no role in the fit to the known observables of the odd nuclei. These points are relevant as well for the remainder of our discussion.

Self-consistency: quadrupole matrix elements.—In the reference Hamiltonian (1) there occur three quadrupole coupling constants. In the case under discussion, the experimental electric quadrupole matrix elements are in good agreement with rigid rotor values. For the CPC calculations we then assume proportionality between neutron and proton mass quadrupole elements, as expressed by the relation

$$\langle IMK|Q^n|I'M'K'\rangle = \eta\langle IMK|Q^p|I'M'K'\rangle, \quad (8)$$

where η is a constant evaluated below. It follows that for the core-particle theory, we can work with the proton quadrupole moment alone provided we introduce different effective coupling strengths for the neutron and proton spectra, according to the equations

$$\kappa_p^{\rm eff} \equiv (\kappa_{pp} + \eta\kappa_{pn}), \quad (9)$$

TABLE I. Particle number, actual and calculated, for $^{158}_{64}$Gd.

$\langle N\rangle$	Actual	Calculated
Neutrons +	44	45.06
Neutrons −	52	50.64
Neutrons total	94	95.70
Protons +	38	36.26
Protons −	26	28.90
Protons total	64	65.16

$$\kappa_n^{\rm eff} \equiv (\eta\kappa_{nn} + \kappa_{pn}). \quad (10)$$

Thus, in fitting CPC to the data in the odd nuclei, we are allowed to choose and indeed find slightly different values for the effective coupling constants. For these purposes and for the further development, the actual value of η is reflected only in the value that has to be assigned to the effective coupling strengths.

Since we are dealing with operators of the form

$$\hat{Q}^i = \sum_{\alpha\gamma} q_{\alpha i,\gamma i} a_{\alpha i}^\dagger a_{\gamma i}, \quad (11)$$

their core matrix elements are again quadratic sums in the same set of CFP as enter the calculation of the number. The first test of self-consistency is that these sums have a "shape" consistent with the rigid rotor assumption, as expressed in (8), a test that is passed with flying colors. This is seen partly from Fig. 1, which emphasizes the fact that not only is the angular momentum dependence of the electric quadrupole matrix elements given correctly, but also their magnitudes and signs. From the fact that the neutron quadrupole matrix elements follow parallel curves, we deduce the value $\eta = 1.1$.

Self-consistency: pairing.—For the pairing matrix elements, which are linear combinations of matrix elements of type

$$\langle IMn(n-1)|a_{\overline{\alpha}}a_\alpha|I'M'n'(N+1)\rangle = \sum_{J\mu\nu} U^*_{J\mu\nu}(\alpha; IMn)V_{J\mu\nu}(\alpha; I'M'n'), \quad (12)$$

there are again two tests. First there is the requirement that the matrix elements be independent of angular momentum, as was assumed in the input. Second we must reproduce the value of this matrix element. For

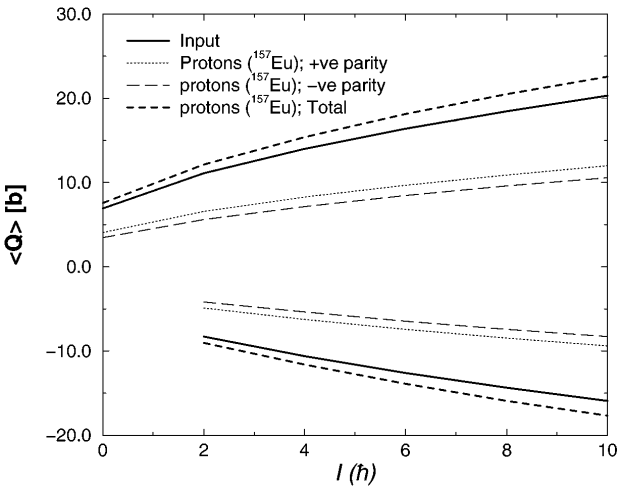

FIG. 1. Values of the matrix elements of $\hat{Q}^p$ for ^{158}Gd. The negative values represent the diagonal elements $\langle IK = 0\|Q^p\|IK = 0\rangle$, whereas the positive values show the off-diagonal elements $\langle IK = 0\|Q^p\|I + 2K = 0\rangle$.

TABLE II. Contributions to the moment of inertia arising from the different terms in the Hamiltonian. Here sp refers to the single particle contribution, Q to the quadrupole contribution, and Δ to the pairing term.

$E_2 - E_0$	$\mathcal{I}_{\rm sp}$	$\mathcal{I}_Q$	$\mathcal{I}_\Delta$	$\mathcal{I}_{\rm total}$	$\mathcal{I}_{\rm exp}$
Neutron +	0.00291	⋯	0.00121		
Neutron −	0.00532	⋯	−0.00236	⋯	
Neutron total	0.00823	⋯	−0.00157	⋯	
Proton +	0.001943	0.00141	−0.00232	⋯	
Proton −	0.001272	0.000523	0.00194	⋯	
Proton total	0.003215	0.001933	−0.00126	⋯	
Total	0.01145	−0.000643	0.001144	0.011951	0.0124

the neutron pairing, the diagonal matrix elements vary monotonically between 1.859 for $I = 0$ and 1.814 for $I = 8$, compared with the experimental value of 1.65 for the gap parameter. The corresponding values for the proton pairing are 1.672 for $I = 0$ and 1.612 for $I = 8$, compared with the experimental value of 1.321.

Self-consistency: moment of inertia.—There remains the test of the self consistency of the excitation spectrum. This requires first that the diagonal elements of (1) satisfy the rigid rotor equation

$$E_I = \langle IM|H|IM\rangle = \frac{I(I+1)}{2\mathcal{I}}, \qquad (13)$$

and second that the experimental value of $\mathcal{I}$ be reproduced. The first of these requirements is well-satisfied, and therefore we can confine our attention to the moment of inertia. In Table II, we display not only the final calculated value of the moment of inertia, but also the contributions of individual terms of H, broken down according to nucleonic charge. The absence of contributions from the neutron quadrupole moment simply reflects the fact that we organized the calculation so that the quadrupole term is expressed completely in terms of the proton quadrupole operator and of the effective coupling strengths. Notice that the major contribution comes overwhelmingly from the single-particle term and that the contribution of the quadrupole term is insignificant. (This term then contributes only deformation energy.) The self-consistency is as close as one has a right to expect, in view of the well-known effect of the quadrupole pairing interaction [7], which is not in our calculation.

The results of this Letter imply that for a limited number of states we have demonstrated a new route for passing directly from a spherical shell model to the properties of a deformed rare-earth nucleus. The immediate next steps are twofold: to add to the working Hamiltonian the additional simple interactions mentioned in the text and to add to the algorithm a proper formulation for normalization of the coefficients of fractional parentage.

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