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# THE COUPLING OF VALENCE SHELL AND PARTICLE-HOLE DEGREES OF FREEDOM IN A PARTIAL RANDOM PHASE APPROXIMATION

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**Abstract:** It is well known that the random phase approximation breaks down in the absence of a substantial energy gap between occupied and unoccupied single-particle states. Particle-hole excitations are then inevitably accompanied by substantial rearrangements of the particles in the neighbourhood of the Fermi surface. To accommodate this situation, a partial RPA is introduced which corresponds to replacing only the particle-hole degrees of freedom by bosons but leaving the valence space degrees of freedom intact. The PRPA is therefore a mapping of the many-fermion dynamics into the dynamics of a coupled boson-valence space. In application of the PRPA, algebraic methods, of either a fermionic or Lie algebra type, can be introduced, if desired, to facilitate the treatment of the valence space degrees of freedom. Results of applications are presented in which the valence space particles are treated in the rotational and SU(3) models, and are coupled strongly to giant dipole and quadrupole resonances.

## 1. Introduction

The equations of motion approach [1]) to the quantum mechanics of many fermion systems gives a very succinct expression of the independent quasi-particle approximations of Hartree-Fock and Hartree-Bogolyubov theory and the Tamm-Dancoff and RPA (random phase approximation) theories of vibrational states [2]).

The latter theories can be regarded as first approximations to boson expansion theories in which the many-fermion hamiltonian is mapped into a harmonic hamiltonian of the type

$$H_b = W_0 + \sum_\nu \hbar\omega_\nu b_\nu^\dagger b_\nu , \tag{1}$$

where $b_\nu^\dagger$ and $b_\nu$ are boson creation and annihilation operators that satisfy the boson commutation relations

$$\begin{aligned} [b_\mu, b_\nu] &= [b_\mu^\dagger, b_\nu^\dagger] = 0 , \\ [b_\mu, b_\nu^\dagger] &= \delta_{\mu\nu} . \end{aligned} \tag{2}$$

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Motivated by the successes of these first order theories, many authors have developed sophisticated boson expansion techniques to describe more general situations such as, for example, rotations [cf. refs. [3,4]) and other references quoted therein]. More sophisticated equations of motion (such as those of Kerman and Klein [5])) have also been devised for more general situations. Although very important, these approaches lack the simplicity of the harmonic vibrational equations. Furthermore, boson expansion or equations of motion techniques are not always the most appropriate for low-lying positive-parity valence-shell degrees of freedom. For example, SU(3) [ref. [6])] or pseudo-SU(3) [ref. [7])] or simply straightforward shell model techniques may be better.

In particular, it appears to be rather artificial to describe the degrees of freedom of the last nucleon in an odd-mass nucleus, or the last several nucleons in an open-shell nucleus, in terms of bosons. Several authors have therefore suggested that one should consider mappings into spaces which admit both bosonic and fermionic degrees of freedom [8-10]). For example, Suzuki and Matsuyanagi [8]) obtained a description of seniority in which pairs of nucleons coupled to zero are bosonized while other kinds of pairs retain a fermion-like character. Of particular relevance to the present analysis is the suggestion by Marshalek [10]) that only the particle-hole excitations of a closed core should be treated as bosons but that the additional valence particles (or holes) should retain their fermion character. It will be shown in this paper that one can get the best of all worlds by using extended RPA techniques to describe the particle-hole degrees of freedom and other (e.g. shell model or even more sophisticated equations-of-motion) techniques for the more complicated rearrangement degrees of freedom of the valence space.

The outcome is the replacement of the infinite dimensional nuclear Hilbert space by a finite dimensional valence space coupled to vibrational degrees of freedom. Such a replacement was recently advocated by Carvalho *et al.* [11]) and shown to be an accurate representation of the nuclear shell model for medium and heavy nuclei. What is further achieved in this paper is an RPA framework for extracting the hamiltonian in such a representation. Thus, for example, a way is provided to renormalize valence shell states by coupling to giant resonance vibrations and to calculate the deformation splitting of giant resonances and other particle-hole excitations. The possibility of renormalizing valence shell states in this way was recently considered by Le Blanc *et al.* [12]) in the context of the symplectic shell model [11,13,14]). The partial RPA approach achieves the same result but in a simpler way that obviates the necessity of invoking the symplectic algebra. It is also more general in as much as it is not restricted to monopole and quadrupole vibrations but applies to vibrations of any multipolarity.

Underlying this development is the important concept of "partial second quantization". Recall that second quantization is fundamentally a technique for realizing physical operators as polynomials in boson or fermion annihilation and creation operators. The technique is extremely useful in handling, for example, infinite dimensional Hilbert and Fock spaces. In particular, hamiltonians that are quadratic in either boson or fermion operators are very easy to diagonalize even on infinite dimensional spaces. The Hartree-Fock independent-particle model, the BCS theory of superconductivity [15]) and the RPA theory of vibrations [16]) are notable examples that exploit this simplicity.

The idea of bosonizing (or second quantizing) only a subset of nuclear degrees of freedom was exploited recently in the U(3)-boson model [17]). This model augments the Bohr-Mottelson (boson) model [18]) with an intrinsic U(3) structure which represents the valence space degrees of freedom and thereby admits vortex spin degrees of freedom.

Parallel techniques were also found recently to have a major application to Lie algebra theory [19,20]). Recall that a standard way to obtain a boson representation of a Lie algebra is via coherent state theory [3]). Thus coherent state theory can be regarded as a technique of second quantization. Partial second quantization then corresponds to expressing the elements of a Lie algebra in terms of a combination of bosons and the elements of a subalgebra. This underlies a recently formulated vector coherent state (also called partially coherent state [20])) theory [19]).

An application of central interest to this paper is to the so-called broken symmetries in nuclear physics. One recalls that the Bohr-Mottelson collective model [18]) of quadrupole rotations and vibrations is expressible in terms of five pairs of quadrupole boson operators ($d^\dagger_\nu$, $d_\nu$; $\nu = 0, \pm 1, \pm 2$). In the harmonic vibrational limit, the ground state of the nucleus is represented as a simple boson vacuum. However, to describe rotations in this model, one needs the concept of a phase transition to a broken symmetry state. In the broken symmetry state, the model nucleus assumes a deformed equilibrium shape. On the other hand, if one admits an intrinsic structure as, for example, in the U(3)-boson model [17]) (the hydrodynamic limit of the microscopic symplectic model) or (more or less equivalently) as arising from the valence particle degrees of freedom, as we consider here, the essential ingredients of a rotational spectrum may already be present in the intrinsic structure, thus giving a very different perspective on the concept of a phase transition. The introduction of a partial RPA therefore accommodates this very common situation. We shall also show that it is appropriate to redefine the concept of the valence space.

## 2. The equations of motion formalism

### 2.1. THE BASIC EQUATIONS

The basic equation-of-motion formalism was presented in ref. [1]). Let $|\Psi_0\rangle$ denote the nuclear ground state and $|\Psi_\lambda\rangle$ an excited state of excitation energy $\hbar\omega_\lambda$. There then exists excitation operators $O^\dagger_\lambda$ such that

$$O^\dagger_\lambda|\Psi_0\rangle = |\Psi_\lambda\rangle\,,$$
$$O_\lambda|\Psi_0\rangle = 0\,. \tag{3}$$

These operators obey the dynamical equations of motion

$$\langle\Psi_0|[O_\kappa, H, O^\dagger_\lambda]|\Psi_0\rangle = \hbar\omega_\lambda\langle\Psi_0|[O_\kappa, O^\dagger_\lambda]|\Psi_0\rangle = \hbar\omega_\lambda\delta_{\kappa\lambda}\,,$$
$$\langle\Psi_0|[O_\kappa, H, O_\lambda]|\Psi_0\rangle = -\hbar\omega_\lambda\langle\Psi_0|[O_\kappa, O_\lambda]|\Psi_0\rangle = 0\,, \tag{4}$$

where the symmetrized double commutators are defined

$$2[O_\kappa, H, O^\dagger_\lambda] = [O_\kappa, [H, O^\dagger_\lambda]] + [[O_\kappa, H], O^\dagger_\lambda]\,. \tag{5}$$

If $X$ is a transition operator, then its matrix element between the ground and an excited state can be expressed

$$\langle\Psi_\lambda|X|\Psi_0\rangle = \langle\Psi_0|[O_\lambda, X]|\Psi_0\rangle\,. \tag{6}$$

Thus the equations of motion express the properties of excited states in terms of ground state expectation values.

To derive their properties in the equations of motion formalism, one must make some approximation $|0\rangle$ for the ground state $|\Psi_0\rangle$ and choose a basis $(\eta^\dagger_\nu, \eta_\nu)$ for the linear space of operators in which the excitation and de-excitation operators $(O^\dagger_\lambda, O_\lambda)$ are presumed to reside. It is convenient to choose basis operators that satisfy the so-called weak boson commutation relations

$$\langle 0|[\eta_\mu, \eta^\dagger_\nu]|0\rangle = \delta_{\mu\nu}\,,$$
$$\langle 0|[\eta_\mu, \eta_\nu]|0\rangle = \langle 0|[\eta^\dagger_\mu, \eta^\dagger_\nu]|0\rangle = 0\,. \tag{7}$$

By choosing basis operators in this way, we automatically ensure their linear independence and, hence, that any potential problems of overcounting excitation modes of the nucleus are avoided [21]).

The linear transformation to the required operators

$$O^\dagger_\lambda = \sum_\nu (Y_\nu(\lambda)\eta^\dagger_\nu - Z_\nu(\lambda)\eta_\nu)\,,$$
$$O_\lambda = \sum_\nu (Y^*_\nu(\lambda)\eta_\nu - Z^*_\nu(\lambda)\eta^\dagger_\nu) \tag{8}$$

must then preserve the weak boson commutation relations; i.e.

$$\langle 0|[O_\kappa, O^\dagger_\lambda]|0\rangle = \delta_{\kappa\lambda}\,,$$
$$\langle 0|[O_\kappa, O_\lambda]|0\rangle = \langle 0|[O^\dagger_\kappa, O^\dagger_\lambda]|0\rangle = 0\,. \tag{9}$$

Thus it is required that the transformation coefficients satisfy

$$\sum_\nu [Y^*_\nu(\kappa)Y_\nu(\lambda) - Z^*_\nu(\kappa)Z_\nu(\lambda)] = \delta_{\kappa\lambda}\,; \tag{10}$$

i.e., the transformation (8) is symplectic.

Finally, the solution of the equations of motion (4), corresponds to solving the eigenvalue equation

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} = \hbar\omega_\lambda\begin{pmatrix} Y(\lambda) \\ Z(\lambda) \end{pmatrix} \tag{11}$$

with

$$A_{\mu\nu} = \langle 0|[\eta_\mu, H, \eta^\dagger_\nu]|0\rangle ,$$
$$B_{\mu\nu} = -\langle 0|[\eta_\mu, H, \eta_\nu]|0\rangle . \quad (12)$$

### 2.2. THE RANDOM PHASE APPROXIMATION (RPA)

The single particle states of the nuclear shell model are conventionally separated into occupied, unoccupied and valence shells. A shell model calculation of low-lying states cutomarily restricts the nuclear Hilbert space to an active space obtained by distributing a relatively small number of extra-core particles over the valence shells as illustrated in fig. 1.

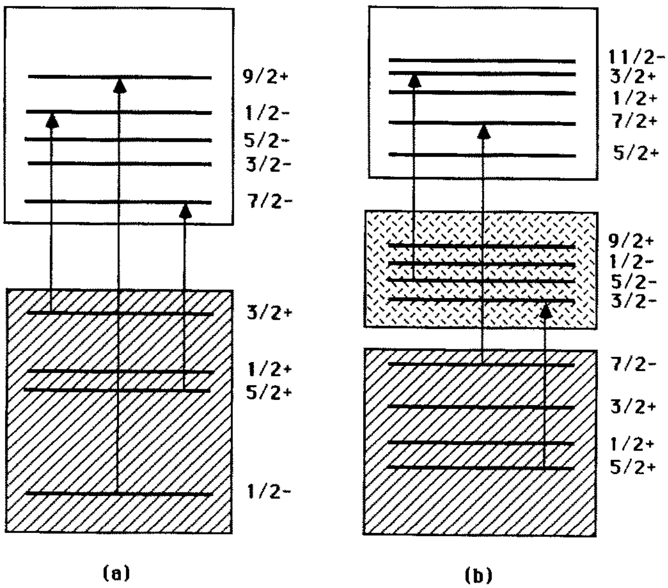


Fig. 1. Single-particle shells and particle-hole raising operators for (a) a closed-shell nucleus and (b) an open-shell nucleus.

For a closed shell nucleus, the valence shells form an empty set and there is a unique closed shell state. In the RPA, the closed shell state is adopted as the approximate (uncorrelated) ground state for the solution of the equations of motion (11) and (12). The basic operators are taken to be the single-particle raising operators

$$\eta^\dagger_{ph} = a^\dagger_p a_h \quad (13)$$

which lift a particle from one of the occupied (particle) shells to one of the unoccupied (hole) shells of the closed shell nucleus, as illustrated in fig. 1(a). These operators evidently satisfy the weak boson commutation relations (7).

For an even open shell nucleus, the uncorrelated ground state $|0\rangle$ of the open shell RPA (OSRPA) [ref. [22]] is taken to be the $J^\pi = 0^+$ ground state of the hamiltonian restricted to the valence space. In other words, the state $|0\rangle$ contains a closed shell core of fully occupied single particle states, together with a shell model distribution of extra core particles over the single particle valence states. The basic operators $(\eta_\nu^\dagger)$ are now taken to be single-particle raising operators of the type indicated in fig. 1(b). Let $a_\alpha^\dagger a_\beta$ denote such a raising operator. Since

$$\langle 0|[a_{\beta'}^\dagger a_{\alpha'}, a_\alpha^\dagger a_\beta]|0\rangle = \delta_{\alpha\alpha'}\delta_{\beta\beta'}(n_\beta - n_\alpha)\,,$$

where

$$n_\alpha = \langle 0|a_\alpha^\dagger a_\alpha|0\rangle\,,$$

we restrict to raising operators for which

$$n_\beta - n_\alpha > 0$$

and define

$$\eta_{\alpha\beta}^\dagger = (n_\beta - n_\alpha)^{-1/2} a_\alpha^\dagger a_\beta\,. \tag{14}$$

These operators then satisfy the weak boson commutation relations and define a basis for the OSRPA.

### 2.3. EQUATIONS OF MOTION THEORY AS A BOSON MAPPING

It is known that all the predictions of any model based on the above equations of motion formalism are reproduced by the boson hamiltonian

$$H_{\rm b} = W_0 + \sum_{\mu\nu} (A_{\mu\nu} b_\mu^\dagger b_\nu + \tfrac{1}{2}B_{\mu\nu} b_\mu^\dagger b_\nu^\dagger + \tfrac{1}{2}B_{\mu\nu}^* b_\nu b_\mu)\,, \tag{15}$$

where $(b_\nu^\dagger, b_\nu)$ are boson operators satisfying the commutation relations (2) and $A_{\mu\nu}$ and $B_{\mu\nu}$ are defined by eq. (12).

To prove this observation, one has only to note that by construction

$$\begin{aligned}\langle 0|[\eta_\mu, \eta_\nu^\dagger]|0\rangle &= [b_\mu, b_\nu^\dagger] = \delta_{\mu\nu}\,,\\ \langle 0|[\eta_\mu, \eta_\nu]|0\rangle &= [b_\mu, b_\nu] = 0\,,\\ \langle 0|[\eta_\mu^\dagger, \eta_\nu^\dagger]|0\rangle &= [b_\mu^\dagger, b_\nu^\dagger] = 0\end{aligned} \tag{16}$$

and, by definition,

$$\begin{aligned}\langle 0|[\eta_\mu, H, \eta_\nu^\dagger]|0\rangle &= A_{\mu\nu} = [b_\mu, H_{\rm b}, b_\nu^\dagger]\,,\\ \langle 0|[\eta_\mu, H, \eta_\nu]|0\rangle &= -B_{\mu\nu} = [b_\mu, H_{\rm b}, b_\nu]\,.\end{aligned} \tag{17}$$

It is important to note that the observation is valid even though a given pair of operators $(\eta_\nu^\dagger, \eta_\nu)$ may be a very poor approximation to boson operators in the full nuclear Hilbert space. It is sufficient that they satisfy the weak boson commutation relations. Thus if $\mathbb{H}_b$ denotes an irreducible representation space for the boson algebra, the standard equation-of-motion formalism may be regarded as the replacement of the nuclear Hilbert space $\mathbb{H}$ by $\mathbb{H}_b$; i.e. $\mathbb{H} \to \mathbb{H}_b$.

For example, if we restrict to five quadrupole bosons, $\mathbb{H}_b$ is the Hilbert space of the Bohr-Mottelson model [18]).

### 2.4. THE INCLUSION OF REARRANGEMENT

The OSRPA has been quite successful particularly at describing negative parity excited states [23]). However, it has some obvious defects. One is that it gives an unsatisfactory description of low-lying positive parity states that are excited predominantly by rearrangement of the particles in the valence shells. Another is that it assumes that all excited states, that it does purport to describe, are obtained from the ground state by a linear combination of single-particle raising and lowering operators but again without any rearrangement of the valence particles.

To rectify these deficiencies, we therefore seek equations of motion corresponding to a coupled valence-shell boson hamiltonian of the form

$$H_{\text{v.b.}} = H_{\text{v}} + \sum_{\nu} (C_\nu b_\nu^\dagger + C_\nu^\dagger b_\nu) + \sum_{\mu\nu} (A_{\mu\nu} b_\mu^\dagger b_\nu + \tfrac{1}{2} B_{\mu\nu} b_\mu^\dagger b_\nu^\dagger + \tfrac{1}{2} B_{\mu\nu}^\dagger b_\mu b_\nu) , \quad (18)$$

where $H_{\text{v}}$, $C_\nu$, $A_{\mu\nu}$, and $B_{\mu\nu}$ are now operators that act between valence shell states and the $(b_\nu^\dagger)$ are the boson images of one-body raising operators $(\eta_\nu^\dagger)$.

Let $S = \{|\alpha\rangle\}$ denote an orthonormal basis for the valence shell space

$$\mathbb{H}_{\text{v}} = \text{span}\,\{|\alpha\rangle\} .$$

$\mathbb{H}_{\text{v}}$ may be the whole valence space or simply a selected subspace according to the generality of the model one wishes to construct. For example, in the OSRPA, one retains only the ground state of the nuclear hamiltonian restricted to the valence space. Other sets of interest might include the ground and first excited state or even a "rotational" sequence of states if such should occur in a preliminary valence shell diagonalization.

Now since the states $\{|\alpha\rangle\}$ are all annihilated by the one-body lowering operators, i.e.

$$\eta_\nu |\alpha\rangle = 0 , \quad (19)$$

it makes sense to identify them with boson vacuum states and to think of the valence shell degrees of freedom as the "intrinsic" degrees of freedom of a collective vibrational model. It must, of course, be recognized that the valence space also contains highly collective degrees of freedom. This is clear from the appearance of lowlying rotational states in many valence shell model calculations. However, the fact remains that, regardless of what one calls them, the valence shell and particle-hole degrees of freedom are quite distinct. Thus the extended equation-of-motion formalism corresponds to a mapping

$$\mathbb{H} \rightarrow \mathbb{H}_v \times \mathbb{H}_b \tag{20}$$

of the full Hilbert space into a simple product space in which $\mathbb{H}_b$ is a boson space and the valence space $\mathbb{H}_v$ is finite dimensional. The dependence of the coefficients in the hamiltonian $H_{v.b.}$ on the valence shell degrees of freedom clearly allows the possibility of strong coupling between the valence and particle-hole (boson) degrees of freedom.

In the partial RPA, we select one-body raising operators ($\eta_\nu^\dagger$) as in the OSRPA such that

$$\langle 0|[\eta_\mu, \eta_\nu^\dagger]|0\rangle = \delta_{\mu\nu} \tag{21}$$

for $|0\rangle$ the ground state of a preliminary shell model calculation restricted to the valence space. The hamiltonian $H_{v.b.}$ is then defined by the matrix elements of the operators $H_v$, $C_\nu$, $A_{\mu\nu}$, and $B_{\mu\nu}$ which in turn are defined by

$$\begin{aligned} \langle\alpha|H_v|\beta\rangle &= \langle\alpha|H|\beta\rangle \quad , \\ \langle\alpha|C_\nu|\beta\rangle &= \langle\alpha|[\eta_\nu, H]|\beta\rangle , \\ \langle\alpha|A_{\mu\nu}|\beta\rangle &= \langle\alpha|[\eta_\mu, H, \eta_\nu^\dagger]|\beta\rangle , \\ \langle\alpha|B_{\mu\nu}|\beta\rangle &= -\langle\alpha|[\eta_\mu, H, \eta_\nu]|\beta\rangle , \end{aligned} \tag{22}$$

where $H$ is the original hamiltonian and $|\alpha\rangle$ and $|\beta\rangle$ belong to the selected basis $S$ of valence space states.

In addition to the usual validity conditions of the RPA, needed to justify the replacement of $H$ by the coupled valence-shell-boson hamiltonian $H_{v.b.}$ of eq. (18), we also require that, to a good approximation, the extended weak boson commutation relations

$$\langle\alpha|[\eta_\mu, \eta_\nu^\dagger]|\beta\rangle \cong [b_\mu, b_\nu^\dagger] = \delta_{\mu\nu} \tag{23}$$

are satisfied for any $|\alpha\rangle, |\beta\rangle \in \mathbb{H}_v$. This is clearly a more stringent condition than the simple condition (16) that is satisfied by construction. It should be noted, however, that the kinds of vibrational states that couple strongly to a sizeable number of valence space states tend to be the highly collective states whose excitation operators satisfy the weak boson commutation relations to a good approximation. Examples are given in sects. 3 and 4.

### 2.5. MORE GENERAL DEFINITION OF ELEMENTARY EXCITATIONS AND THE VALENCE SPACE

The above discussion makes use of an independent-particle basis for the shell model in order to give meaning to the concept of particle-hole excitations and the many-particle valence space. Thus, a many-particle valence state is defined as a distribution of nucleons over the single-particle valence states. However, if one first selects a set of elementary raising operators ($\eta^\dagger_\nu$) as operators which lift particles across single-particle shells (for any convenient definition of single-particle shells), one can also define the many-particle valence space by eq. (19); i.e. as the vacuum of the chosen elementary operators.

It immediately becomes clear that the more elementary raising operators one retains the smaller the valence space and vice versa. For example, given any selected set of $N$ single-particle states, arbitrarily indexed by integers $h=1,\ldots,N$, and a set of elementary raising operators

$$\eta^\dagger_{ph} = a^\dagger_p a_h\,, \qquad p > N\,, \qquad h \leqslant N\,,$$

the vacuum space of these particle-hole operators is spanned by a single Slater determinant as in Hartree–Fock theory. At another extreme, if the raising operator set includes only centre-of-mass $1\hbar\omega$ dipole operators, then the vacuum is simply the infinite dimensional subspace of the full shell model space in which the c.m. is in its harmonic oscillator ground state; i.e. the space of the translationally invariant shell model. If the raising operators include all the negative parity operators of any multipolarity that lift a particle from one harmonic oscillator shell to the next (i.e. the set of all $1\hbar\omega$ operators) then the vacuum space is precisely the valence space of the harmonic oscillator shell model. In the symplectic shell model [11,13]), the excitation operators are restricted to just six $2\hbar\omega$ raising operators of angular momentum 0 and 2. The valence space of the symplectic shell model is then observed to be infinite dimensional [11]). Clearly many possibilities exist and one has to decide on the basis of the physics what elementary excitations to choose and what subspace of the resultant valence space to retain in a practical calculation. The important characteristic of the formalism is that it provides a convenient framework for model making and automatically avoids potential problems of overcounting.

To clarify the last remark, note that in a generalization to an open-shell nucleus of the second RPA, in which one includes both one and two particle-hole excitation operators, there is a potential problem for overcounting because a two particle-hole operator that lifts a particle from an occupied to a valence level and then lifts a particle from a valence level to an unoccupied level can be equivalent to a one particle-hole operator that lifts a particle directly from an occupied to an unoccupied level. However, such problems are avoided when one spans the space of excitation operators with basis operators that satisfy the weak boson commutation relations (7) as shown in ref. [21]).

## 3. Deformation splitting of the giant dipole resonance

Consider a model Hamiltonian of the form

$$H_{\text{v.b.}} = H_{\text{v}} + H_{\text{dip}} + H_{\text{coup}}\,, \tag{24}$$

where $H_v$ is the restriction of the full hamiltonian $H$ to $\mathbb{H}_v$, the selected valence space, $H_{dip}$ is of the form

$$H_{dip} = \hbar\omega_1 p^\dagger \cdot p\,, \tag{25}$$

where $p^\dagger$ is a $J^\pi = 1^-$ boson excitation operator for the giant dipole resonance and $H_{coup}$ couples the giant dipole and valence shell states. For simplicity, suppose that $H_{coup}$ is of the form

$$H_{coup} = \chi \mathbb{Q} \cdot (p^\dagger \times p)^{(2)}\,, \tag{26}$$

where

$$(p^\dagger \times p)^{(2)}_M = \sum_m (-1)^m (11\, M-m m|2M) p^\dagger_{M-m} p_{-m}$$

and $\mathbb{Q}$ is a $J=2$ valence space operator. A model hamiltonian of this type was considered, for example, in ref. [24]) in the context of an extension of the SU(3) model to include the giant dipole degrees of freedom and it is of interest to derive the parameters of such a model from a microscopic hamiltonian.

We first consider a suitable choice for the elementary dipole excitation operators. Recall that the $z$-component of the electric dipole operator is given by

$$\mathcal{M}(\text{E1}; 0) = e\frac{NZ}{A}\left(\frac{1}{Z}\sum_{i=1}^{Z} z_i - \frac{1}{N}\sum_{j=1}^{N} z_j\right),$$

where $z_i$ is the $z$-coordinate of the $i$th proton and $z_j$ is the $z$-coordinate of the $j$th neutron. These coordinates can be expressed in terms of single-particle harmonic oscillator raising and lowering operators

$$z_i = \sqrt{\frac{\hbar}{2m\omega}}(b^\dagger_{i0} + b_{i0})$$

giving

$$\mathcal{M}(\text{E1}; 0) = e\sqrt{\frac{\hbar NZ}{2m\omega A}}(\eta^\dagger_0 + \eta_0)\,,$$

where

$$\eta^\dagger_0 = \sqrt{\frac{NZ}{A}}\left[\frac{1}{Z}\sum_{i=1}^{Z} b^\dagger_{i0} - \frac{1}{N}\sum_{j=1}^{N} b^\dagger_{j0}\right]. \tag{27}$$

With this normalization, $\eta^\dagger_0$ is the $z$-component of a dipole boson operator $\eta^\dagger$ and satisfies the strong boson commutation relations

$$[\eta_0, \eta^\dagger_0] = 1\,. \tag{28}$$

We therefore determine $H_{dip}$ with

$$p^\dagger_0 = Y\eta^\dagger_0 - Z\eta_0\,, \tag{29}$$

by solving the equations of motion

$$AY + BZ = \hbar\omega_1 Y,$$
$$B^* Y + A^* Z = -\hbar\omega_1 Z \tag{30}$$

with

$$A = \langle 0|[\eta_0, H, \eta_0^\dagger]|0\rangle,$$
$$B = -\langle 0|[\eta_0, H, \eta_0]|0\rangle. \tag{31}$$

To determine $H_{\rm coup}$, observe that

$$[p, H_{\rm coup}, p^\dagger]^{(2)} = \chi \mathbb{Q}, \tag{32}$$

where $[\cdot, \cdot]^{(2)}$ is a commutator of spherical tensors coupled to angular momentum 2. We therefore define $\chi\mathbb{Q}$ by its valence space matrix elements

$$\chi\langle\alpha\|\mathbb{Q}\|\beta\rangle = \langle\alpha\|[p, H, p^\dagger]^{(2)}\|\beta\rangle. \tag{33}$$

For simplicity, consider a valence space spanned by a rotation-like spectrum of states $S = \{|0\rangle, |2\rangle, |4\rangle, \dots\}$ of even angular momentum. A giant dipole state $(J=1)$

$$|\alpha J\rangle = \sum_{L=J-1}^{J+1} C_{\alpha LJ}(p^\dagger \times |L\rangle)^{(J)} \tag{34}$$

then involves at most two non-zero coefficients. Having determined the hamiltonian $H_{\rm v.b.}$ its spectrum is therefore obtained by the diagonalization of at most $2\times2$ matrices.

To give an idea of the kind of results obtainable, we show the spectrum of $H_{\rm v.b.}$ calculated under the assumption that the valence shell spectrum and matrix elements follow the rotational model predictions; i.e. the valence shell energies are assumed to be given by

$$\langle L|H_{\rm v}|L\rangle = E_0 + AL(L+1) \tag{35}$$

and the quadrupole matrix elements by

$$\langle L'\|\mathbb{Q}\|L\rangle = \sqrt{2L+1}(L200|L'0)q, \tag{36}$$

where $q$ is an "intrinsic" quadrupole moment.

The spectrum obtained for the parameter values

$$A = 15\ {\rm keV}, \qquad \chi q = 2.45\ {\rm MeV}, \qquad \hbar\omega_1 = 14\ {\rm MeV}$$

is shown in fig. 2. For comparison, the results of diagonalizing the same hamiltonian in the adiabatic approximation are also shown. (Recall that the adiabatic approximation is given by assuming the rotational frequencies to be small in comparison with vibrational frequencies.)

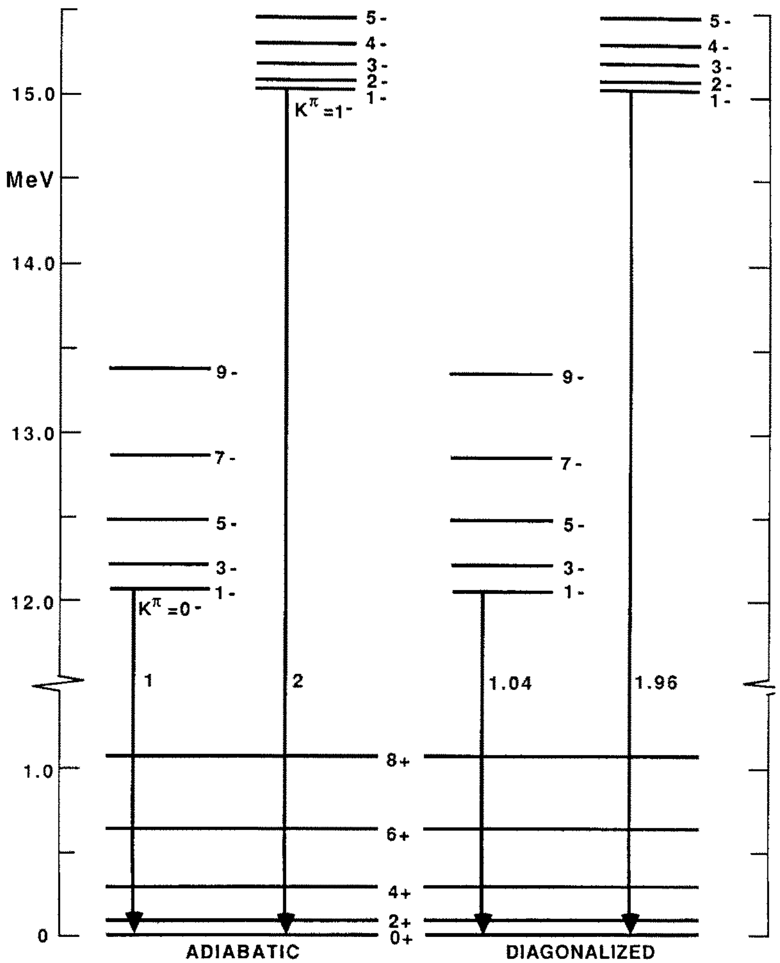


Fig. 2. Spectrum for the hamiltonian of eq. (24) calculated in the adiabatic approximation and by exact diagonalization.

The results are consistent with what one expects from a collective model analysis and from an RPA treatment in a deformed Hartree-Fock basis. What is further achieved, however, is the ability to derive such results from a fully microscopic analysis without the necessity for (deformed) independent-particle approximations. Furthermore, the formalism applies regardless of whether or not the valence space matrix elements of the quadrupole operators can be approximated by eq. (36).

An apparent limitation of the above analysis is the restriction to the valence space of the states coupled to the giant dipole degrees of freedom. One knows that, in fact, the low-lying "rotational" states of deformed nuclei are highly renormalized by coupling to the giant quadrupole degrees of freedom. As a consequence, the quadrupole matrix elements for low-lying states are much larger than those obtained by restricting to the valence space. Such renormalizations clearly need to be taken into account if one is to obtain a realistic description, from first principles, of the deformation structure of the giant dipole resonance. One possibility is to admit an explicit coupling between the giant dipole and giant quadrupole degrees of freedom. A much simpler approach, however, is to consider first the coupling of the valence shell states to the giant quadrupole degrees of freedom and then to replace the valence shell states, in the above analysis of the giant dipole resonance, by the coupled low-lying states. We therefore consider, in the following section, the renormalization of the low-lying spectrum by coupling to the giant quadrupole resonance and, conversely, the deformation splitting of giant quadrupole resonance states.

## 4. Collective quadrupole states

We now consider a model hamiltonian of the type

$$H_{\text{v.b.}} = H_{\text{v}} + A_0 d^\dagger \cdot d + \tfrac{1}{2}B_0(d^\dagger \cdot d^\dagger + d \cdot d) + k_1 D_1 \cdot (d^\dagger + d)$$
$$+ k_2 D_2 \cdot (d^\dagger \times d)^{(2)} + k_3 D_3 \cdot [(d^\dagger \times d^\dagger)^{(2)} + (d \times d)^{(2)}]\,. \qquad (37)$$

Such a hamiltonian (with $k_3 = 0$) was considered by Le Blanc *et al.* [12,25]) in the context of their coupled rotor-vibrator model and it is of interest, therefore, to derive the components of such a model from a microscopic hamiltonian.

We first consider a suitable definition for the elementary excitation operators. The 0-component $Q_0$ of the mass quadrupole operator is given in dimensionless harmonic oscillator units by

$$Q_0 = \frac{m\omega}{\hbar} \sum_{s=1}^{A} (2z_s^2 - x_s^2 - y_s^2)\,. \qquad (38)$$

Thus, in terms of single particle harmonic oscillator raising and lowering operators, it is expressed

$$Q_0 = \mathbb{Q}_0 + Q_0^+ + Q_0^-\,, \qquad (39)$$

where $\mathbb{Q}_0$ is Elliott's SU(3) quadrupole operator and

$$Q_0^+ = \tfrac{1}{2}\sum_s (2b_{sz}^\dagger b_{sz}^\dagger - b_{sx}^\dagger b_{sx}^\dagger - b_{sy}^\dagger b_{sy}^\dagger)\,,$$
$$Q_0^- = (Q_0^+)^\dagger\,. \qquad (40)$$

Thus $Q_0^+$ and $Q_0^-$ are respectively $2\hbar\omega$ raising and lowering operators. Let $|0\rangle$ be the ground state for $H_{\text{v}}$. We then have

$$\langle 0|[Q_0^-, Q_0^+]|0\rangle = 2N_0\,, \qquad (41)$$

where

$$N_0 = \langle 0|(C_{xx} + C_{yy} + C_{zz})|0\rangle \qquad (42)$$

and, for example,

$$C_{xx} = \tfrac{1}{2} \sum_{s=1}^{A} (b^\dagger_{sx} b_{sx} + b_{sx} b^\dagger_{sx}) .$$

In other words, $N_0 \hbar\omega$ is the ground state expectation of the independent particle harmonic oscillator hamiltonian

$$H_{\text{h.o.}} = (C_{xx} + C_{yy} + C_{zz}) \hbar\omega . \tag{43}$$

It is appropriate therefore to define the elementary quadrupole raising operators by

$$\eta^\dagger_\nu = \frac{1}{\sqrt{2N_0}} Q^+_\nu , \qquad \nu = 0, \pm 1, \pm 2 . \tag{44}$$

These operators, by construction, satisfy the commutation relations

$$\langle 0 | [\eta_\mu, \eta^\dagger_\nu] | 0 \rangle = \delta_{\mu\nu} .$$

Furthermore, it is known that they are boson operators to a high degree of accuracy. Indeed, the second order terms in a boson expansion of $\eta^\dagger_\nu$ have been given in ref. [19]) and are very small for large values of $N_0$. Note also that

$$N_0 \cong 0.9 A^{4/3}$$

is indeed a large number for medium and heavy nuclei.

Let $S = \{|\alpha\rangle, |\beta\rangle, \dots\}$ be a selected set of quadrupole vacuum states; i.e. they satisfy eq. (19). The equations of motion then give immediately

$$\begin{aligned}
\langle \alpha | A_0 | \beta \rangle &= \sqrt{\tfrac{1}{5}} \langle \alpha | [\eta, H, \eta^\dagger]^{(0)} | \beta \rangle , \\
\langle \alpha | B_0 | \beta \rangle &= -\sqrt{\tfrac{1}{5}} \langle \alpha | [\eta, H, \eta]^{(0)} | \beta \rangle , \\
k_1 \langle \alpha \| D_1 \| \beta \rangle &= \langle \alpha \| [\eta, H]^{(2)} \| \beta \rangle , \\
k_2 \langle \alpha \| D_2 \| \beta \rangle &= \langle \alpha \| [\eta, H, \eta^\dagger]^{(2)} \| \beta \rangle , \\
k_3 \langle \alpha \| D_3 \| \beta \rangle &= -\tfrac{1}{2} \langle \alpha \| [\eta, H, \eta]^{(2)} \| \beta \rangle .
\end{aligned} \tag{45}$$

To illustrate the kinds of results one can obtain, it is useful to consider a specific hamiltonian. The structure of the conventional RPA was illustrated very effectively by Brown, Evans and Thouless [26]) with a schematic hamiltonian of the type

$$H = H_0 - \tfrac{1}{2} \chi Q \cdot Q , \tag{46}$$

where $H_0$ is an independent-particle hamiltonian and $Q$ is the corresponding multipole operator for the excitations under consideration. Such a hamiltonian was given a foundation in the context of the vibrating potential model (VPM) in ref. [27]) and was used, for example, by Suzuki and Rowe [28]) to analyse the structure of giant multipole states of open shell nuclei. For purposes of illustration we therefore consider this hamiltonian with $Q$ the quadrupole operator (38), and set $H_0 = H_{\text{h.o.}}$, the independent particle harmonic oscillator hamiltonian of eq. (43). From eqs. (45), we then obtain

$$H_{\text{v.b.}} = E_0 - \tfrac{1}{2}\chi \mathbb{Q}\cdot\mathbb{Q} + 2\hbar\omega d^\dagger\cdot d - \chi\mathbb{Q}\cdot\mathcal{Q} - \tfrac{1}{2}\chi\mathcal{Q}\cdot\mathcal{Q}$$
$$+\sqrt{14}\chi\mathbb{Q}\cdot[2(d^\dagger\times d)^{(2)} + \tfrac{1}{2}(d^\dagger\times d^\dagger)^{(2)} + \tfrac{1}{2}(d\times d)^{(2)}]\,, \tag{47}$$

where $\mathbb{Q}$ is again the restriction of the quadrupole tensor operator $Q$ to the valence space,

$$\mathcal{Q} = \sqrt{2N_0}(d^\dagger + d) \tag{48}$$

and we have retained only the leading order terms of each type in the small parameter $1/N_0$. With these definitions, the full quadrupole operator is given by

$$Q_{\text{v.b.}} = \mathbb{Q} + \mathcal{Q} - \sqrt{14}(d^\dagger\times d)^{(2)}\,. \tag{49}$$

Note that we have not neglected exchange terms in this analysis as is common practice in using separable interactions of this type.

If we restrict the valence space states to a single $J=0$ state (e.g. the ground state of a preliminary valence space diagonalization) as in the OSRPA, then $H_{\text{v.b.}}$ reduces to the simple form

$$H_{\text{v.b.}} = E_0 + 2\hbar\omega d^\dagger\cdot d - N_0\chi(d^\dagger + d)\cdot(d^\dagger + d)\,. \tag{50}$$

This hamiltonian is of standard RPA form. It is easily diagonalized [25]) and gives a giant quadrupole state at excitation energy

$$\hbar\omega_2 = 2\hbar\omega(1 - 2N_0\chi/\hbar\omega)^{1/2}\,. \tag{51}$$

The VPM model estimate [27]) for the coupling constant,

$$\chi = \frac{\hbar\omega}{4N_0}\,, \tag{52}$$

based on a self-consistency argument, then clearly gives

$$\hbar\omega_2 = \sqrt{2}\hbar\omega \tag{53}$$

in agreement with the estimates of Suzuki and Rowe [28]) for a spherical nucleus.

If instead of giving $\chi$ its VPM value, one regards it as an adjustable parameter, then it is clear from eq. (51) that for

$$\kappa = 2N_0\chi/\hbar\omega > 1 \tag{54}$$

the RPA returns an imaginary root. Now, by Thouless' stability theorem [29]), one knows that the appearance of an imaginary RPA root indicates that the given vacuum state is unstable against particle-hole excitations and that a "broken symmetry" vacuum exists. An imaginary RPA root has therefore been heralded as the signature of a phase transition in the following sense. If one plots the spectrum for the hamiltonian (50) as a function of the coupling constant, one expects to see a vibrational spectrum with excitation energies given reasonably accurately by the RPA for $\kappa < 1$ and a rotational spectrum for $\kappa > 1$. However, this is not the only mechanism for a phase transition as becomes transparent when one admits a multiplicity of vacuum states in the partial RPA.

Consider, for the moment, a harmonic oscillator closed shell nucleus, such as $^{16}O$ or $^{40}Ca$. The relatively large RPA excitation energy $\sqrt{2}\hbar\omega$ would appear to indicate a considerable measure of stability of their closed shell states against quadrupole deformation whereas, in fact, one believes that already at 6.06 MeV in $^{16}O$ and at 3.35 MeV in $^{40}Ca$ there are highly deformed excited states with rotational bands built upon them [30]). In $^{16}O$ for example, the excited rotational states are believed to be predominantly 4 particle-4 hole states obtained by promoting four particles from the 1p shell into the 2s1d shell. The maximally deformed states that one can make in this way are the states of the SU(3) $(\lambda, \mu) = (8, 4)$ representation. Now observe that such states are also vacuum states for the above defined quadrupole excitation operators. Thus they can be included within the active valence space of the partial RPA.

The full spectrum for the hamiltonian $H_{\text{v.b.}}$ of eq. (47) is seen, by inspection, to be the superposition of the spectra based on all the irreducible SU(3) subspaces of valence space states calculated separately. The energy of the correlated $J = 0$ state for any such representation is particularly easy to calculate. For example, the ground state of the $0\hbar\omega$ closed shell based spectrum is given by the well-known RPA result

$$E(0,0) = E_0 + \tfrac{5}{2}(\hbar\omega_2 - 2\hbar\omega)\,. \tag{55}$$

For an $n\hbar\omega$ $(\lambda, \mu)$ irrep, one obtains to leading order in $1/N_0$

$$E(\lambda,\mu) = E_0 + n\hbar\omega + \tfrac{5}{2}(\hbar\omega_2 - 2\hbar\omega) - \frac{1}{N_0}(\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu)\frac{\kappa}{1-\kappa}\hbar\omega\,. \tag{56}$$

Then, for the $4\hbar\omega$ (8, 4) irrep of $^{16}O$ one obtains

$$\hbar\omega_0 = E(\lambda,\mu) - E(0,0) = 4\hbar\omega - 3.84\frac{\kappa}{1-\kappa}\hbar\omega\,. \tag{57}$$

This excitation energy, which is plotted in comparison with the giant quadrupole energy $\hbar\omega_2$ as a function of $\kappa$ in fig. 3 indicates the occurrence of a phase transition for values of $\kappa$ marginally larger than the VPM value ($\kappa = 0.5$).

The simple schematic hamiltonian (46) which ignores, for example, the pairing interactions, no doubt overemphasizes the importance of quadrupole correlations. A more realistic hamiltonian would also allow some interactions between the excitations built on different SU(3) valence states. The model nevertheless provides a very simple explanation for the appearance of deformed excited configurations in the low energy spectra of 'spherical' nuclei. For heavier deformed nuclei, we

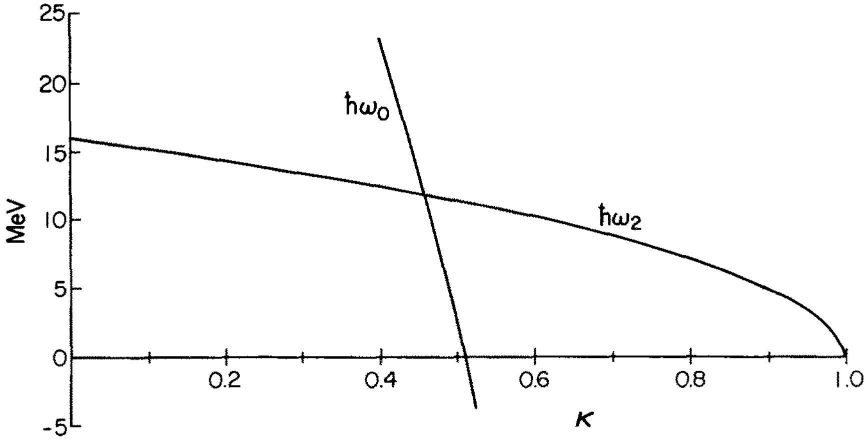


Fig. 3. The giant quadrupole excitation energy $\hbar\omega_2$ and the excitation energy $\hbar\omega_0$ of the $J=0$ band head for the deformed (8, 4) band of $^{16}O$ relative to the energy of the correlated closed shell state plotted as a function of $\kappa = 2N_0\chi/\hbar\omega$.

suggest that many such excited configurations will fall below the conventional shell model valence shell states. An important problem is therefore to identify the configurations that will lead to the lowest energy states. An analysis of this problem using the above schematic hamiltonian has therefore been undertaken recently by Dagum [31]).

Let us now consider the full spectrum of states for $H_{\text{v.b.}}$ for a valence space consisting of an arbitrary SU(3) irrep $(\lambda, \mu)$. This spectrum is particularly easy to calculate for an irrep $(\lambda=0, \mu=0)$ or for an irrep for which the value of the SU(3) Casimir invariant

$$\langle\lambda\mu|\mathbb{C}|\lambda\mu\rangle = 4(\lambda^2+\mu^2+\lambda\mu+3\lambda+3\mu) \tag{58}$$

is large. For a (0, 0) irrep, containing as it does a single $J=0$ state, the solution is identical to that of the conventional RPA and OSRPA considered above. We therefore consider the other limit.

To diagonalize the hamiltonian $H_{\text{v.b.}}$, we first invoke the identity

$$\mathbb{Q}\cdot\mathbb{Q} = \mathbb{C} - 3L^2 . \tag{59}$$

Making this substitution lets us eliminate all terms in $H_{\text{v.b.}}$ that are quadratic in $\mathbb{Q}$. We then make use of the well-known fact that the SU(3) quadrupole operators commute with each other to within terms of order $1/\langle\mathbb{C}\rangle$. Thus we obtain the spectrum of $H_{\text{v.b.}}$ to leading order in $1/\langle\mathbb{C}\rangle$.

The spectrum obtained for the representation $(\lambda, \mu) = (108, 0)$ considered appropriate for $^{166}Er$ with $N_0 = 811.5$, $\hbar\omega = 7.46$, and $\chi = \hbar\omega/4N_0$ is shown in fig. 4. The relative $B$(E2) values for decay of the giant quadrupole $2^+$ states to the ground state are shown in units in which, without enhancement by RPA ground state correlations, the $2^+$ states of the $K=0$, 1 and 2 bands would have values of

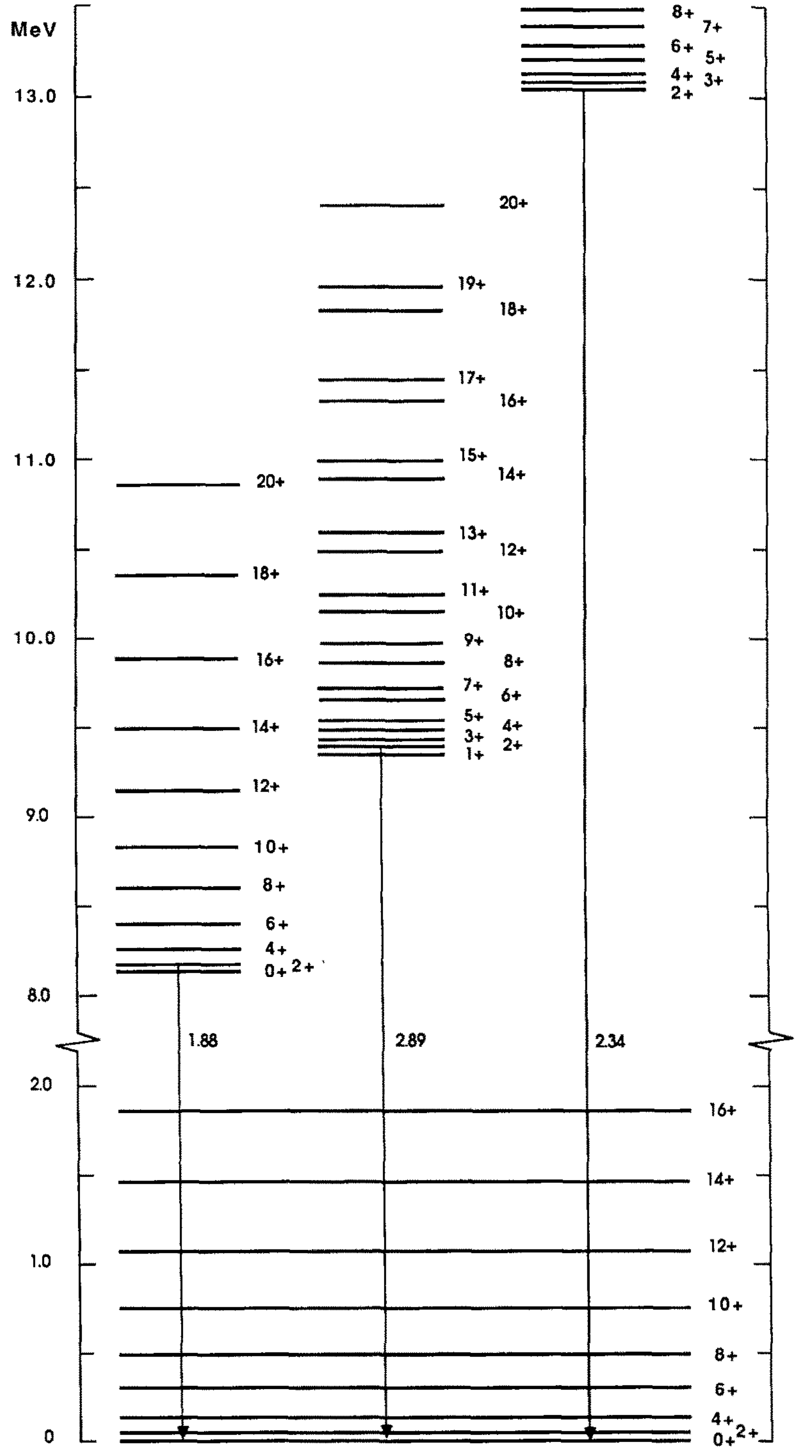


Fig. 4. Spectrum for $^{166}$Er in the partial RPA for the schematic hamiltonian of eq. (46).

1, 2 and 2, respectively, in the adiabatic approximation. Although not shown on the figure, the $B(\mathrm{E2})$ values between states of the ground state are precisely four times what they would be without coupling to the giant quadrupole resonance as previously discovered by Le Blanc *et al.* [25]).

It is gratifying to observe that the results are essentially consistent with what one expects from a collective model analysis or from an RPA treatment in a deformed Hartree-Fock basis. There is, however, a fundamental difference in that this equations of motion analysis is executed in a spherical basis. It does not rely on any independent-particle approximation. Furthermore, it can be applied regardless of whether or not the valence shell states form a rotational band or have symplectic symmetry.

## 5. Discussion

The basic theory of the quantum mechanics of many-body systems is founded on the Hartree-Fock and random phase approximations. In parallel with classical mechanics, HF theory gives an (approximate) ground state and the RPA describes its normal mode vibrations about equilibrium. However, as is well known, this approach leaves much to be desired in the generic open-shell situation in which the HF approximation returns a deformed state without good angular momentum. This is, in principle, a consequence of the HF independent-particle constraint which is manifestly unrealistic in the open-shell situation. One can of course proceed by angular momentum projection. Alternatively, one can interpret the deformed HF state as the intrinsic state of a phenomenological rotational model. These approaches are intuitively appealing and give remarkably good results but they are conceptually unsatisfactory.

The essential problem with the HF approach is that it insists on labelling single-particle states as either occupied or empty whereas, for open shell nuclei, in particular, there is a relatively smooth fall-off in occupancy. One can extend to a Hartree-Bogolyubov approximation but this only compounds the problem by violating particle number as well as angular momentum conversation. To come to terms with the dilemma, it has been suggested (for example in ref. [32])) that, instead of seeking a single Slater determinant $|\Phi\rangle$ with minimal energy one should instead seek a many-particle valence space, $\mathbb{H}_v$, of states by minimizing the trace of the hamiltonian over $\mathbb{H}_v$. Thus, instead of solving the HF variational equation

$$\delta\langle\Phi|H|\Phi\rangle = 0\,,$$

one should solve

$$\delta\,\mathrm{Tr}\langle H\rangle = 0\,.$$

Given a deformed HF solution $|\Phi\rangle$, one can apply the conventional RPA to calculate the so-called "intrinsic" vibrational excitations. This makes sense in the strong coupling limit, in which the HF state realistically represents the intrinsic state of a rotational nucleus. Alternatively, one can project states of good angular momentum from $|\Phi\rangle$ and apply the OSRPA to the projected ground state. This corresponds to the weak coupling limit and makes sense when the projected states are not those of a strongly deformed rotor or when the vibrational excitations do not couple strongly to the rotations. In contast, given a valence space of states $\mathbb{H}_v$, one can apply the partial RPA. One can then describe a full range of weak, intermediate and strong coupling situations. Furthermore, one can describe virtually any situation regardless of the character of its valence shell states.

A desirable feature of a partial RPA calculation, particularly when used in conjunction with an algebraic model for the valence space, is that the results of calculations are interpretable in collective model terms. The formalism simply provides a mechanism for deriving the parameters of the collective hamiltonian from a microscopic hamiltonian and of allowing coupling of the collective (particle-hole) degrees of freedom to selected valence shell degrees of freedom. Furthermore, it does so without imposing independent-particle constraints or violating angular momentum conservation.

The examples given are two of the many possibilities worth considering. For example, it is of interest to consider the possibility of describing the intrinsic valence space dynamics algebraically in order to obtain models with composite algebraic structures. For example, the U(6)-based interacting boson model for the valence space naturally extends to a U(6)-dipole boson or a U(6)-quadrupole boson model by inclusion of the giant dipole and giant quadrupole degrees of freedom. Such models have in fact already been proposed in refs. [24,33]). We note too that Elliott's SU(3) model for the valence space naturally augments to the U(3)-boson model on inclusion of both the giant monopole and quadrupole degrees of freedom. This model was discovered [17]) as the hydrodynamic limit of the symplectic model. The significance of the present equations of motion formalism is that it provides a mechanism for deriving the hamiltonians and other operators of such models microscopically.

Finally, as suggested in refs. [8-10]), one can use fermionic algebras to describe the valence space and so obtain composite algebraic structures with both fermionic and bosonic components. Since the fermions obey anti-commutation relations and the bosons obey commutation relations, one is then naturally led to composite (i.e. graded Lie) algebras with both commutator and anti-commutator components. Such algebras have been used, for example, in the interacting boson-fermion model [34]). However, in nuclear physics applications to date, only graded Lie algebras have been considered in which the elementary boson and fermion operators, from which they have been constructed, are mutually commuting. The interesting possibility is then suggested of taking into account the fermionic substructure of the bosons by relaxing this inessential restriction. For example, the phonon raising operators of a many-fermion system may well be excellent (or very good) bosons. Yet they may be expressible as (possibly infinite) sums of fermion operators

$$b_\lambda^\dagger = \sum_{\mu\nu} C_{\mu\nu}^\lambda a_\mu^\dagger a_\nu .$$

For example, the giant dipole p-bosons of sect. 3 are perfect bosons but can be second quantized and expressed in terms of fermion operators in this way. It would then follow that the bosons and fermions in combination have the elementary (but non-trivial) graded Lie algebra structure with, for example,

$$\{a_\mu, a_\nu^\dagger\} = \delta_{\mu\nu} ,$$

$$[b_\kappa, b_\lambda^\dagger] = \delta_{\kappa\lambda} ,$$

$$[a_\mu, b_\lambda^\dagger] = \sum_\nu C_{\mu\nu}^\lambda a_\nu .$$

The very significant advantage of using graded Lie algebras in boson-fermion mapping theories is that the representation theory then automatically looks after the common situation in which the bosonic and fermionic degrees of freedom may not be completely independent. One recalls, for example, that this was the problem addressed in refs. [8-10]).

Further discussion of the partial RPA can be found in ref. [35]).

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