Tensor equations of motion for the excitations of rotationally invariant or charge-independent systems

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A tensor equations-of-motion formalism for the excitation of a many-body system is presented, following the same general approach as the uncoupled formalism presented in a previous article. It is designed to take explicit account of the geometrical constraints imposed on excitation operators by the requirements that stationary states should have good angular momentum and, for a charge-independent nuclear Hamiltonian, good isospin. These developments are particularly relevant for application to molecular, atomic, and nuclear systems. By recognizing the geometrical constraints and exploiting the invariance properties of the excitation operators, the equations of motion become more readily applicable to nonscalar systems; i.e. to systems with nonzero angular momentum and/or isospin.

CONTENTS

I. INTRODUCTION

Equations-of-motion methods have contributed significantly to the conceptual development of many-body theory. For this reason, they have received considerable attention in recent years and have been put on a much more rigorous basis (Kerman and Klein, 1963; Do Dang and Klein, 1964; Dreizler *et al.* 1967; Belyaev and Zelevinsky, 1962; Marumori *et al.* 1964a; Marumori *et al.* 1964b; D. J. Rowe, 1968a). We focus here on the double-commutator formalism, introduced in paper I (Rowe, 1968a), which is formally exact, very simple and which has proved to be extremely useful. The reader is referred to Rowe (1972) for a summary of some of its achievements. Not only does it provide a very compact statement of a number of basic many-body theories, including the HF (Hartree–Fock), Hartree–Bogolyubov, RPA (Random Phase Approximation) and Quasiparticle RPA theories, it also leads naturally to generalizations of the above in a systematic, straightforward and computationally practical manner.

One seeks excitation operators $O_\lambda^\dagger$ which relate excited states $|\lambda\rangle$ to some parent state $|0\rangle$ according to the equations

$$O_\lambda^\dagger |0\rangle = |\lambda\rangle,$$
$$O_\lambda |0\rangle = 0. \tag{1.1}$$

For simplicity, and to accord with previous practice, we shall usually refer to $|0\rangle$ as the *ground state*, although it could itself be an excited state.

In the early linearization methods (Lane, 1964) one attempted to determine the $O_\lambda^\dagger$ by solution of the equation

$$[H, O_\lambda^\dagger] = \omega_\lambda O_\lambda^\dagger.$$

Now, in general, this equation does not have *simple* solutions, which is apparent from the fact that, if the Hamiltonian contains two-body interactions, the left-hand side is an operator of particle rank one greater than the right. This difficulty was circumvented by linearizing the equations of motion in one of several more or less equivalent ways. One method was to make a normal ordered expansion of the left-hand side, with respect to a particle–hole vacuum state, and to discard the term of highest particle rank. Without this term the equation could then be solved. This method was used to derive the B.C.S. theory of superconductivity (Anderson, 1958) and the RPA theory of excited states (Sawada, 1957; Baranger, 1960; Sawicki, 1961).

In paper I, the rather arbitrary linearization procedures were clarified and superceded by the observation that a set of operators satisfying Eq. (1.1) obey the formally *exact* equations of motion

$$\langle 0|[O_\kappa, H, O_\lambda^\dagger]_\pm|0\rangle = \omega_\lambda\langle 0|[O_\kappa, O_\lambda^\dagger]_\pm|0\rangle$$
$$= \delta_{\kappa\lambda}\omega_\lambda, \tag{1.2}$$

where the double commutator (anticommutator) is defined

$$2[O_\kappa, H, O_\lambda^\dagger]_- \equiv [O_\kappa, [H, O_\lambda^\dagger]] + [[O_\kappa, H], O_\lambda^\dagger],$$

$$2[O_\kappa, H, O_\lambda^\dagger]_+ \equiv \{O_\kappa, [H, O_\lambda^\dagger]\} + \{[O_\kappa, H], O_\lambda^\dagger\}. \quad (1.3)$$

The equations with commutators (rather than anticommutators) are relevant if the states $|0\rangle$ and $|\lambda\rangle$ are in the same system or differ by an even number of fermions. The operator $O_\lambda^\dagger$ is then said to be 'Bose-like' on account of the fact that the commutator of two Bose-like operators is simpler (i.e., of particle rank at least one lower) than the product. For this reason the maximum possible number of commutations has been introduced into Eq. (1.2) in order to exploit to the full the Bose-like character of the operators.

Similarly, the equations with anticommutators are relevant if the states $|0\rangle$ and $|\lambda\rangle$ differ by an odd number of fermions. The operator $O_\lambda^\dagger$ is then said to be 'Fermi-like' on account of the fact that the anticommutator of two Fermi-like operators is simpler (i.e., of particle rank at least one lower) than the product.

The equations of motion (1.2) will be referred to in this paper as the 'uncoupled' equations to distinguish them from the new tensor-coupled equations to be presented. The uncoupled equations have been discussed in detail in previous papers and their versatility has been demonstrated in a number of applications. They are appropriate equations to use whenever one has reason to expect the excitation operator $O_\lambda^\dagger$ to be simple compared with the stationary states, $|0\rangle$ and $|\lambda\rangle$, that it relates. If the reverse were the situation, static approaches, such as the conventional shell-model approach to the solution of the stationary state Schrödinger equation would manifestly be preferable.

One particularly appropriate application of the above equations-of-motion method is to the collective density vibrational excitations of even (i.e., $J=0$) nuclei, which have been very successfully described in the RPA (Sawada, 1957; Baranger, 1960; Sawicki, 1961; Rowe and Wong, 1970). If the ground state $|0\rangle$ in Eq. (1.2) is approximated by the HF particle–hole vacuum state and if a particle–hole expansion is made for $O_\lambda^\dagger$, the standard RPA equations immediately result, as pointed out in paper I (Rowe, 1968a); cf., Sec. V.A. In the nuclear physics context, the RPA is particularly significant because of its close relationship, via the time-dependent HF formulation, with the unified and collective vibrational models (Rowe, 1970).

However, unlike the linearization and other many-body methods, the double commutator formalism is not wedded to a HF approximation for the ground state; for it does not depend on an independent particle representation, like the time-dependent HF method (Ferrell, 1957; Goldstone and Gottfried, 1959), nor does it depend on a particle–hole vacuum for a normal ordered expansion or the use of diagrammatic techniques. The double commutator equations of motion have the enormous advantage that they can be used with *any* ground state and this makes it possible, for example, to extend the HF definition of single-particle states and the RPA theory of excitations to systems with highly correlated ground states; e.g., to spin zero (i.e., $J=T=0$) open-shell nuclei[1] (Rowe, 1972; Rowe and Wong, 1970). The tensor equations of motion, introduced in Sec. III also make it possible to include $J\neq 0$ or $T\neq 0$ systems (assuming isospin is a relevant quantum number) (Ngo-Trong and Rowe, 1971; Ngo-Trong, 1972).

The generalization of the RPA to open-shell nuclei was important in order that there should be a single microscopic theory of the collective excitations, such as the giant dipole resonance and the highly collective octupole vibrations, which are characteristic of both open- and closed-shell nuclei and which are equally described by the phenomenological collective models.

The extension of the RPA to open-shell nuclei has also opened up the possibility for calculation of many excited states of nuclei which were hitherto inaccessible to realistic microscopic investigation; for example, the giant resonances of open-shell nuclei of dipole and higher multipolarities (Satchler, 1972) which are nowadays the object of considerable experimental interest in photonuclear reactions, electron scattering, μ^--capture, nucleon scattering, and other direct reaction processes.

Note that direct reactions are extremely important probes of the dynamic structure of any many-body system for the reason that they only populate states that can be excited by simple one-body operators. This observation is particularly significant for the equations-of-motion method. For, while the solutions obtained for some $O_\lambda^\dagger$ in a space of one-body operators may not correspond very precisely to the individual eigenstates of the system, they do correspond to the "doorway" states by which the compound states are reached.

We now come to the objective of this paper, which is to show how equations of motion may be formulated to exploit the spherical tensor properties of stationary states and the rotational invariance (and charge independence) of the Hamiltonian in order that equations-of-motion calculations might be as economic and as realistic as possible.

It has been emphasized above and in previous papers that the equations of motion (1.2) are formally exact, and in principle, completely general, but that they are only of practical use if the excitation operators $O_\lambda^\dagger$ are simple. Now a moment's reflection convinces one that, if the objective is simplicity, the definition (1.1) of the excitation operators is not the optimum for a non-scalar system; i.e. a system whose ground state angular momentum is not zero.[2] This is because the operators $O_\lambda^\dagger$ are considerably complicated, for a non-scalar system, by the geometrical requirement of generating states of good angular momentum.

[1] Note that similar generalizations of other many-body formalisms may also be possible. For example, it has been shown that general time-dependent variational excitations also give the equations of motion (1.2) for Bose-like excitations (Rowe, 1968b). Schuck and Ethofer (1973) have also suggested parallel generalizations of Green's function methods.

[2] For the purposes of this paper we use the expression "angular momentum," unless otherwise qualified, to denote whatever set of total angular momentum, spin and isospin is relevant. In nuclear physics, for example, this set might be just the total angular momentum and/or isospin, if the latter is considered to be a good quantum number. In atomic physics, it might be either the total angular momentum or the orbital angular momentum and spin.

This is illustrated by the following simple example. Suppose that $|J_0M_0 = J_0\rangle$ is a member of a $(2J_0+1)$ degenerate ground state and that an excited state $|J_eJ_e\rangle$ can be expressed

$$|J_eJ_e\rangle = O_{\lambda\mu=\lambda}{}^\dagger\,|J_0J_0\rangle, \tag{1.4}$$

where $O_{\lambda\mu}{}^\dagger$ is the μ component of a spherical tensor of angular momentum $\lambda = J_e - J_0$. The excited state with $M_e = J_e - 1$ is therefore

$$|J_eJ_e-1\rangle = (2J_e)^{-1/2}J_-\,|J_eJ_e\rangle = (2J_e)^{-1/2}J_-O_{\lambda\lambda}{}^\dagger\,|J_0J_0\rangle,$$

where $J_- = J_x - iJ_y$ is the usual angular momentum step-down operator (Messiah, 1966). Now, if $O_{\lambda\lambda}{}^\dagger$ is a simple one-body operator, it follows that the excitation operator for the state $|J_eJ_e-1\rangle$ is a two-body operator; i.e., the operator $(2J_e)^{-1/2}J_-O_{\lambda\lambda}{}^\dagger$. However, the complication is purely geometrical in origin and the essential simplicity of the excitation process reappears if the excited states are re-expressed as coupled spherical tensor products; viz.,

$$|J_eM_e\rangle = \sum_{\mu M_0} (\lambda\, J_0\, \mu\, M_0\,|\,J_eM_e)\; O_{\lambda\mu}{}^\dagger\,|J_0M_0\rangle, \tag{1.5}$$

where $(\lambda\, J_0\, \mu\, M_0\,|\,J_eM_e)$ is a vector coupling (Clebsch–Gordon) coefficient.

Apart from the simplifications that result, there are also very significant physical reasons for considering coupled tensor products. Consider, for example, a single particle weakly coupled to a $J=0$ core (de-Shalit, 1965). If the core has an excited vibrational state, the coupled particle–core system exhibits a multiplet of excited states which will be split if the particle-core interaction depends on the geometrical orientation of the particle's orbit with respect to the excited core.

Pursuing this example, we also see that polarization by the particle can modify the character of the core excitation and even introduce, into the excited state, components with core excitations of other multipolarity. Thus there is no real physical reason why the angular momentum of the excitation operator should be a good quantum number. And certainly there is no reason why it should adopt the maximum possible value as supposed in Eq. (1.4). The right-hand side of Eq. (1.5) should therefore be allowed to include more than one λ component, the amplitudes of which remain to be determined by the equations of motion. Clearly the magnitudes of the various components will have considerable physical significance in portraying the character of the excitation.

The extension of Eq. (1.1) proposed thus closely parallels the extension of the single-particle model to the weak coupling of a nucleon to a non-spin-zero nucleus (de-Shalit, 1965). The generalizations of the equations of motion that result are likewise closely related to French's generalizations of the standard sum rules to multipole sum rules for non-scalar nuclei (French, 1966).

In the following section, we summarize the properties of second quantized spherical tensors. This section is based heavily on the more complete treatment of this subject by French (1966). It contains all the basic algebraic relationships needed for equations-of-motion purposes and enables subsequent sections to distinguish the physics from the algebra.

The new tensor equations of motion are introduced in Sec. III, and their properties are given in Sec. IV.

The particular application of the tensor equations to a scalar system is discussed in Sec. V. It is shown that, in this case, the tensor equations of motion are equivalent to the previous uncoupled equations. Some applications to open- and closed-shell nuclei are discussed, and it is shown that the coupled form of the equations is more useful than the uncoupled form for practical purposes.

Applications to non-scalar systems are discussed in Section VI. Multipole field equations are given for the motion of a nucleon coupled to a non-zero angular momentum core, and RPA equations are presented for the excitations of good isospin of a doubly magic $N > Z$ nucleus.

The conclusions and further possible applications are summarized in Sec. VII.

II. SOME DEFINITIONS AND PROPERTIES OF SPHERICAL TENSORS

The algebra involved in this work is considerably simplified by using the very elegant tensorial techniques for second quantized operators developed by French (1966). We present here our notations and the particular properties and algebraic relationships needed for this paper.

A. Tensor products

Let R^Γ denote a spherical tensor of rank Γ and $R_\mu{}^\Gamma$ one of its $(2\Gamma+1)$ components.

The coupled product of two tensors R^{Γ_1} and S^{Γ_2} to form a tensor of rank Γ will be written

$$(R^{\Gamma_1}\times S^{\Gamma_2})_\mu{}^\Gamma \equiv \sum_{\mu_1(\mu_2)} (\Gamma_1\Gamma_2\mu_1\mu_2\,|\,\Gamma\mu)\,R_{\mu_1}{}^{\Gamma_1}S_{\mu_2}{}^{\Gamma_2}, \tag{2.1}$$

where $(\Gamma_1\Gamma_2\mu_1\mu_2\,|\,\Gamma\mu)$ is a CG (Clebsch–Gordon) coefficient. The symmetry properties of CG coefficients are listed in any book on angular momentum. We note here only the well-known relations:

$$(\Gamma_1\Gamma_2\mu_1\mu_2\,|\,\Gamma\mu)$$

$$= (-1)^{\Gamma_1+\Gamma_2-\Gamma}(\Gamma_1\Gamma_2-\mu_1-\mu_2\,|\,\Gamma-\mu), \tag{2.2a}$$

$$= (-1)^{\Gamma_1+\Gamma_2-\Gamma}(\Gamma_2\Gamma_1\mu_2\mu_1\,|\,\Gamma\mu), \tag{2.2b}$$

$$= (-1)^{\Gamma_1-\mu_1}\hat{\Gamma}\hat{\Gamma}_2{}^{-1}(\Gamma\Gamma_1\mu-\mu_1\,|\,\Gamma_2\mu_2), \tag{2.2c}$$

$$(\Gamma\Gamma-\mu\mu\,|\,00) = (-1)^{\Gamma+\mu}\hat{\Gamma}^{-1}, \tag{2.2d}$$

where $\hat{\Gamma}$ is an abbreviation for $(2\Gamma+1)^{1/2}$.

B. Racah recoupling

For more than two tensors, the coupled product is well-defined only when the internal couplings are specified. The well-known Racah recoupling relation is written in this notation

$$((R^{\Gamma_1}\times S^{\Gamma_2})^{\Gamma_{12}}\times T^{\Gamma_3})^{\Gamma} = \sum_{\Gamma_{23}} \hat{\Gamma}_{12}\hat{\Gamma}_{23} W(\Gamma_1\Gamma_2\Gamma\Gamma_3;\Gamma_{12}\Gamma_{23})(R^{\Gamma_1}\times(S^{\Gamma_2}\times T^{\Gamma_3})^{\Gamma_{23}})^{\Gamma}, \quad (2.3)$$

where $W(\Gamma_1\Gamma_2\Gamma\Gamma_3;\Gamma_{12}\Gamma_{23})$ is the standard Racah coefficient.

We note, the following useful relationships:

$$W(abcd;ef) = W(badc;ef) = W(acbd;fe), \quad (2.4a)$$

$$W(abab;f0) = W(aabb;0f) = (-1)^{a+b-f}\hat{a}^{-1}\hat{b}^{-1}, \quad (2.4b)$$

$$W(aabb;fa+b) = \hat{f}^{-2}(aaa-a\mid f0)(bbb-b\mid f0). \quad (2.4c)^3$$

C. Direct product spaces

Frequently more than one vector space is needed to describe physical quantities. Depending on the nature of the Hamiltonian, we may choose to describe the system in a direct product space; e.g., (L, S), (L, S, T) or (J, T). Thus suppose R^{Γ_1}, S^{Γ_2}, T^{Γ_3} are all spherical tensors in the direct product space (J, T), the above relations are understood by means of the following direct product notation:

$$\Gamma_1 \equiv (J_1, T_1),$$
$$(-1)^{\Gamma_1} \equiv (-1)^{J_1+T_1},$$
$$\hat{\Gamma}_1 \equiv \hat{J}_1\hat{T}_1 \equiv (2J_1+1)^{1/2}(2T_1+1)^{1/2},$$
$$W(\Gamma_1\Gamma_2\Gamma\Gamma_3;\Gamma_{12}\Gamma_{23}) \equiv W(J_1J_2JJ_3;J_{12}J_{23})W(T_1T_2TT_3;T_{12}T_{23}), \quad \text{etc.} \quad (2.5)$$

D. Tensor states

We denote by $|\Gamma\rangle\rangle$ a tensor state, whose $(2\Gamma+1)$ components $|\Gamma\mu\rangle$ are the usual Dirac ket vectors. The action of a tensor operator on such a tensor state is then expressed

$$(R^{\Gamma_1}\times|\Gamma_2\rangle\rangle)_{\mu}{}^{\Gamma} = \sum_{\mu_1(\mu_2)} (\Gamma_1\Gamma_2\mu_1\mu_2\mid\Gamma\mu)R_{\mu_1}{}^{\Gamma_1}|\Gamma_2\mu_2\rangle. \quad (2.6)$$

E. Excitation operators

Because of previous practice, excitation operators of spherical tensor rank λ are written $O_\lambda{}^\dagger$, with a dagger. Their μ components are conventionally written $O_{\lambda\mu}{}^\dagger$, by which is meant

$$O_{\lambda\mu}{}^\dagger \equiv (O_\lambda{}^\dagger)_\mu. \quad (2.7)$$

Excitation operators fall into two classes; those which are Bose-like, for which λ is an integer, and those which are Fermi-like, for which λ is a half-odd integer. Particular examples are the pure boson creation operators $\eta_{\lambda\mu}{}^\dagger$ of the harmonic oscillator Hamiltonian, and the pure fermion creation operators $a_{\lambda\mu}{}^\dagger$ of the independent-particle Hamiltonian.

F. De-excitation operators and adjoints

Whereas the excitation operator $O_{\lambda\mu}{}^\dagger$ is the μ component of a λ-tensor, its Hermitian adjoint, the de-excitation operator $O_{\lambda\mu}$, is not. This is for the same reason that the complex conjugate of the spherical harmonic

$$Y_{lm}{}^* = (-1)^m Y_{l-m}$$

is not the component of a tensor because of the $(-1)^m$ phase factor. Thus we define the *Hermitian adjoint tensor* O_λ, as the tensor whose μ component is

$$(O_\lambda)_\mu = (-1)^\mu O_{\lambda-\mu}. \quad (2.8)$$

For a Fermi-like operator, the phase factor $(-1)^\mu$ will clearly be imaginary, which can be inconvenient. It is sometimes useful therefore to employ another operator $O_{\bar{\lambda}}$ related to O_λ by a phase factor

$$O_{\bar{\lambda}} \equiv (-1)^\lambda O_\lambda. \quad (2.9)$$

This operator is a spherical tensor of rank λ with μ component

$$O_{\bar{\lambda}\mu} \equiv (-1)^{\lambda+\mu} O_{\lambda-\mu}. \quad (2.10)$$

The operator $O_{\bar{\lambda}\mu}$ is in fact related to $O_{\lambda\mu}$ simply by a rotation of the coordinate system through 180° about the y axis. In a particular phase convention, it is also the time-reverse of $O_{\lambda\mu}$ [see for example Appendix A of Rowe (1970)]. Particular examples are the fermion creation and annihilation tensor operators, $a_\lambda{}^\dagger$ and $a_{\bar{\lambda}}$, used, for example, in nuclear applications of the BCS theory of superconductivity.

Using the above definitions one readily derives the Hermitian adjoint of a coupled product of tensors:

$$(R^{\Gamma_1}\times S^{\Gamma_2})^{\Gamma\dagger} = (S^{\Gamma_2\dagger}\times R^{\Gamma_1\dagger})^{\Gamma}. \quad (2.11)$$

The Hermitian adjoint of a tensor state $|\Gamma\rangle\rangle$ will be written $\langle\langle\Gamma|$. It is a spherical tensor of rank Γ with μ component

$$(\langle\langle\Gamma|)_\mu \equiv (-1)^\mu\langle\Gamma-\mu|. \quad (2.12)$$

G. Tensor products of excitation and de-excitation operators

Frequently products of excitation and de-excitation operators are encountered which need to be expressed in coupled form; e.g.,

$$O_{x\lambda\mu}O_{y\lambda'\mu'}{}^\dagger = \sum_{\Gamma}(-1)^{\lambda-\mu}(\lambda\lambda'-\mu\mu'\mid\Gamma\mu'-\mu)(O_{x\bar{\lambda}}\times O_{y\lambda'}{}^\dagger)_{\mu'-\mu}{}^{\Gamma}, \quad (2.13)$$

[3] Equation (2.4c) is perhaps not well-known. It is derived by comparing the expressions given by Brink and Satchler (1962) for the particular Racah coefficient appearing on the left with those given by Rose (1957) for the CG coefficient on the right.

where we now use the subscripts x and y to distinguish different operators of the same tensor rank. This expression is especially useful when only a subset of possible values for Γ contribute in a particular application. For example, the expectation of (2.13) in a scalar (i.e., zero angular momentum) state $|0\rangle$ has contributions only from $\Gamma = 0$. Using Eq. (2.2d) for the CG coefficient, we therefore obtain

$$\langle 0 | O_{x\lambda\mu} O_{y\lambda'\mu'}^\dagger | 0\rangle = \delta_{\lambda\lambda'}, \delta_{\mu\mu'} (-1)^{2\lambda} \hat{\lambda}^{-1} \langle 0 | (O_{x\bar{\lambda}} \times O_{y\lambda}^\dagger)^0 | 0\rangle \tag{2.14}$$

which can also be written, using Eq. (2.9),

$$\langle 0 | O_{x\lambda\mu} O_{y\lambda'\mu'}^\dagger | 0\rangle = \delta_{\lambda\lambda'} \delta_{\mu\mu'} (-1)^{-\lambda} \hat{\lambda}^{-1} \langle 0 | (O_{x\lambda} \times O_{y\lambda})^0 | 0\rangle. \tag{2.15}$$

In a similar way one derives

$$\langle x\lambda\mu | y\lambda'\mu'\rangle = \delta_{\lambda\lambda'} \delta_{\mu\mu'} (-1)^{-\lambda} \hat{\lambda}^{-1} (\langle\langle x\lambda | \times | y\lambda\rangle\rangle)^0 \tag{2.16}$$

giving

$$(\langle\langle x\lambda | \times | y\lambda'\rangle\rangle)^0 = \delta_{xy} \delta_{\lambda\lambda'} (-1)^\lambda \hat{\lambda}. \tag{2.17}$$

H. Commutation relations

Based on Eq. (2.13), we define coupled commutators of tensor operators

$$[O_{x\bar{\lambda}}, O_{y\lambda'}^\dagger]_k^\Gamma = \sum_{\mu(\mu')} (-1)^{\lambda-\mu} (\lambda\lambda' - \mu\mu' | \Gamma k) [O_{x\lambda\mu}, O_{y\lambda'\mu'}^\dagger]. \tag{2.18}$$

Anticommutators are defined in a parallel way.

These commutators carry the same information as the more conventional uncoupled commutators. For example, pure boson or pure Fermi operators obey the uncoupled commutation (anticommutation) relations

$$[\eta_{x\lambda\mu}, \eta_{y\lambda'\mu'}^\dagger] = \delta_{xy} \delta_{\lambda\lambda'} \delta_{\mu\mu'},$$

$$\{a_{x\lambda\mu}, a_{y\lambda'\mu'}^\dagger\} = \delta_{xy} \delta_{\lambda\lambda'} \delta_{\mu\mu'},$$

respectively. Inserting these expressions into Eq. (2.18) one readily derives

$$[\eta_{x\bar{\lambda}}, \eta_{y\lambda'}^\dagger]^\Gamma = \delta_{xy} \delta_{\lambda\lambda'} \delta_{\Gamma 0} (-1)^{2\lambda} \hat{\lambda},$$

$$\{a_{x\bar{\lambda}}, a_{y\lambda'}^\dagger\}^\Gamma = \delta_{xy} \delta_{\lambda\lambda'} \delta_{\Gamma 0} (-1)^{2\lambda} \hat{\lambda}. \tag{2.19}$$

I. Reduced matrix elements

The matrix elements of a tensor operator W^λ can be written

$$\langle \Gamma\mu | W_\nu^\lambda | \Gamma_1\mu_1\rangle = (\lambda\Gamma_1\nu\mu_1 | \Gamma\mu) \langle \Gamma\mu | (W^\lambda \times | \Gamma_1\rangle\rangle)_\mu^\Gamma.$$

Reordering the CG coefficient, using Eq. (2.2b), and expressing the matrix element in the form (2.16), gives

$$\langle \Gamma\mu | W_\nu^\lambda | \Gamma_1\mu_1\rangle = (-1)^{\lambda+\Gamma_1-2\Gamma} (\Gamma_1\lambda\mu_1\nu | \Gamma\mu) \hat{\Gamma}^{-1} (\langle\langle \Gamma | \times W^\lambda \times | \Gamma_1\rangle\rangle)^0.$$

Comparing this expression with the Wigner–Eckart theorem

$$\langle \Gamma\mu | W_\nu^\lambda | \Gamma_1\mu_1\rangle = (\Gamma_1\lambda\mu_1\nu | \Gamma\mu) \hat{\Gamma}^{-1} \langle \Gamma \| W^\lambda \| \Gamma_1\rangle, \tag{2.20}$$

one obtains the very useful identity

$$(\langle\langle \Gamma | \times W^\lambda \times | \Gamma_1\rangle\rangle)^0 = (-1)^{2\Gamma-\lambda-\Gamma_1} \langle \Gamma \| W^\lambda \| \Gamma_1\rangle. \tag{2.21}$$

J. One-body tensor operators

If W^Ω is a one-body tensor operator, it can be expressed in terms of its one-body matrix elements in the uncoupled second-quantized form

$$W_k^\Omega = \sum_{\alpha\beta} \sum_{\mu(\nu)} \langle \alpha\mu | W_k^\Omega | \beta - \nu\rangle a_{\alpha\mu}^\dagger a_{\beta-\nu}.$$

Expanding the matrix element, with the Wigner–Eckart theorem (2.20), and re-ordering the CG coefficients using Eq. (2.2c) gives

$$W_k^\Omega = \sum_{\alpha\beta} \sum_{\mu(\nu)} \hat{\Omega}^{-1} \langle \alpha \| W^\Omega \| \beta\rangle (\alpha\beta\mu\nu | \Omega k) (-1)^{\beta+\nu} a_{\alpha\mu}^\dagger a_{\beta-\nu}$$

which can be expressed as the tensor identity

$$W^\Omega = \sum_{\alpha\beta} \hat{\Omega}^{-1} \langle \alpha \| W^\Omega \| \beta\rangle A_{\alpha\beta}^\dagger(\Omega), \tag{2.22}$$

where $A_{\alpha\beta}^\dagger(\Omega)$ is defined

$$A_{\alpha\beta}^\dagger(\Omega) = (a_\alpha^\dagger \times a_{\bar{\beta}})^\Omega. \tag{2.23}$$

For later convenience we note the identity

$$A_{\beta\alpha}^\dagger(\Omega) = (-1)^{\Omega+\alpha-\beta} A_{\alpha\beta}(\bar{\Omega}) \tag{2.24}$$

which follows from Eq. (2.11), and the definition (2.9).

K. The Hamiltonian

In uncoupled form, the Hamiltonian can be expressed

$$H = \sum_{\mu\nu} T_{\mu\nu} a_\mu^\dagger a_\nu + \tfrac{1}{4} \sum_{\mu\nu\mu'\nu'} V_{\mu\nu\mu'\nu'} a_\mu^\dagger a_\nu^\dagger a_{\nu'} a_{\mu'}, \tag{2.25}$$

where T includes the kinetic energy, one-body spin–orbit interaction, etc., and V is the two-body interaction.

This Hamiltonian may also be expressed

$$H = H_0 + V_{\text{res}},$$

$$H_0 = \sum_{\mu\nu} \epsilon_{\mu\nu} a_\mu^\dagger a_\nu, \tag{2.26}$$

where the one-body part, H_0, includes a single particle potential representing the interaction of each particle with the fields produced by the other particles, and V_{res} is the *residual* interaction. For example, in HF theory,

$$\epsilon_{\mu\nu} = \delta_{\mu\nu}\epsilon_\nu, \tag{2.27}$$

where ϵ_ν is a HF single-particle energy.

In expressing H in coupled form, we assume it to be a scalar. Obviously this need not be the case in all direct product spaces. For example, H may contain tensor forces in an (L, S) space or charge-dependent forces in a (J, T) space. We nevertheless suppose that a space has been chosen in which H is a scalar, although this is not necessary and may not always be desirable.

The one- and two-body components of H can then be expressed

$$H^{(1)} = \sum_{\mu\nu} \hat{\nu}\epsilon_{\mu\nu}(a_\mu{}^\dagger \times a_{\bar{\nu}})^0, \tag{2.28a}$$

$$H^{(2)} = -\tfrac{1}{4} \sum_{\mu\nu\mu'\nu'} \hat{\Omega} V_{\mu\nu\mu'\nu'}{}^{\Omega}((a_\mu{}^\dagger \times a_\nu{}^\dagger)^\Omega \times (a_{\bar{\mu}'} \times a_{\bar{\nu}'})^\Omega)^0, \tag{2.28b}$$

where

$$\epsilon_{\mu\nu} = \langle \mu \mid H^{(1)} \mid \nu \rangle, \tag{2.29a}$$

$$V_{\mu\nu\mu'\nu'}{}^{\Omega} = \langle (\mu\nu)\Omega \mid H^{(2)} \mid (\mu'\nu')\Omega \rangle (1 + \delta_{\mu\nu})^{1/2} (1 + \delta_{\mu'\nu'})^{1/2}, \tag{2.29b}$$

with $\mid \nu \rangle$ a single-particle state and $\mid (\mu\nu)\Omega \rangle$ a normalized antisymmetrized two-particle state of angular momentum Ω. Note that $H^{(1)}$ and $H^{(2)}$ may be, respectively, either T and V or H_0 and V_{res}.

III. TENSOR EQUATIONS OF MOTION

If we denote the ground state by the tensor state $\mid \Delta \rangle\rangle$, and an excited state by $\mid x\Lambda \rangle\rangle$, we can define excitation operators $O_{x\lambda}{}^\dagger$ of tensor rank λ such that

$$(O_{x\lambda}{}^\dagger \times \mid \Delta \rangle\rangle)^\Lambda = \mid x\Lambda \rangle\rangle, \tag{3.1a}$$

$$O_{x\lambda} \mid \Delta \rangle\rangle = 0. \tag{3.1b}$$

In the first equation the usual tensorial coupling is shown explicitly, whereas in the second equation all possible coupled products are required to vanish.

Formally there is a whole continuum of operators $O_{x\lambda}{}^\dagger$ that satisfy Eq. (3.1); e.g., the set of operators

$$O_{x\lambda}{}^\dagger = N(\mid x\Lambda \rangle\rangle \times \langle\langle \Delta \mid)^\lambda + \sum_{\mu,\nu \neq \Delta} C_{\mu\nu}(\mid \mu \rangle\rangle \times \langle\langle \nu \mid)^\lambda, \tag{3.2}$$

where

$$N = (-1)^{\Delta-\lambda}\hat{\Lambda}/\hat{\lambda},$$

and the $C_{\mu\nu}$ are arbitrary. Furthermore any value of λ which satisfies the triangle relations, i.e.,

$$\mid \Delta - \Lambda \mid \leq \lambda \leq \Delta + \Lambda,$$

is permissible. Thus the most general excitation operators which satisfy Eq. (3.1) are of mixed tensor rank

$$Q_{x\Lambda}{}^\dagger = \sum_i O_{x\lambda_i}{}^\dagger. \tag{3.3}$$

This lack of uniqueness is a considerable practical advantage since it improves the chances of finding a good excitation operator within a given finite operator space. Furthermore we believe that the amplitudes of the various multipole components of $Q^\dagger$ have considerable physical significance, as discussed in the introduction. Thus we adopt the general form (3.3).

From Eq. (3.1a) we have immediately

$$([H, Q_{x\Lambda}{}^\dagger] \times \mid \Delta \rangle\rangle)^\Lambda = \omega_{x\Lambda}(Q_{x\Lambda}{}^\dagger \times \mid \Delta \rangle\rangle)^\Lambda, \tag{3.4}$$

where $\omega_{x\Lambda}$ is the excitation energy of the state $\mid x\Lambda \rangle\rangle$. This equation can be converted to an equality between two numbers by zero-coupling both sides to $\langle\langle y\Lambda \mid$, the Hermitian adjoint of another excited state

$$\begin{aligned} &(\langle\langle y\Lambda \mid \times [H, Q_{x\Lambda}{}^\dagger] \times \mid \Delta \rangle\rangle)^0 \\ &= \omega_{x\Lambda}(\langle\langle y\Lambda \mid \times Q_{x\Lambda}{}^\dagger \times \mid \Delta \rangle\rangle)^0 \\ &= \delta_{xy}(-1)^\Lambda \hat{\Lambda}\omega_{x\Lambda}, \end{aligned} \tag{3.5}$$

where we have used Eq. (2.17).

Written out explicitly, Eq. (3.5) becomes

$$\begin{aligned} &\sum_{ij} (((\langle\langle \Delta \mid \times O_{y\lambda_i})^\Lambda \times ([H, O_{x\lambda_j}{}^\dagger] \times \mid \Delta \rangle\rangle)^\Lambda)^0, \\ &= \omega_{x\Lambda} \sum_{ij} (((\langle\langle \Delta \mid \times O_{y\lambda_i})^\Lambda \times (O_{x\lambda_j}{}^\dagger \times \mid \Delta \rangle\rangle)^\Lambda)^0, \\ &= \delta_{xy}(-1)^\Lambda \hat{\Lambda}\omega_{x\Lambda}, \end{aligned}$$

or, making a Racah recoupling and using Eq. (2.21),

$$\begin{aligned} &\sum_{ij\Gamma} (-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat{\Gamma} W(\lambda_i\lambda_j\Delta\Delta; \Gamma\Lambda) \\ &\times \langle \Delta \| (O_{y\bar{\lambda}_i} \times [H, O_{x\lambda_j}{}^\dagger])^\Gamma \| \Delta \rangle \\ &= \omega_{x\Lambda} \sum_{ij\Gamma} (-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat{\Gamma} W(\lambda_i\lambda_j\Delta\Delta; \Gamma\Lambda) \\ &\times \langle \Delta \| (O_{y\bar{\lambda}_i} \times O_{x\lambda_j}{}^\dagger)^\Gamma \| \Delta \rangle \\ &= \delta_{xy}\omega_{x\Lambda}. \end{aligned} \tag{3.6}$$

Now, using the constraint imposed on the excitation operators by Eq. (3.1a), we can replace the products inside the matrix elements by commutators. Thus the matrix elements become

$$\langle\Delta\,\|\,(O_{y\bar\lambda_i}\times[H,O_{x\lambda_j}{}^\dagger])^\Gamma\,\|\,\Delta\rangle = \langle\Delta\,\|\,[O_{y\bar\lambda_i},[H,O_{x\lambda_j}{}^\dagger]]_\pm{}^\Gamma\,\|\,\Delta\rangle,$$

$$\langle\Delta\,\|\,(O_{y\bar\lambda_i}\times O_{x\lambda_j}{}^\dagger)^\Gamma\,\|\,\Delta\rangle = \langle\Delta\,\|\,[O_{y\lambda_i},O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma\,\|\,\Delta\rangle. \tag{3.7}$$

Furthermore the symmetry of the equations can be emphasized by further replacing the double commutator by the symmetrized double commutator, defined by Eq. (1.3)

$$\langle\Delta\,\|\,[O_{y\bar\lambda_i},[H,O_{x\lambda_j}{}^\dagger]]_\pm{}^\Gamma\,\|\,\Delta\rangle = \langle\Delta\,\|\,[O_{y\bar\lambda_i},H,O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma\,\|\,\Delta\rangle. \tag{3.8}$$

Equation (3.8) follows if

$$\langle\Delta\,\|\,[[O_{y\bar\lambda_i},O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma,H]\,\|\,\Delta\rangle = 0 \tag{3.9}$$

which holds for *any* operators $O_{y\bar\lambda_i}$ and $O_{x\lambda_j}{}^\dagger$ provided only that $|\,\Delta\rangle\rangle$ is an eigenstate of H, which it is supposed to be.

Thus the tensor equations of motion finally become

$$\begin{aligned}\sum_{ij\Gamma}&(-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat\Gamma W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)\\&\times\langle\Delta\,\|\,[O_{y\bar\lambda_i},H,O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma\,\|\,\Delta\rangle,\\&=\omega_{x\Lambda}\sum_{ij\Gamma}(-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat\Gamma W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)\\&\times\langle\Delta\,\|\,[O_{y\bar\lambda_i},O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma\,\|\,\Delta\rangle,\\&=\delta_{xy}\omega_{x\Lambda}.\end{aligned} \tag{3.10}$$

Since the relationships (3.7) and (3.8) are exact identities for the true ground state and excitation operators, Eq. (3.10) is formally equivalent to (3.6). We make the distinction, however, because, in practical application, some approximation must be made for the ground state and the operator space must be truncated. Equation (3.10) is therefore fashioned such that it is as insensitive as possible to the approximations and, furthermore, retains the symmetries of the exact equations. Thus it contains commutators rather than products, because they are of lower particle rank, and the double commutators are symmetrized in order that approximate solutions exist and that they will be orthonormal. The justification for the latter observation will be given later.

To solve Eq. (3.10) some approximation must be made for the ground state $|\,\Delta\rangle\rangle$, and the excitation operators must be restricted to a finite space of basis operators $\{\eta_\alpha{}^\dagger(\lambda_i)\}$, which may or may not include the adjoint operators $\eta_\alpha(\bar\lambda_i)$. Inserting the expansion

$$Q_{x\Lambda}{}^\dagger=\sum_{\alpha i}X_{\alpha i}(x)\eta_\alpha{}^\dagger(\lambda_i) \tag{3.11}$$

into the equation of motion (3.10) gives the matrix equation for the coefficients

$$MX(x)=\omega_x NX(x), \tag{3.12}$$

where the matrices M and N are defined

$$\begin{aligned}M_{\alpha i,\beta j}&=\sum_\Gamma(-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat\Gamma W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)\\&\quad\times\langle\Delta\,\|\,[\eta_\alpha(\bar\lambda_i),H,\eta_\beta{}^\dagger(\lambda_j)]_\pm{}^\Gamma\,\|\,\Delta\rangle,\\N_{\alpha i,\beta j}&=\sum_\Gamma(-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat\Gamma W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)\\&\quad\times\langle\Delta\,\|\,[\eta_\alpha(\bar\lambda_i),\eta_\beta{}^\dagger(\lambda_j)]_\pm{}^\Gamma\,\|\,\Delta\rangle.\end{aligned} \tag{3.13}$$

The matrices M and N are both Hermitian. Equation (3.12) can therefore be reduced to the form of a standard eigenvalue equation by the method discussed in Section V and in Rowe (1969). As a consequence, solutions of the approximated equations exist and retain the orthonormality properties of the exact solutions. This would not in general be the case had we used the nonsymmetric double commutators, given on the left-hand side of Eq. (3.8), in the equations of motion, since the identity (3.9) may not hold exactly for $|\,\Delta\rangle\rangle$ an approximate eigenstate.

A particular case of Eq. (3.10) is when the excitation operator is restricted to a single tensor component of maximal rank; i.e., $\lambda=\Lambda-\Delta$. As noted at the beginning of this section, such an operator always exists [cf. Eq. (3.2)] although it need not be simple. Using the identity (2.4c), Eq. (3.10) then reduces to the simpler equation

$$\begin{aligned}\sum_\Gamma&\hat\Gamma^{-1}(\lambda\lambda-\lambda\lambda\,|\,\Gamma 0)(\Delta\Delta\Delta-\Delta\,|\,\Gamma 0)\\&\times\langle\Delta\,\|\,[0_{y\bar\lambda},H,O_{x\lambda}{}^\dagger]_\pm{}^\Gamma\,\|\,\Delta\rangle\\&=\omega_{x\Lambda}\sum_\Gamma\hat\Gamma^{-1}(\lambda\lambda-\lambda\lambda\,|\,\Gamma 0)(\Delta\Delta\Delta-\Delta\,|\,\Gamma 0)\\&\times\langle\Delta\,\|\,[O_{y\bar\lambda},O_{x\lambda}{}^\dagger]^\Gamma\,\|\,\Delta\rangle,\\&=\delta_{xy}\omega_{x\Lambda}.\end{aligned} \tag{3.14}$$

This equation of motion could in fact have been derived from the uncoupled equations of motion (1.2) due to the fact that the coupled product (1.5) is, in this particular case, also the simple product (1.4).

An even more particular case is when $\Delta=0$; i.e., the ground state is a scalar. The excitation operator is then automatically restricted to a single component of maximal rank, $\lambda=\Lambda$. Furthermore only $\Gamma=0$ contributes in Eq. (3.14). Since this is a very common situation, we consider it in more detail in Sec. V.

IV. PROPERTIES OF THE TENSOR EQUATIONS OF MOTION

A. Orthogonality and normalization

Consider two solutions $X(x)$ and $X(y)$ of Eq. (3.12). Since the matrices M and N are Hermitian,

$$\begin{aligned}X^\dagger(y)MX(x)&=\omega_x X^\dagger(y)NX(x),\\&=\omega_y{}^*X^\dagger(y)NX(x).\end{aligned} \tag{4.1}$$

Unless ω_x and $\omega_y{}^*$ are equal, therefore, both sides of this equation must vanish. Furthermore, since $X^\dagger(x)NX(x)$ is real, we may choose the normalization to give orthogonality relations

$$X^\dagger(y)NX(x) = \pm\delta_{xy} \qquad (\omega_x \ \text{real})$$
$$= 0 \qquad (\omega_x \ \text{complex}). \tag{4.2}$$

Zero energy solutions ($\omega_x = 0$) may or may not be normalizeable.

In order that the excited states should be orthonormal, Eq. (3.10) tells us that the excitation operators should satisfy the equation

$$\sum_{ij\Gamma} (-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat{\Gamma}W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)$$
$$\times \langle\Delta \,||\, [O_{y\bar{\lambda}_i}, O_{x\lambda_j}{}^\dagger]_\pm{}^\Gamma \,||\, \Delta\rangle = \delta_{xy}. \tag{4.3}$$

Furthermore, physical excitation energies should be real. Inserting the expansion (3.11) into (4.3) gives the orthonormality requirement in matrix form

$$X^\dagger(y)NX(x) = \delta_{xy}.$$

However, we can only require that "physical" solutions of the equations which truly correspond to *excitation* operators be normalizeable in this way. Solutions with the other normalizations, given in Eq. (4.2), can and do occur. For if the space of basis operators $\{\eta_\alpha{}^\dagger(\lambda_i)\}$ includes the adjoint operators $\eta_\alpha(\bar{\lambda}_i)$, it includes not only the excitation operators $Q_{x\Lambda}{}^\dagger$ but also their adjoints. It follows therefore that solutions to the equations of motion exist which correspond to *de-excitation* operators or linear combinations of them. Such solutions will be described as "unphysical." They are a well-known feature of, for example, the standard RPA equations.

Since the unphysical solutions do not necessarily have positive norm, the sign of the normalization in Eq. (4.2) provides one means of eliminating unphysical solutions. Unfortunately it is not in general sufficient identification and one may have to identify some unphysical solutions of positive norm by inspection. Fortunately this does not appear to present any problems in practice. The situation arises, for example, in the BCS theory of superconductivity where quasiparticle creation and annihilation operators both have positive norm as a consequence of the symmetry of the anticommutation relations

$$\{\alpha_\mu, \alpha_\nu{}^\dagger\} = \{\alpha_\mu{}^\dagger, \alpha_\nu\} = \delta_{\mu\nu}.$$

Note that, in certain situations, ω can take both positive and negative values for physical solutions. This is possible even if $|\,\Delta\rangle\rangle$ is a true ground state because the excited state $|\,x\Lambda\rangle\rangle$ may appear in a system of different particle number, for example a neighboring nucleus, in which case $|\,x\Lambda\rangle\rangle$ may quite legitimately have lower energy than $|\,\Delta\rangle\rangle$.

B. Transition matrix elements

Given the solutions to the equations of motion, we wish to evaluate the reduced matrix elements $\langle x\Lambda \,||\, W^\Omega \,||\, \Delta\rangle$ for a given transition operator W^Ω.

Using Eq. (2.21) we can express the matrix element

$$\langle x\Lambda \,||\, W^\Omega \,||\, \Delta\rangle$$
$$= (-1)^{\Omega+\Delta-2\Lambda} \sum_i (((\langle\langle\Delta \,|\, \times O_{x\lambda_i})^\Lambda \times W^\Omega \times |\,\Delta\rangle\rangle)^0$$

or making a Racah recoupling,

$$\langle x\Lambda \,||\, W^\Omega \,||\, \Delta\rangle$$
$$= (-1)^{\Omega+\Delta-2\Lambda} \sum_{i\Gamma} \hat{\Lambda}\hat{\Gamma}W(\lambda_i\Omega\Delta\Delta;\Gamma\Lambda)$$
$$\times (\langle\langle\Delta \,|\, \times (O_{x\lambda_i} \times W^\Omega)^\Gamma \times |\,\Delta\rangle\rangle)^0.$$

Now, according to the philosophy of the equations of motion method, we use the constraint (3.1b) to insert a commutator into the matrix element on the right-hand side. Then again using Eq. (2.21) and the definition (2.9), we obtain

$$\langle x\Lambda \,||\, W^\Omega \,||\, \Delta\rangle$$
$$= (-1)^{\Omega+\Delta-\Lambda}\hat{\Lambda} \sum_{i\Gamma} (-1)^{\Delta-\Lambda-\Gamma-\lambda_i}\hat{\Gamma}W(\lambda_i\Omega\Delta\Delta;\Gamma\Lambda)$$
$$\times \langle\Delta \,||\, [O_{x\bar{\lambda}_i}, W^\Omega]_\pm{}^\Gamma \,||\, \Delta\rangle. \tag{4.4}$$

Suppose, for example, that W^Ω is a one-body operator, cf. Eq. (2.22), having matrix elements between many-body states given by

$$\langle x\Lambda \,||\, W^\Omega \,||\, \Delta\rangle$$
$$= \sum_{\alpha\beta} \hat{\Omega}^{-1}\langle\alpha \,||\, W^\Omega \,||\, \beta\rangle\langle x\Lambda \,||\, A_{\alpha\beta}{}^\dagger(\Omega) \,||\, \Delta\rangle. \tag{4.5}$$

To evaluate such matrix elements we have therefore to determine the matrix elements of the unit one-body tensor operators $A_{\alpha\beta}{}^\dagger(\Omega)$.

By way of illustration, suppose that $A_{\alpha\beta}{}^\dagger(\Omega)$ is a member of the set of basis operators, $\eta_\gamma{}^\dagger(\lambda_j)$. Replacing W^Ω by $\eta_\gamma{}^\dagger(\lambda_j)$ in Eq. (4.4) then gives

$$\langle x\Lambda \,||\, \eta_\gamma{}^\dagger(\lambda_j) \,||\, \Delta\rangle = (-1)^{\lambda_j+\Delta-\Lambda}\hat{\Lambda} \sum_{\alpha i\Gamma} (-1)^{\Delta-\Lambda-\Gamma-\lambda_i}$$
$$\times \hat{\Gamma}W(\lambda_i\lambda_j\Delta\Delta;\Gamma\Lambda)X_{\alpha i}{}^*\langle\Delta \,||\, [\eta_\alpha(\bar{\lambda}_i), \eta_\gamma{}^\dagger(\lambda_j)]_\pm{}^\Gamma \,||\, \Delta\rangle,$$

or

$$\langle x\Lambda \,||\, \eta_\gamma{}^\dagger(\lambda_j) \,||\, \Delta\rangle = (-1)^{\lambda_j+\Delta-\Lambda}\hat{\Lambda} \sum_{\alpha i} X_{\alpha i}{}^*N_{\alpha i,\gamma j}. \tag{4.6}$$

V. APPLICATION TO SCALAR SYSTEMS

If the ground state is a scalar, the excitation operator must carry the angular momentum of the corresponding excited state. Thus the vector coupled product in Eq. (3.1) reduces to a simple product:

$$O_{x\lambda\mu}{}^\dagger \,|\, 0\rangle = |\, x\lambda\mu\rangle,$$
$$O_{x\lambda\mu} \,|\, 0\rangle = 0. \tag{5.1}$$

The equations of motion (3.10) and (3.14) also simplify

$$\begin{aligned}(-1)^{2\lambda}\hat{\lambda}^{-1}\langle 0 \mid [O_{y\bar{\lambda}}, H, O_{x\lambda}{}^{\dagger}]_{\pm}{}^{0} \mid 0\rangle, \\ = \omega_{x\lambda}(-1)^{2\lambda}\hat{\lambda}^{-1}\langle 0 \mid [O_{y\lambda}, O_{x\lambda}{}^{\dagger}]_{\pm}{}^{0} \mid 0\rangle, \\ = \delta_{xy}\omega_{x\lambda}.\end{aligned} \tag{5.2}$$

Comparison with (2.14) makes it clear that Eq. (5.2) can be written in the uncoupled form

$$\begin{aligned}\langle 0 \mid [O_{y\lambda\mu}, H, O_{x\lambda\mu}]_{\pm} \mid 0\rangle \\ = \omega_{x\lambda}\langle 0 \mid [O_{y\lambda\mu}, O_{x\lambda\mu}{}^{\dagger}]_{\pm} \mid 0\rangle = \delta_{xy}\omega_{x\lambda}\end{aligned} \tag{5.3}$$

whence it becomes apparent that, in the particular case of a scalar ground state, the new tensor equations of motion and the old uncoupled equations, Eq. (1.2), are equivalent.

In fact Eq. (5.3) was expressed in the more useful coupled form (5.2) and used to calculate the excited states of even open-shell nuclei (Rowe and Wong; 1970) before the general tensor equations were derived. The coupled equations (5.2) are much preferable to (5.3) for practical purposes because they contain only ground state expectations of *scalar* operators, rather than operators of mixed tensorial rank. This is a considerable advantage, as will be indicated below.

In the interest of clarity we shall consider only the commutator equations of motion for 'Bose-like' operators for the remainder of this section. The parallel development of the anticommutator equations for 'Fermi-like' operators will be self-evident.

To solve the equations, the excitation operators are approximated by an expansion

$$O_{x\lambda}{}^{\dagger} = \sum_{\alpha} \{Y_{\alpha}(x)\eta_{\alpha}{}^{\dagger}(\lambda) - Z_{\alpha}(x)\eta_{\alpha}(\bar{\lambda})\} \tag{5.4}$$

in a *finite* set of basis operators, which we suppose includes the adjoint operators, $\eta_{\alpha}(\bar{\lambda})$, although it need not. The equations of motion (5.2) then give the expansion coefficients as solutions of the matrix equation

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} Y(x) \\ Z(x) \end{pmatrix} = \omega_x \begin{pmatrix} U & V \\ -V^* & -U^* \end{pmatrix}\begin{pmatrix} Y(x) \\ Z(x) \end{pmatrix} \tag{5.5}$$

with submatrices

$$\begin{aligned}A_{\alpha\beta}{}^{\lambda} &= \hat{\lambda}^{-1}\langle 0 \mid [\eta_{\alpha}(\bar{\lambda}), H, \eta_{\beta}{}^{\dagger}(\lambda)]^{0} \mid 0\rangle \quad &\text{(Hermitian)}\\ B_{\alpha\beta}{}^{\lambda} &= -\hat{\lambda}^{-1}\langle 0 \mid [\eta_{\alpha}(\bar{\lambda}), H, \eta_{\beta}(\bar{\lambda})]^{0} \mid 0\rangle \quad &\text{(symmetric)}\\ U_{\alpha\beta}{}^{\lambda} &= \hat{\lambda}^{-1}\langle 0 \mid [\eta_{\alpha}(\bar{\lambda}), \eta_{\beta}{}^{\dagger}(\lambda)]^{0} \mid 0\rangle \quad &\text{(Hermitian)}\\ V_{\alpha\beta}{}^{\lambda} &= -\lambda^{-1}\langle 0 \mid [\eta_{\alpha}(\bar{\lambda}), \eta_{\beta}(\bar{\lambda})]^{0} \mid 0\rangle \quad &\text{(antisymmetric).}\end{aligned} \tag{5.6}$$

The supermatrices on both sides of Eq. (5.5) are manifestly Hermitian. To obtain the solutions, one therefore begins by diagonalizing the metric matrix on the right-hand side. A transformation of the equation can then be made to standard RPA form

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} Y(x) \\ Z(x) \end{pmatrix} = \omega_x \begin{pmatrix} Y(x) \\ Z(x) \end{pmatrix}. \tag{5.7}$$

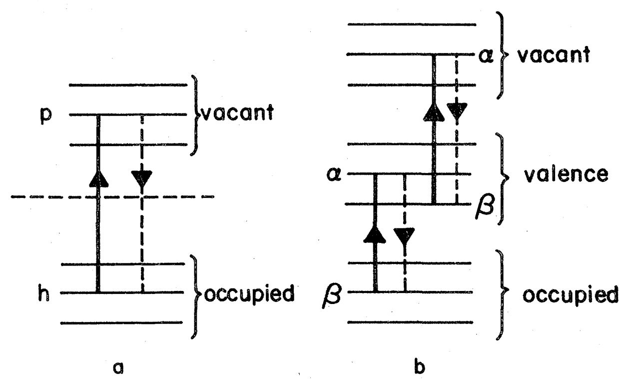

FIG. 1. Forward and backward going excitation processes (a) for a closed-shell nucleus and (b) for an open-shell nucleus.

This method is described in detail in Rowe (1969). In this form it is an eigenvalue equation but for a non-Hermitian matrix. It can be solved either by direct diagonalization or, if the matrix elements are real as they invariably are, by a procedure in which only real symmetric matrices are diagonalized (Ullah and Rowe, 1971).

Having obtained the excitation operators, transition matrix elements for some spherical tensor operator, W^{λ} can be evaluated from the general equation (4.4) which for a scalar ground state reduces to

$$\langle x\lambda \| W^{\lambda} \| 0\rangle = \langle 0 \mid [O_{x\bar{\lambda}}, W^{\lambda}]^{0} \mid 0\rangle. \tag{5.8}$$

Inserting the expansion (5.4) we obtain

$$\begin{aligned}\langle x\lambda \| W^{\lambda} \| 0\rangle = \sum_{\alpha} \{Y_{\alpha}{}^{*}(x)\langle 0 \mid [\eta_{\alpha}(\bar{\lambda}), W^{\lambda}]^{0} \mid 0\rangle \\ + Z_{\alpha}{}^{*}(x)\langle 0 \mid [W^{\lambda}, \eta_{\alpha}{}^{\dagger}(\lambda)]^{0} \mid 0\rangle\}.\end{aligned} \tag{5.9}$$

Other properties of the scalar equations of motion, which are identical to those of the uncoupled equations, are not discussed here because they have been discussed at length elsewhere (Rowe, 1972; Rowe, 1968).

A. Application to closed-shell nuclei

For a closed-shell nucleus (or atom), the equations can be solved with a closed-shell approximation for the ground state and with $O_{x\lambda}{}^{\dagger}$ expanded in a particle–hole space. Thus if we label occupied single-particle states by h, and vacant single-particle states by p, as illustrated in Fig. 1(a), the expansion for $O_{x\lambda}{}^{\dagger}$ becomes

$$O_{x\lambda}{}^{\dagger} = \sum_{ph} \{Y_{ph}(x)A_{ph}{}^{\dagger}(\lambda) - Z_{ph}(x)A_{ph}(\bar{\lambda})\}, \tag{5.10}$$

where $A_{ph}{}^{\dagger}(\lambda)$ is defined by Eq. (2.24).

The equations that result from the above two approximations are those of the standard closed-shell RPA. Evaluation of the matrix elements is particularly simple in this approximation because of the very special relationship that exists between the closed-shell state (the particle–hole vacuum) and the particle–hole operators. Thus the U matrix, of Eq. (5.5) becomes the unit matrix, and the V matrix vanishes.

If the Hamiltonian is expressed as in Eq. (2.28), one obtains the well-known expressions

$$A_{ph,p'h'} = \epsilon_{pp'}\delta_{hh'} - \epsilon_{h'h}\delta_{pp'} - \sum_{\Omega} \hat{\Omega} W(phh'p'; \Gamma\Omega) V_{h'php'}{}^{\Omega}$$

$$B_{ph,p'h'} = \sum_{\Omega} \hat{\Omega} W(p\Omega\Gamma h'; p'h) V_{p'ph'h}{}^{\Omega}. \tag{5.11}$$

Substitution of Eq. (5.10) into (5.9) using the expansion (2.22) for W^{λ} also leads readily to

$$\langle x\lambda \| W^{\lambda} \| 0\rangle = \sum_{ph} \{Y_{ph}{}^{*}(x) \langle p \| W^{\lambda} \| h\rangle + (-1)^{\lambda+p-h} Z_{ph}{}^{*}(x) \langle h \| W^{\lambda} \| p\rangle\}. \tag{5.12}$$

If the backward going terms in the expansion for $O_{x\lambda}{}^{\dagger}$ are omitted, i.e., the Z coefficients are put identically equal to zero, the equations reduce to those of the standard TDA (Tamm–Dancoff Approximation) (cf., e.g., Rowe, 1970).

Although the TDA and RPA equations can be derived in a large variety of other ways, the above equations-of-motion derivation is extremely simple and straightforward, and has the very significant merit that it exposes very clearly the approximations involved. Thus it is immediately apparent how to go to higher levels of approximation; one either employs a better (correlated) ground state (Rowe *et al.*, 1971) or includes higher order excitation processes into the operator expansion (Sawicki, 1962; Tamura and Udagawa, 1964). Both such extensions can and have been made.

The vital ingredient of the present formulation, that makes the former extension possible, is that the double commutators

$$[(a_{\alpha}{}^{\dagger} \times a_{\bar{\beta}})^{\lambda}, H, (a_{\gamma}{}^{\dagger} \times a_{\bar{\delta}})^{\lambda}]^{0}$$

can be evaluated, without reference to the ground state or even to the nucleus. They are 0-, one- and two-body *scalar* operators, just as the Hamiltonian, and can be expressed in terms of their 0-, one- and two-body matrix elements. Detailed expressions are given in Rowe and Wong (1970). These matrix elements can be determined for any given Hamiltonian and single-particle basis, by a general computer code which can and has been programmed.

Having generated the double commutators, their expectations can be evaluated for *any* approximate ground state of *any* nucleus or atom. Thus unlike almost all other derivations of the RPA, the closed-shell particle–hole vacuum state no longer plays an essential role and for this reason it is a straightforward matter to extend the RPA to correlated ground states and open-shell nuclei.

B. Application to open-shell nuclei

For an open-shell nucleus the single-particle states fall into three categories, as illustrated in Fig. 1(b); viz. the occupied, the valence and the vacant shells, according to the shell model classification.

In the shell-model, the ground state and other lowlying positive parity states are customarily obtained by diagonalization of the Hamiltonian within the space defined as the valence space. Negative parity excitations, on the other hand, necessarily require the transfer of a nucleon across a major shell boundary. This brings the occupied and vacant shells into the calculation and generally raises the dimensions of the shell model calculation beyond practical limits. The open-shell RPA makes the negative parity excitations also accessible to calculation.

In the open-shell RPA, the equations of motion are solved for the shell-model ground state, restricted to the valence space. The excitation operators are expanded

$$O_{x\lambda}{}^{\dagger} = \sum_{\alpha>\beta} \{Y_{\alpha\beta}(x) A_{\alpha\beta}{}^{\dagger}(\lambda) - Z_{\alpha\beta}(x) A_{\alpha\beta}(\bar{\lambda})\}, \tag{5.13}$$

where the operator $A_{\alpha\beta}{}^{\dagger}(\lambda)$ either promotes a nucleon from an occupied to a valence shell or from a valence to a vacant shell, as illustrated in Fig. 1(b). If the valence space includes both positive and negative parity single-particle states, transitions between different valence shells of opposite parity can also be included.

Insertion of these approximations into the general equations of motion gives a matrix equation (5.5) for which the metric matrix is again already diagonal (provided there are no two single-particle shells in the valence space of identical spin and parity) and which therefore reduces trivially to standard RPA form.

At this stage it is worth pausing to consider why the dimensions of an open-shell RPA matrix are an order of magnitude smaller than those of a comparable shell model calculation. The reduction is achieved by neglecting the large number of possible rearrangements of valence nucleons that occur, in a true eigenstate, in addition to the particle–hole excitations. However an excitation induced by a direct reaction must proceed via a single–particle excitation channel. Rearrangements subsequently occur as the primary excitation (the doorway state) thermalizes its energy among the other degrees of freedom. This thermalization clearly leads to broadening and additional structure of the excitation spectrum, which the open-shell RPA does not describe. However the open-shell RPA can be expected to give the gross structure, corresponding to the correct positions and over-all strengths of the doorway states.

The scalar open-shell RPA has been applied to a number of light nuclei in the $1p$ and $2s1d$ shells, with considerable success (Rowe and Wong; 1970, Wong, Rowe and Parikh, 1974). It is particularly useful for calculating the inelastic electron scattering form factors for the many states in the giant resonance region [cf., Appendix by T. W. Donnelly to Rowe (1972)].

The anticommutator equations can be similarly used to derive independent particle and quasiparticle theories of open- and closed-shell nuclei. Other possibilities, such as their application to weak-coupling and two-particle transfer reactions, have yet to be fully explored.

VI. APPLICATIONS TO NONSCALAR SYSTEMS

By way of illustrating some of the ways in which the general tensor equations of motion might be used, we consider two examples, one for a Fermi-like excitation and one for a Bose-like excitation.

A. Single-particle states for a tensor nucleus

In the self-consistent field theory of single-particle states (Rowe, 1968, 1972; Rowe and Wong, 1970; Rowe and Rosensteel, 1975), one considers the motion of each particle in a potential well which represents the interaction of that particle with the fields produced by all the other particles. The single-particle states are thus eigenstates of a Hamiltonian

$$H_0 = T + U = \sum_{\mu\nu} \epsilon_{\mu\nu} a_\mu{}^\dagger a_\nu, \tag{6.1}$$

where U is the self-consistent field.

In the uncoupled equations-of-motion formalism, the single-particle matrix elements are defined

$$\epsilon_{\mu\nu} \equiv \langle 0 \mid \{a_\mu, H, a_\nu{}^\dagger\} \mid 0 \rangle, \tag{6.2}$$

where H is the full Hamiltonian, and $\mid 0\rangle$ is the many-particle ground state. Inserting the expression (2.25) for H, Eq. (6.2) becomes

$$\epsilon_{\mu\nu} = T_{\mu\nu} + \sum_{\mu'\nu'} V_{\mu\mu'\nu\nu'} \langle 0 \mid a_{\mu'}{}^\dagger a_{\nu'} \mid 0 \rangle, \tag{6.3}$$

which defines $U_{\mu\nu}$.

In HF theory, it is assumed that $\mid 0\rangle$ is a determinant of A single-particle states. But it may be more general and include the correlations of a more realistic ground state.

Now if $\mid 0\rangle$ is an angular momentum zero state, it is clear that H_0 is a scalar. This is demonstrated explicitly by rewriting the above expression for the field

$$U_{\mu\nu} = \sum_{\mu'\nu'\Omega} (\hat{\Omega}^2/\hat{p}^2\hat{p}') V_{\mu\mu'\nu\nu'}{}^\Omega \langle 0 \mid (a_{\mu'}{}^\dagger \times a_{\bar{\nu}'})^0 \mid 0 \rangle. \tag{6.4}$$

Thus the single-particle creation operators

$$\alpha_x{}^\dagger = \sum_\nu X_\nu(x) a_\nu{}^\dagger, \tag{6.5}$$

which diagonalize H_0, have good angular momentum. Similarly the $(A \pm 1)$-particle states, $\alpha_x{}^\dagger \mid 0\rangle$ and $\alpha_y \mid 0\rangle$, have good angular momentum and are immediately interpretable in terms of the $(A \pm 1)$-particle eigenstates. However if $\mid 0\rangle$ is not a scalar, neither is U and the states $\alpha_x{}^\dagger \mid 0\rangle$ and $\alpha_y \mid 0\rangle$ do not have good angular momentum.

For a tensor parent state $\mid \Delta\rangle\rangle$, we therefore consider Fermi-like excitation operators $\alpha_x{}^\dagger$, for the $(A + 1)$-particle states, such that

$$\begin{aligned} &\mid x\Lambda\rangle\rangle = (\alpha_x{}^\dagger \times \mid \Delta\rangle\rangle)^\Lambda, \\ &\alpha_x \mid \Delta\rangle\rangle = 0. \end{aligned} \tag{6.6}$$

The parent state $\mid \Delta\rangle\rangle$ might be, for example, a vibrational excited state of an even nucleus, and we wish to consider the states $\mid x\Lambda\rangle\rangle$ formed by the addition of a nucleon.

For the purpose of defining single-particle states, we suppose that $\alpha_x{}^\dagger$ can be expanded, according to Eq. (6.5), in terms of pure fermion operators. It will be assumed that each *basis* operator $a_\nu{}^\dagger$ creates a fermion in a state of good angular momentum but no such restriction will be imposed on $\alpha_x{}^\dagger$ itself. Substituting (6.5) into the general tensor equations of motion (3.10) gives the coefficients $X_\nu(x)$ as solutions of the equation

$$\sum_\nu M_{\mu\nu} X_\nu(x) = \epsilon_x \sum_\nu N_{\mu\nu} X_\nu(x), \tag{6.7}$$

where

$$\begin{aligned} M_{\mu\nu} = &\sum_\Gamma (-1)^{\Delta-\Lambda-\Gamma-\mu} \hat{\Gamma} W(\mu\nu\Delta\Delta;\Gamma\Lambda) \\ &\times \langle \Delta \,||\, \{a_{\bar{\mu}}, H, a_\nu{}^\dagger\}^\Gamma \,||\, \Delta\rangle, \end{aligned} \tag{6.8}$$

$$\begin{aligned} N_{\mu\nu} = &\sum_\Gamma (-1)^{\Delta-\Lambda-\Gamma-\mu} \hat{\Gamma} W(\mu\nu\Delta\Delta;\Gamma\Lambda) \\ &\times \langle \Delta \,||\, \{a_{\bar{\mu}}, a_\nu{}^\dagger\}^\Gamma \,||\, \Delta\rangle. \end{aligned} \tag{6.9}$$

Substituting the expression (2.19) for the fermion anti-commutator, Eq. (6.9) becomes

$$N_{\mu\nu} = \delta_{\mu\nu}, \tag{6.10}$$

and inserting the expansion (2.28) for H, Eq. (6.8) becomes

$$M_{\mu\nu} = T_{\mu\nu} + \sum_\Gamma U_{\mu\nu}{}^\Gamma, \tag{6.11}$$

with

$$\begin{aligned} U_{\mu\nu}{}^\Gamma = &\sum_{\mu'\nu'\Omega} (-1)^{\Delta-\Lambda-\Omega-\nu'} \hat{\Gamma}\hat{\Omega}^2 W(\mu\nu\Delta\Delta;\Gamma\Lambda) W(\mu\mu'\nu\nu';\Omega\Gamma) \\ &\times V_{\mu\mu'\nu\nu'}{}^\Omega \langle \Delta \,||\, (a_{\mu'}{}^\dagger \times a_{\bar{\nu}'})^\Gamma \,||\, \Delta\rangle. \end{aligned} \tag{6.12}$$

Consider, for example, the $\Gamma = 0$ component of U. For $\Gamma = 0$, Eq. (6.12) reduces to

$$U_{\mu\nu}{}^{\Gamma=0} = \sum_{\mu'\nu'\Omega} (\hat{\Omega}^2/\hat{p}^2\hat{p}'\hat{\Delta}) V_{\mu\mu'\nu\nu'}{}^\Omega \langle \Delta \,||\, (a_{\mu'}{}^\dagger \times a_{\bar{\nu}'})^0 \,||\, \Delta\rangle,$$

which is seen to be a natural generalization of Eq. (6.4). However, for $\Delta \neq 0$, the field contains other multipoles. Furthermore, since U represents the interaction between the particle and the parent state, it is not surprising that these other multipoles should depend on the geometrical factors expressing the coupling of the particle to the core.

To our knowledge, no applications have been made to date of the above "multipole" field equations.

B. RPA theory of isospin splitting in N > Z nuclei

Consider, for example, the giant dipole resonance of a doubly magic nucleus for which the number N of neutrons exceeds the number Z of protons. For example, ^{88}Sr has 50 neutrons which close the $1g_{9/2}$ shell and 38 protons which close the $1f_{7/2}$ shell. The ground state of such a nucleus has vanishing angular momentum but nonvanishing isospin

$$\begin{aligned} &J_0 = 0, \\ &T_0 = \tfrac{1}{2}(N - Z), \qquad T_3 = T_0, \end{aligned}$$

where T_3 is the third component of isospin.

In the long wavelength limit, the electromagnetic operator for absorption of an electric dipole gamma ray is a tensor operator of both angular momentum and isospin unity. It excites states primarily in the neighborhood of 80 $A^{-1/3}$ MeV, where $A = N + Z$ is the mass number, giving rise to

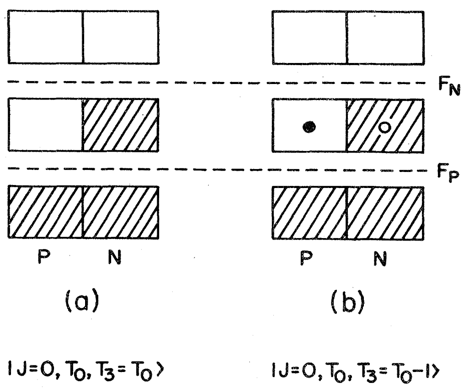

FIG. 2. Closed, valence, and open shells for an $N > Z$ nucleus (a) for a doubly closed-shell state and (b) for an isobaric analog of a doubly closed-shell state. F_N and F_P denote the Fermi surfaces for the neutrons and protons, respectively.

the well-known phenomenon of the giant dipole resonance. Now, if $T_0 \neq 0$, an $E1$ excitation can populate states of $T_e = T_0$ and $T_0 + 1$.[4] Thus for an $N > Z$ nucleus the giant dipole resonance splits into two components. This splitting was predicted by Fallieros *et al.* (1965), and observed in a number of photonuclear experiments.

The description of such excitations of good isospin is straightforward in the tensor equations-of-motion formalism. We denote by

$$\begin{aligned} |\Delta\rangle\rangle &= |J_0 = 0, T_0\rangle\rangle \qquad T_0 \neq 0, \\ |x\Lambda\rangle\rangle &= |xJ, T_e\rangle\rangle \qquad T_e = T_0, T_0 \pm 1, \end{aligned} \tag{6.13}$$

respectively, the tensor ground and excited states whose components constitute the isobaric multiplets of these states. Note, however, that among the states of the ground state isobaric multiplet, only the state of maximum $T_3 = T_0$ is in fact a closed-shell state (or is approximated as such in the shell model); cf., Fig. 2(a). The other members of the multiplet are isobaric analogs of this closed-shell state, one member of which is illustrated in Fig. 2(b).

Consider now excited particle–hole states of isospin $T_e = T_0 + 1$. Figure 3(a) illustrates the member of an isobaric multiplet of maximum $T_3 = T_0 + 1$. It is generated from the closed-shell state by a particle–hole operator which annihilates a proton and creates a neutron. Such an operator manifestly has isospin unity. In solving for the $T_0 + 1$ states in the RPA, we therefore consider excitation operators

$$\begin{aligned} Q_{x\Lambda\tau}^\dagger = \sum_{\alpha>F_N,\beta<F_P} \{ &Y_{\alpha\beta}(x) A_{\alpha\beta}^\dagger(J, T_i = 1, \tau) \\ &- Z_{\alpha\beta}(x) A_{\alpha\beta}(\bar{J}, T_i = 1, -\tau) \}, \end{aligned} \tag{6.14}$$

where τ is the third component of isospin, and F_N and F_P are, respectively, the neutron and proton Fermi surfaces.

It is instructive to note that if the parent state shown in Fig. 2(a) is the doubly closed-shell nucleus ${}^{88}\mathrm{Sr}_{50}{}^{38}$, for example, then the member of the excited multiplet of maximum $T_3 = T_0 + 1$, shown in Fig. 3(a), belongs to the nucleus ${}^{88}\mathrm{Rb}_{51}{}^{37}$; i.e., the nucleus with one less proton, and one more neutron. The analog state in ^{88}Sr is constructed by further operating with T_-, the isospin lowering operator. The result is illustrated in Fig. 3(b) and is seen to contain two-particle two-hole configurations. The necessity for such configurations in a state of good isospin was pointed out by Fallieros *et al.* (1965) and taken into account in their shell-model calculations (Goulard *et al.* 1968) of the dipole states of ^{88}Sr. In the tensor equations of motion formalism, they are automatically included as a result of the vector coupling of the excitation operator to the tensor ground state. Thus it is sufficient to consider only one particle–hole components in the excitation operator.

To generate excited states of $T_e = T_0$ it is possible (but not desirable) to consider only excitation operators of isospin zero. The excited particle–hole configurations are then of the type shown in Figs. 4(a) and 4(b). For excitations of the type shown in Fig. 4(a) it is in fact immaterial whether or not one chooses particle–hole operators of isospin zero or one, since it can readily be shown that

$$\begin{aligned} &A_{\alpha\beta}^\dagger(JT_i = 1 \ \tau = 0) \,|\, 0T_0T_0\rangle \\ &\quad = \pm A_{\alpha\beta}^\dagger(JT_i = 0, \tau = 0) \,|\, 0T_0T_0\rangle, \end{aligned} \tag{6.15}$$

according as $\beta > F_p$ or $\alpha < F_N$. This is due to the fact that for $\alpha < F_N$ only proton excitations are permitted by the Pauli principle, while for $\beta > F_P$ only neutron excitations are permitted. For the same reason it can easily be shown that

$$\begin{aligned} &\hat{J}^{-1}\langle 0T_0T_0 \,|\, [A_{\alpha\beta}(\bar{J}T_i = 0), A_{\gamma\delta}^\dagger(JT_i = 0)]^0 \,|\, 0T_0T_0\rangle \\ &\quad = \zeta_{\alpha\beta}{}^{-2}\delta_{\alpha\gamma}\delta_{\beta\delta}, \end{aligned} \tag{6.16}$$

where

$$\begin{aligned} \zeta_{\alpha\beta} &= (2)^{1/2} \qquad \text{if} \quad \alpha < F_N \quad \text{or} \quad \beta > F_P \\ &= 1 \qquad \text{otherwise}. \end{aligned} \tag{6.17}$$

It is therefore convenient to consider the "orthonormal" basis operators $\zeta_{\alpha\beta} A_{\alpha\beta}^\dagger(J0)$.

If we wish, we may include both isospin zero and one operators for $\alpha > F_N$, $\beta < F_P$, in which case we admit configurations of the type shown in Fig. 4(c) in parallel with those for $T_e = T_0 + 1$. In solving for the T_0 excited states in the RPA we therefore consider excitation operators

$$Q_{x\Lambda}^\dagger = \sum_i O_{xJT_i}{}^\dagger, \tag{6.18}$$

where

$$\begin{aligned} O_{xJ0}^\dagger &= \sum_{\alpha>\beta} \{ Y_{\alpha\beta0}(x) \zeta_{\alpha\beta} A_{\alpha\beta}^\dagger(J0) - Z_{\alpha\beta0}(x) \zeta_{\alpha\beta} A_{\alpha\beta}(\bar{J}0) \}, \\ O_{xJ1}^\dagger &= \sum_{\alpha>F_N,\beta<F_P} \{ Y_{\alpha\beta1}(x) \zeta_{\alpha\beta} A_{\alpha\beta}^\dagger(J1) \\ &\quad - Z_{\alpha\beta1}(x) \zeta_{\alpha\beta} A_{\alpha\beta}(J1). \end{aligned} \tag{6.19}$$

With the observation that $O_{xJ0}^\dagger$ vanishes identically for $T_e = T_0 + 1$, Eqs. (6.18) and (6.19) cover both cases $T_e = T_0$ and $T_0 + 1$. For convenience of notation, we shall also simply remember the restriction on the summation over α and β; namely that $\alpha > F_N$ and $B < F_P$ for $O_{xJ1}^\dagger$.

Since the ground state $|\Delta\rangle\rangle = |J_0 = 0T_0\rangle\rangle$ is a scalar

[4] Note that states of isospin $T_e = T_0 - 1$ cannot occur for $T_3 = T_0$. They can occur, however, in the neighboring nucleus of smaller T_3.

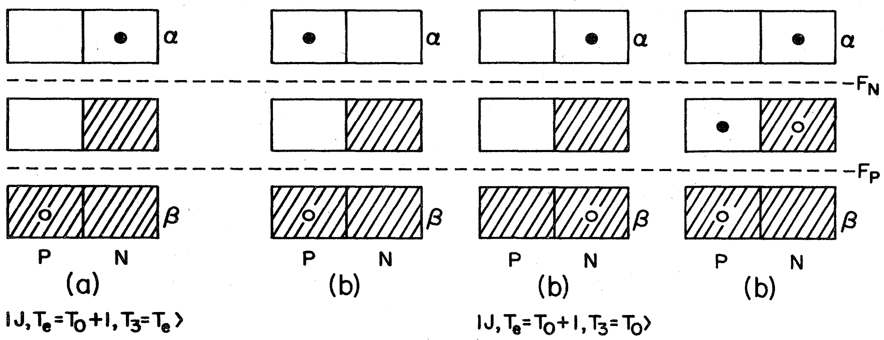

FIG. 3. Particle-hole configurations in a $T_e = T_0 + 1$ excited multiplet of a closed-shell nucleus (a) for the state of maximum $T_3 = T_0 + 1$ and (b) for the analog state of $T_3 = T_0$.

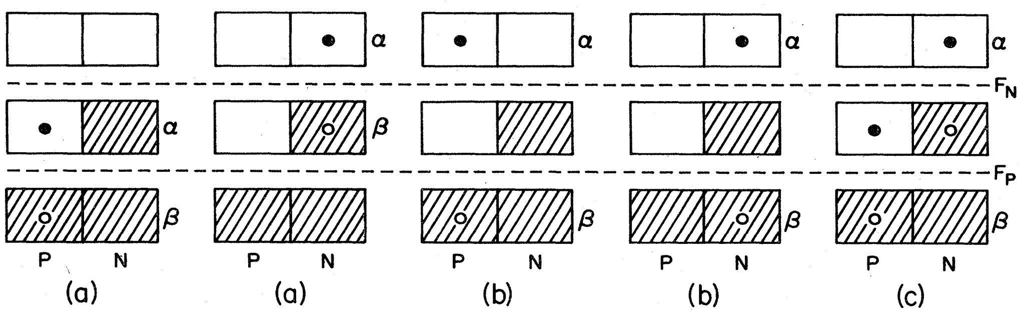

FIG. 4. Particle–hole configurations in a $T_e = T_0$ excited multiplet of a closed-shell nucleus.

in angular momentum (but not isospin) space, the tensor equations of motion (3.10) partially simplify to Eq. (5.2) and for integer J become

$$\begin{aligned}\sum_{ijT} &\hat{J}^{-1}\hat{T}(-1)^{T_0-T_e-T-T_i}W(T_iT_jT_0T_0;TT_e)\\ &\times\langle 0T_0\,||\,[O_{y\bar{J}\bar{T}_i},H,O_{xJT_j}{}^\dagger]^{OT}\,||\,0T_0\rangle\\ &=\omega_{x\Lambda}\sum_{ijT}\hat{J}^{-1}T(-1)^{T_0-T_e-T-T_i}W(T_iT_jT_0T_0;TT_e)\\ &\times\langle 0T_0\,||\,[O_{y\bar{J}\bar{T}_i},O_{xJT_j}{}^\dagger]^{OT}\,||\,0T_0\rangle,\\ &=\delta_{xy}\omega_{x\Lambda},\end{aligned}\tag{6.20}$$

where the superscript OT on the commutators signifies that they are coupled to angular momentum O and isospin T.

In order to exploit the simplifications that result for a closed-shell ground state (i.e., a particle–hole vacuum state) it is convenient to use the Wigner–Eckart theorem, Eq. (2.20), to write

$$\begin{aligned}&\langle OT_0\,||\,[O_{y\bar{J}\bar{T}_i},H,O_{xJT_j}{}^\dagger]^{OT}\,||\,OT_0\rangle\\ &=\sum_\tau[\hat{T}_0/(T_0TT_0O\mid T_0T_0)](-1)^{T_i-\tau}(T_iT_j-\tau\tau\mid TO)\\ &\times\langle OT_0T_0\mid[O_{y\bar{J}T_{i\tau}},H,O_{xJT_{j\tau}}{}^\dagger]^0\mid OT_0T_0\rangle,\end{aligned}$$

where we have also used Eq. (2.13) to decouple the commutator in isospin space. The equations of motion thus become

$$\begin{aligned}\sum_{ij\tau}&\hat{J}^{-1}C_{ij\tau}\langle OT_0T_0\mid[O_{y\bar{J}T_{i\tau}},H,O_{xJT_{j\tau}}{}^\dagger]^0\mid OT_0T_0\rangle\\ &=\omega_{x\Lambda}\sum_{ij\tau}\hat{J}^{-1}C_{ij\tau}\langle OT_0T_0\mid[O_{y\bar{J}T_{i\tau}},O_{xJT_{j\tau}}{}^\dagger]^0\mid OT_0T_0\rangle,\\ &=\delta_{xy}\omega_{x\Lambda},\end{aligned}\tag{6.21}$$

where

$$\begin{aligned}C_{ij\tau}=\sum_T&\hat{T}\hat{T}_0(-1)^{T_0-T_e-T-\tau}\\ &\times[(T_iT_j-\tau\tau\mid TO)/(T_0TT_0O\mid T_0T_0)]\\ &\times W(T_iT_jT_0T_0;TT_e).\end{aligned}\tag{6.22}$$

Substituting the expansion (6.19) into (6.21) readily gives the RPA equations, in matrix form,[5]

$$\begin{pmatrix}A & B\\ B^\dagger & D\end{pmatrix}\begin{pmatrix}Y\\ Z\end{pmatrix}=\omega\begin{pmatrix}Y\\ -Z\end{pmatrix},\tag{6.23}$$

with

$$\begin{aligned}A_{\alpha\beta i,\gamma\delta j}&=\sum_\tau\hat{J}^{-1}C_{ij\tau}\zeta_{\alpha\beta}\zeta_{\gamma\delta}\\ &\times\langle OT_0T_0\mid[A_{\alpha\beta}(\bar{J}T_{i\tau}),H,A_{\gamma\delta}{}^\dagger(JT_{j\tau})]^0\mid OT_0T_0\rangle,\\ B_{\alpha\beta i,\gamma\delta j}&=-\sum_\tau\hat{J}^{-1}C_{ij\tau}\zeta_{\alpha\beta}\zeta_{\gamma\delta}\\ &\times\langle OT_0T_0\mid[A_{\alpha\beta}(\bar{J}T_{i\tau}),H,A_{\gamma\delta}(\bar{J}\bar{T}_{j\tau})]^0\mid OT_0T_0\rangle,\\ D_{\alpha\beta i,\gamma\delta j}&=\sum_\tau\hat{J}^{-1}C_{ij\tau}\zeta_{\alpha\beta}\zeta_{\gamma\delta}\\ &\times\langle OT_0T_0\mid[A_{\alpha\beta}{}^\dagger(J\bar{T}_{i\tau}),H,A_{\gamma\delta}(\bar{J}\bar{T}_{j\tau})]^0\mid OT_0T_0\rangle.\end{aligned}\tag{6.24}$$

[5] In deriving the RPA equations, it is useful to observe the identities

$$C_{ij\tau}=C_{ji\tau},$$

$$\sum_\tau\delta_{ij}C_{ij\tau}=\delta_{ij}.$$

Inspection reveals that A and D are Hermitian matrices. Thus the supermatrix on the lhs of Eq. (6.23) is also Hermitian, as such an equations-of-motion matrix should be. But it has less symmetry than the familiar RPA matrix for an $N = Z$ nucleus, cf., Eq. (5.7).

If the solutions are normalized in the usual way, i.e.,

$$\sum_{\alpha\beta i} \{ | Y_{\alpha\beta i}(x\Lambda) |^2 - | Z_{\alpha\beta i}(x\Lambda) |^2 \} = \pm 1, \tag{6.25}$$

it can readily be shown, by substitution, that the excitation operators are orthonormal in the usual RPA sense; *viz.*

$$\sum_{ij\tau} \hat{J}^{-1} C_{ij\tau} \langle OT_0T_0 | [O_{y\bar{J}T_i\tau}, O_{xJT_j\tau}{}^\dagger]^0 | OT_0T_0 \rangle = \pm \delta_{xy}, \tag{6.26}$$

where the "physical" solutions have positive norm.

The general expression for reduced transition matrix elements of a one-body tensor operator W^{JT_j} is given by Eq. (4.4), which simplifies in angular momentum (but not isospin) space, according to Eq. (5.8), to

$$\begin{aligned} &\langle xJT_e \| W^{JT_j} \| OT_0 \rangle \\ &= (-1)^{T_j+T_0-T_e} T_e \sum_{iT} (-1)^{T_0-T_e-T-T_i} \\ &\times \hat{T} W(T_iT_jT_0T_0; TT_e) \\ &\times \langle OT_0 \| [O_{x\bar{J}\bar{T}_i}, W^{JT_j}]^{OT} \| OT_0 \rangle. \end{aligned} \tag{6.27}$$

Expressing the rhs in terms of closed-shell matrix elements as before, we obtain

$$\begin{aligned} \langle xJT_e \| W^{JT_j} \| OT_0 \rangle &= (-1)^{T_j+T_0-T_e} \hat{T}_e \sum_{i\tau} C_{ij\tau} \\ &\times \langle OT_0T_0 | [O_{x\bar{J}T_i\tau}, W_\tau{}^{JT_j}]^0 | OT_0T_0 \rangle. \end{aligned} \tag{6.28}$$

To evaluate this expression, we use Eq. (2.22) and the identity (2.24) to express the transition operator

$$\begin{aligned} W^\Omega = &\sum_{\alpha>\beta} \hat{\Omega}^{-1} \{ \langle \alpha \| W^\Omega \| \beta \rangle A_{\alpha\beta}{}^\dagger(\Omega) \\ &+ (-1)^{\Omega+\alpha-\beta} \langle \beta \| W^\Omega \| \alpha \rangle A_{\alpha\beta}(\bar{\Omega}) \} \\ &+ \text{noncontributing components}, \end{aligned} \tag{6.29}$$

where $\Omega = JT_j$.

The evaluation of Eq. (6.29) is now straightforward if $T_e = T_0 + 1$ or if $T_e = T_0$ and $T_j = 0$. However if $T_e = T_0$ and $T_j = 1$ we have to be more careful because the particle–hole operators $A_{\alpha\beta}{}^\dagger(JO)$ and $A_{\alpha\beta}{}^\dagger(J1)$ are not orthogonal when $\alpha < F_N$ or $\beta > F_P$; cf., Eq. (6.15). In fact one can show that

$$\begin{aligned} &\zeta_{\alpha\beta} \langle OT_0T_0 | [A_{\alpha\beta}(\bar{J}O), A_{\gamma\delta}{}^\dagger(J1O)]^0 | OT_0T_0 \rangle \zeta_{\gamma\delta} \\ &= \hat{J} \delta_{\alpha\gamma} \delta_{\beta\delta} \xi_{\alpha\beta}, \end{aligned} \tag{6.30}$$

where

$$\begin{aligned} \xi_{\alpha\beta} = &-1 \quad \text{if} \quad \alpha < F_N, \beta < F_P, \\ &+1 \quad \text{if} \quad \alpha > F_N, \beta > F_P, \\ &\;\;0 \quad \text{if} \quad \alpha > F_N, \beta < F_P. \end{aligned} \tag{6.31}$$

Thus one obtains the expression for transition matrix elements

$$\begin{aligned} \langle xJT_e \| W^{JT_j} \| OT_0 \rangle &= (-1)^{T_j+T_0-T_e} \hat{T}_e \hat{T}_j{}^{-1} \\ &\times [\sum_{\alpha>\beta} \zeta_{\alpha\beta}{}^{-1} \{ Y_{\alpha\beta j}{}^*(x) \langle \alpha \| W^{JT_j} \| \beta \rangle + (-1)^{J+T_j+\alpha-\beta} \\ &\times Z_{\alpha\beta j}{}^*(x) \langle \beta \| W^{JT_j} \| \alpha \rangle \} \\ &- [(T_0+1)/T_0]^{1/2} \delta_{T_eT_0} \delta_{T_j1} \\ &\times \sum_{\alpha>\beta} \zeta_{\alpha\beta}{}^{-1} \xi_{\alpha\beta} \{ Y_{\alpha\beta 0}{}^*(x) \langle \alpha \| W^{J1} \| \beta \rangle \\ &+ (-1)^{J+\alpha-\beta} Z_{\alpha\beta 0}{}^*(x) \langle \beta \| W^{J1} \| \alpha \rangle \}]. \end{aligned} \tag{6.32}$$

VII. DISCUSSION AND CONCLUSIONS

In paper I and the present paper, an equations-of-motion method has been formulated to describe the dynamic properties of nuclei and other many-body systems. The method is particularly useful for finite systems since no expansions are involved which only converge in the limit of large particle number and there is no violation of the Pauli principle.

The formalism is exact and, in principle, completely general. Nevertheless, as we have emphasized several times, it is only useful for excitation processes which are relatively simple. As a consequence, the equations of motion of paper I were limited, in practice, to systems with scalar ($J = T = 0$) ground states. This is because the excitation operators were considerably complicated by the geometrical requirement of generating excited states of good angular momentum and isospin. In the present paper the equations of motion have been generalized to take explicit account of these geometrical constraints and to exploit the invariance properties of the Hamiltonian and the corresponding spherical tensor properties of the excitation operators, in order that equations-of-motion calculations should be as economic and as realistic as possible, and, in particular, applicable to *any* system.

The extension of the RPA from closed- to open-shell *scalar* nuclei has been made (Rowe and Wong, 1970), using the equations of motion of paper I, and applied to the particle-hole excitation of ^{12}C and a number of even $N = Z$ *sd*-shell nuclei with considerable success (Wong, Rowe and Parikh, 1974). For nonscalar nuclei, the extension of the RPA has been made on the basis of the generalized equations of this paper. Its application to the investigation of the isospin structure of the $N > Z$ Ni isotopes yielded very good accord with experiments. A preliminary report of these calculations has already been published (Ngo-Trong and Rowe, 1971; Ngo-Trong, 1972).

A criticism that has sometimes been levelled against the above equations-of-motion formalism is that it is incomplete inasmuch as it presupposes a ground state but gives no prescription for its derivation. We maintain that this is in fact a major strength. For we do not believe that there is necessarily any simple relationship between the best ways to describe the dynamic excitations of a system and the static properties of its ground state. Of course it is well known that a knowledge of transition densities can provide considerable information about ground state correlations (Sanderson, 1965; Rowe, 1968c) and this information might be used to improve a model ground state and hence the equations of motion solutions in a self-consistent way. But the fact that the equations of motion can be deployed with any static theory of the ground state gives them considerable flexibility in designing realistic model calculations for a diversity of physical situations.

A number of possible applications of equations of motion exist. One possibility is to the two-nucleon transfer reactions. Another is to nucleon scattering and photonuclear reactions by considering excitations into the continuum. For some purposes it may well be that variations or extensions of the equations should be devised; for example, it might be appropriate to couple excitations built on a number of low-lying states $|\Delta_i\rangle\rangle$, i.e.,

$$|x\Lambda\rangle\rangle = \sum_i (Q_{x\Lambda}^\dagger(i) \times |\Delta_i\rangle\rangle)^\Lambda,$$

as in the intermediate coupling model. It is also probable that the constraint on the excitation operators, that their Hermitian adjoints annihilate the ground state, is inappropriate for some types of excitations, e.g., rotational states, and that other constraints and equations of motion should be devised. Some such variations have already been suggested (Nadjakov and Mikhailov, 1970; Bouten *et al.*, 1973). It should also be remarked that the constraint (3.1b) that we imposed on the annihilation operator, although convenient, is not unique. For example, Armstrong (1974) has considered an alternative constraint and derived an open-shell RPA for use in atomic physics, which differs somewhat from that based on the tensor equations of motion presented here. These illustrations indicate that the versatility of equations-of-motion methods have yet to be fully explored.

ACKNOWLEDGMENTS

We wish to thank Dr. J. B. French for stimulating our interest in multipole sum rules and the possibility of using parallel techniques for equations-of-motion purposes. Thanks are also due to Dr. S. S. M. Wong for many invaluable consultations.

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