Higher Random Phase Approximation and Energy Spectra of Spherical Nuclei

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A method which is an extension of the usual random phase approximation (RPA) is proposed in order to study the spectra of spherical nuclei. In contrast to the usual RPA method based on the linearized equations of motion of the one-nucleon excitation operators, in the higher random phase approximation (HRPA) the many-nucleon excitations are also included. Nuclear states are superpositions of the one- and many-nucleon excitations (i.e., particle-hole pairs). We have especially studied the modes consisting of one- and two-nucleon excitations. In this second RPA, one solves the secular problem obtained from the closed system of linearized equations of motion for the one particle-hole pair operators ("doubles") and the two-pair operators ("quadruples"). States of definite nuclear spin, parity, and isotopic spin are considered. The method of the second RPA is illustrated in the example of the 6.06-Mev, $J^\pi=0^+$, $T=0$ state of O^{16}. Satisfactory semiquantitative agreement with the experiment is obtained for this case. The second RPA is also discussed in connection with the "aligned coupling scheme." The importance of the method for the study of the vibrational 4^+ states is indicated.

1. INTRODUCTION

RECENTLY, the method of random phase approximation (RPA) has been successfully applied to the problem of certain types of collective nuclear states. In fact, the RPA method provides only an improvement of the usual shell-model configuration mixing calculations. Namely, it allows for the inclusion of certain correlations in the ground state, i.e., a "diffused" Fermi surface by the so-called "backward-going graphs." This method, also known as the method of the Sawada modes, can be formulated in terms of the linearized equations of motion of the single-particle density matrix (cf., e.g., Sawicki[1] and Sawicki and Soda[2]; reference 2 is hereafter referred to as I). This method was originally applied to the high-density electron gas, and then, by many workers, to nuclear problems. In particular, the basic properties of the giant $E1$ states with $J^\pi=1^-$, $T=1$, the octupole vibrational states, $J^\pi=3^-$, $T=0$, and the low-lying $J^\pi=2^+$, $T=0$ vibrational states of even-even nuclei have been satisfactorily explained with the help of the RPA method. The fact that the $T=0$ collective states lie low and the $T=1$ states lie high in energy relative to the respective basic single-particle excitations, is explained by the effective net particle-hole interaction which is, on the average, attractive in the $T=0$ states, and repulsive in the $T=1$ states.

The operators of the two-nucleon excitations, i.e., the terms quadratic in the off-diagonal components of the single particle density operator $\hat{\rho}$, as given in Eq. (4) of I, have rather small contributions to many types of states as, for example, to the ones mentioned above. If one considers only a finite number of single-particle shell-model levels, than there are present many more such quadratic terms than the linear coupling terms. However, their net contributions may be quite small, on the average, for some types of modes. This smallness is ensured by two effects: (1) the randomness of phases with which such terms contribute, and (2) strong selection rules, especially in spherical nuclei. As an example to illustrate (2), we observe that for the $E1$ states with $J^\pi=1^-$, $T=1$, the basic one-nucleon excitations correspond to the average spacing between two adjacent major shells $\hbar\omega_0$. On the other hand, by parity and angular momentum selection rules, the two-nucleon excitations correspond to basic excitations of the order of $3\hbar\omega_0$. Such large energy denominators ensure the smallness of the contributions of the double excitations from a closed shell.

However, there are nuclear states for which two- and many-nucleon basic excitations are important, or perhaps even more important, than the one-nucleon excitations. For example, the $J^\pi=0^+$, $T=0$ states in O^{16} should be described as superpositions of the one-nucleon excitations $(1s^{-1}2s)$, $(1p^{-1}2p)$, and the two-nucleon excitations $(1p^{-2}2s^2)$, $(1p^{-2}2s1d)$, and $(1p^{-2}1d^2)$. Here, both types of excitations correspond to the average double shell spacing, $2\hbar\omega_0$, and thus enter on the same footing. Another example are the $J^\pi=4^+$, $T=0$ vibrational states, where the two-nucleon basic excitations seem to be essential, in contrast to some recent calculations,[3] with the usual (linearized) Sawada-type theory.

In order to study the correlation and "screening" effects in the ground state of a high density electron gas, Suhl and Werthamer[4] have introduced an extension of the RPA method called the higher random phase approximation (HRPA). We shall now formulate this method for finite systems of fermions, and in order to study the excited states, in particular, the nuclear energy spectra.

If we assume only two-body interactions in the system, the commutator with the Hamiltonian of a product operator $c_{\gamma'}{}^\dagger c_{\delta'}{}^\dagger \cdots c_\delta c_\gamma$, where c_γ destroys one nucleon in the shell-model state γ and $c_{\gamma'}{}^\dagger$ creates one in the state γ', contains products with two more

[1] J. Sawicki, Nuclear Phys. **23**, 285 (1961).
[2] J. Sawicki and T. Soda, Nuclear Phys. **28**, 270 (1961).
[3] L. S. Kisslinger and H. Ogata (private communications).
[4] H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961).

operators. One of these is a destruction and the other a creation operator, i.e., we have one extra operator $c_{\alpha'}{}^{\dagger}c_{\alpha}\equiv\hat{\rho}_{\alpha\alpha'}$ in the products. Consequently, we obtain an infinite chain of equations of motion for the product operators, such that the equation of motion for an N product contains coupling terms with the products of the $N+2$ operators, for which we then write the new equation of motion, *ad infinitum*. Such a chain of equations can be broken off at a certain maximum assumed number of operators in the products N_0 and linearized so that one obtains a closed soluble system of equations.

This can be achieved by the method of contractions, i.e., by extracting from the products up to N_0+2 operators all the possible diagonal components $\hat{\rho}_{\alpha\alpha}=c_{\alpha}{}^{\dagger}c_{\alpha}$, and replacing them by the Fermi sea occupation factors n_{α} ($n_{\alpha}=1$ if the state α lies below the Fermi surface, and $=0$ if it lies above). All of the uncontractable N_0+2 products are neglected. This procedure is valid provided such N_0+2 products can give only small contributions for a given particular type of state.

Let us illustrate the method on the simplest case of the motion of single annihilation operators. Let us assume the Hamiltonian

$$\hat{H}=\hat{H}_0+\hat{V}=\sum_{\alpha}E_{\alpha}{}^{0}c_{\alpha}{}^{\dagger}c_{\alpha}+\tfrac{1}{2}\sum_{\alpha\alpha'\beta\beta'}\langle\alpha'\beta'|V|\alpha\beta\rangle c_{\alpha'}{}^{\dagger}c_{\beta'}{}^{\dagger}c_{\beta}c_{\alpha},\quad(1)$$

where $\hat{H}_0$ is the zero-order shell-model Hamiltonian corresponding to the single-particle energy spectrum $\{E_{\alpha}{}^{0}\}$, and the complete set of eigenfunctions $\{\varphi_{\alpha}{}^{0}\}$; $V=V(1,2)$ is the phenomenological two-body interaction potential called the "residual" interaction. We can now write the equations of motion for the "singles," i.e., the c_{α} operators:

$$i\hbar(\partial/\partial t)c_{\nu}=E_{\nu}{}^{0}c_{\nu}+\sum_{abb'}\langle\nu b'|V|ab\rangle c_{b'}{}^{\dagger}c_{b}c_{a}.\quad(2)$$

Equation (2) can be also rewritten as

$$-(E_{\nu}{}^{0}+E)c_{\nu}=\tfrac{1}{2}\sum_{abb'}\langle\nu b'|U|ab\rangle c_{b'}{}^{\dagger}c_{b}c_{a}=\sum_{b'}\sum_{a<b}\langle\nu b'|U|ab\rangle c_{b'}{}^{\dagger}c_{b}c_{a},\quad(3)$$

where $U=V(12)(1-P_{12})$ is the antisymmetrized two-body exchange operator. In the last sum, Eq. (3), the restriction "$a<b$" avoids repetitions of the same terms. We now write the equations of motion for the "triples"

$$-Ec_{\mu}{}^{\dagger}c_{\nu}c_{\nu'}=(E_{\nu}{}^{0}+E_{\nu'}{}^{0}-E_{\mu}{}^{0})c_{\mu}{}^{\dagger}c_{\nu}c_{\nu'}+\tfrac{1}{2}\sum_{aa'bb'}\langle a'b'|U|ab\rangle(\delta_{b\mu}c_{a'}{}^{\dagger}c_{b'}{}^{\dagger}c_{a}c_{\nu}c_{\nu'}+\delta_{a'\nu}c_{\mu}{}^{\dagger}c_{b'}{}^{\dagger}c_{b}c_{a}c_{\nu'}+\delta_{a'\nu'}c_{\mu}{}^{\dagger}c_{\nu}c_{b'}{}^{\dagger}c_{b}c_{a}).\quad(4)$$

The energy E is the same as in Eq. (2) because our new states are superpositions of our singles and triples. After performing all the possible contractions in Eqs. (3) and (4), we get the final closed systems of equations of motion for singles and the uncontractable triples:

$$-(E_{\nu}{}^{0}+E)c_{\nu}\cong\sum_{a}\langle\nu a|U|ba\rangle n_{a}c_{b}+\tfrac{1}{2}\sum_{\substack{abb'\\ \text{all different}}}\langle\nu b'|U|ab\rangle c_{b'}{}^{\dagger}c_{b}c_{a},\quad(5)$$

$$\begin{aligned}-(E_{\nu}{}^{0}+E_{\nu'}{}^{0}-E_{\mu}{}^{0}+E)c_{\mu}{}^{\dagger}c_{\nu}c_{\nu'}\cong{}&\sum_{a}\langle\nu'\nu|U|a\mu\rangle[n_{\nu}n_{\nu'}+n_{\mu}(1-n_{\nu}-n_{\nu'})]c_{a}\\&+\sum_{a}n_{a}\{\langle\nu'a|U|a\mu\rangle(n_{\mu}-n_{\nu'})c_{\nu}+\langle a\nu|U|a\mu\rangle\\&\times(n_{\mu}-n_{\nu})c_{\nu'}\}+\sum_{a\neq a'}\{\langle a'\nu|U|a\mu\rangle(n_{\mu}-n_{\nu})c_{a'}{}^{\dagger}c_{a}c_{\nu'}\\&+\langle\nu'a'|U|a\mu\rangle(n_{\mu}-n_{\nu'})c_{a'}{}^{\dagger}c_{a}c_{\nu}\\&+\langle\nu'\nu|U|aa'\rangle\tfrac{1}{2}(1-n_{\nu}-n_{\nu'})c_{\mu}{}^{\dagger}c_{a'}c_{a}\}\\&+\sum_{a\neq a'}n_{a}\{-\langle aa'|U|a\mu\rangle c_{a'}{}^{\dagger}c_{\nu}c_{\nu'}+\langle\nu a|U|a'a\rangle\\&\times c_{\mu}{}^{\dagger}c_{a'}c_{\nu'}+\langle\nu'a|U|a'a\rangle c_{\mu}{}^{\dagger}c_{\nu}c_{a'}\}.\end{aligned}\quad(6)$$

A detailed study of the system of Eqs. (5) and (6) with special application to spherical nuclei is in preparation by G. Fano and the author.

In Eqs. (5) and (6) we have discarded all the terms involving the fluctuations of the particle-number operators about the Fermi sea occupation factors, $\hat{\rho}_{\alpha\alpha}-n_{\alpha}$, assuming them to be of a higher order.

All the sums in Eqs. (5) and (6) containing the factor n_a and the diagonal matrix elements $\langle\beta a|U|\alpha a\rangle$ are the self-energy terms which should and could be properly included in the zero-order energies $\{E_{\alpha}{}^{0}\}$. In fact, it is better to define the "residual" interaction operator $\hat{V}$ as the actual $\hat{V}$ involving the true two-body potentials minus the sum over the single-particle interaction potentials to be determined self-consistently from a Hartree-Fock-type calculation. This could be done so that the resulting final system of Eqs. (5) and (6) is as above but contains no diagonal matrix elements of U. A discussion of the neglected $O(\hat{\rho}_{\alpha\alpha}-n_{\alpha})$ terms is also a part of the self-consistency problem. A study of the above questions is in preparation by G. Fano and the author.

2. ONE- AND TWO-NUCLEON EXCITATIONS AND SECOND RANDOM PHASE APPROXIMATION

Now, we shall formulate and discuss in detail the Second RPA, particularly in connection with the problem of the collective states of spherical nuclei.

The equations of motion for the "doubles," i.e., for the operators $\hat{\rho}_{\nu\mu}=c_{\mu}{}^{\dagger}c_{\nu}$, have been given in Eq. (4) of I.

They can be rewritten as

$$(E_\mu^0-E_\nu^0-E)\hat{\rho}_{\nu\mu}\cong(n_\mu-n_\nu)\sum_{\kappa\neq\kappa'}\langle\nu\kappa'|U|\mu\kappa\rangle\hat{\rho}_{\kappa\kappa'}+\sum_{\substack{\kappa\kappa's\\ \text{all different}}}\{\langle\nu\kappa'|V|s\kappa\rangle\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{s\mu}-\langle s\kappa'|V|\mu\kappa\rangle\hat{\rho}_{\nu s}\hat{\rho}_{\kappa\kappa'}\}. \quad (7)$$

The self-energy terms are assumed to be already self-consistently included in the zero-order energies $\{E_\alpha^0\}$, and the fluctuation terms $O(\hat{\rho}_{\alpha\alpha}-n_\alpha)$ are omitted. In practice, we shall not perform any self-consistency calculation in the present paper. In fact, we are primarily interested in the general properties of the double excitations and in the formal structure of the Second RPA. The sum $\sum_{\kappa\kappa's}\langle\nu\kappa'|V|s\kappa\rangle\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{s\mu}$ also can be written as

$$\tfrac{1}{2}\sum_{\kappa\kappa's}\langle\nu\kappa'|U|s\kappa\rangle\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{s\mu}=\sum_{\kappa'}\sum_{\kappa<s}\langle\nu\kappa'|U|s\kappa\rangle\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{s\mu},$$

where the last restriction "$\kappa<s$" avoids the occurrence of the same term twice.

Now, we can write the equations of motion for the uncontractable quadruples $c_{\alpha'}{}^\dagger c_{\beta'}{}^\dagger c_\beta c_\alpha=\hat{\rho}_{\alpha\alpha'}\hat{\rho}_{\beta\beta'}$ in the form

$$[\Delta E^0(\mu\mu';\nu\nu')-E]\hat{\rho}_{\nu\mu}\hat{\rho}_{\nu'\mu'}=\tfrac{1}{2}\sum_{\kappa\kappa' ss'}\langle s'\kappa'|U|s\kappa\rangle\{\delta_{s\mu}c_{s'}{}^\dagger c_{\kappa'}{}^\dagger c_\kappa c_{\mu'}{}^\dagger c_\nu c_{\nu'}+\delta_{s\mu'}c_\mu{}^\dagger c_{s'}{}^\dagger c_{\kappa'}{}^\dagger c_\kappa c_\nu c_{\nu'}+\delta_{\kappa'\nu}c_\mu{}^\dagger c_{\mu'}{}^\dagger c_{s'}{}^\dagger c_{\nu'}c_\kappa c_s+\delta_{\kappa'\nu'}c_\mu{}^\dagger c_{\mu'}{}^\dagger c_\nu c_{s'}{}^\dagger c_\kappa c_s\}, \quad (8)$$

where

$$\Delta E^0(\mu\mu';\nu\nu')=E_\mu{}^0+E_{\mu'}{}^0-E_\nu{}^0-E_{\nu'}{}^0.$$

After all the possible contractions, we obtain the following system of equations:

Note added in proof. If one included the threefold contractions possible in Eq. (8), one would get a constant term in the right-hand side of Eq. (9) equal to $\langle\nu\nu'|U|\mu\mu'\rangle[n_\mu n_{\mu'}(1-n_\nu-n_{\nu'})-n_\nu n_{\nu'}(1-n_\mu-n_{\mu'})]$ $(=\mp\langle\nu\nu'|U|\mu\mu'\rangle$, the upper sign for $n_\nu=n_{\nu'}=1$, $n_\mu=n_{\mu'}=0$, the lower sign for $n_\nu=n_{\nu'}=0$, $n_\mu=n_{\mu'}=1$). Such a constant term of coupling with the ground state can appear formally but only in the case of $J^\pi=0^+$, $T=0$ states. However, in HRPA one calculates only the excitation energies *relative* to the ground state, and a constant commutes with $\hat{H}$. Thus, the constant gets formally decoupled from the quadruples in the HRPA secular matrix. The formal situation is different when we make an ordinary shell model calculation with no backward-going graphs. In a most recent letter [Phys. Rev. Letters 1, 36 (1962)], N. Vinh Mau and G. E. Brown report their shell model calculations of the 0^+ states in O^{16}. They do not consider the case of a correlated ground state. Their results are generally similar to those of our Sec. 3; they then criticize in the light of the most recent experimental data, and suggest that the dynamical nature of the 6.06 state in O^{16} may be more complicated.

$$\begin{aligned}[\Delta E^0(\mu\mu';\nu\nu')-E]\hat{\rho}_{\nu\mu}\hat{\rho}_{\nu'\mu'}\cong&-\sum_\kappa\{\langle\nu'\nu|U|\kappa\mu'\rangle[n_\nu n_{\nu'}+n_{\mu'}(1-n_\nu-n_{\nu'})]\hat{\rho}_{\kappa\mu}\\&+\langle\nu'\nu|U|\mu\kappa\rangle[n_\nu n_{\nu'}+n_\mu(1-n_\nu-n_{\nu'})]\hat{\rho}_{\kappa\mu'}\\&+\langle\kappa\nu'|U|\mu\mu'\rangle[n_\mu n_{\mu'}+n_{\nu'}(1-n_\mu-n_{\mu'})]\hat{\rho}_{\nu\kappa}\\&+\langle\nu\kappa|U|\mu\mu'\rangle[n_\mu n_{\mu'}+n_\nu(1-n_\mu-n_{\mu'})]\hat{\rho}_{\nu'\kappa}\}\\&-\sum_{\kappa\neq\kappa'}\{\langle\nu\kappa'|U|\mu\kappa\rangle(n_\nu-n_\mu)\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{\nu'\mu'}+\langle\kappa'\nu'|U|\mu\kappa\rangle\\&\times(n_{\nu'}-n_\mu)\hat{\rho}_{\kappa\kappa'}\hat{\rho}_{\nu\mu'}+\langle\nu\kappa'|U|\kappa\mu'\rangle(n_\nu-n_{\mu'})\hat{\rho}_{\nu'\mu}\hat{\rho}_{\kappa\kappa'}\\&+\langle\kappa'\nu'|U|\kappa\mu'\rangle(n_{\nu'}-n_{\mu'})\hat{\rho}_{\nu\mu}\hat{\rho}_{\kappa\kappa'}+\tfrac{1}{2}\langle\kappa\kappa'|U|\mu\mu'\rangle\\&\times(1-n_\mu-n_{\mu'})\hat{\rho}_{\nu\kappa}\hat{\rho}_{\nu'\kappa'}+\tfrac{1}{2}\langle\nu'\nu|U|\kappa\kappa'\rangle(1-n_\nu-n_{\nu'})\\&\times\hat{\rho}_{\kappa\mu}\hat{\rho}_{\kappa'\mu'}\}+\text{"proper" self-energy terms.}\end{aligned} \quad (9)$$

The "proper" self-energy terms which belong to ΔE^0 are

$$\sum_{\kappa\neq s}n_\kappa\{\langle\kappa\nu|U|\kappa s\rangle\hat{\rho}_{s\mu}\hat{\rho}_{\nu'\mu'}+\langle\kappa\nu'|U|\kappa s\rangle\hat{\rho}_{\nu\mu}\hat{\rho}_{s\mu'}-\langle\kappa s|U|\kappa\mu\rangle\hat{\rho}_{\nu s}\hat{\rho}_{\nu'\mu'}-\langle\kappa s|U|\kappa\mu'\rangle\hat{\rho}_{\nu\mu}\hat{\rho}_{\nu's}\}.$$

In Eqs. (7) and (9) we see the characteristic particle-hole projection operators in the form of factors $(n_\alpha-n_{\alpha'})$, the particle-particle and hole-hole factors $(1-n_\beta-n_{\beta'})$, and their combinations $[n_\beta n_{\beta'}+n_\alpha(1-n_\beta-n_{\beta'})]$.

We see that the formal structure of our chain of equations is very different from that of the Brueckner theory which deals with the problems of the ground state. The present HRPA theory deals with the excited states and determines only the excitation energies *relative* to the ground state.

The secular matrix of the closed system of Eqs. (7) and (9) is Hermitian if we only confine ourselves to the single and double transitions "up across" the Fermi surface, i.e., with *creations* of one and two particle-hole pairs.

There are also "mixed" double excitations with destructions and creations of one state above and another below the Fermi surface. If such terms are included, the hermiticity of the secular matrix is destroyed. In the following, we shall not treat such "mixed" quadruples and the likewise possible hole-hole and particle-particle doubles. Perhaps, one should attempt to treat those terms as part of the self-consistency problem of the single particle energy spectrum.

In addition, there are also the single and double transitions "down across" the Fermi surface, the so-called backward-going graphs. If these are included, the secular matrix is non-Hermitian but has the simple

properties quite analogous to those for the case of the usual RPA. The eigenvectors can be written as $\{\hat{B}_n^\dagger|\Psi_0\rangle\}$, where $|\Psi_0\rangle$ is the "true" ground state, and

$$\hat{B}_n^\dagger \equiv \sum_{\alpha\neq\alpha'} c_{(n)}(\alpha\alpha')\hat{\rho}_{\alpha\alpha'} + \tfrac{1}{2}\sum_{\alpha\neq\alpha',\beta\neq\beta'} d_{(n)}(\alpha\alpha',\beta\beta')\hat{\rho}_{\alpha\alpha'}\hat{\rho}_{\beta\beta'}.$$

The components c and d satisfy the simple orthonormality relations with an indefinite metric

$$\sum_{\alpha<\alpha_F<\alpha'} [c_{(n)}(\alpha\alpha')c_{(m)}{}^*(\alpha\alpha') - c_{(n)}(\alpha'\alpha)c_{(m)}{}^*(\alpha'\alpha)] + \tfrac{1}{2}\sum_{\alpha<\alpha_F<\alpha'}\sum_{\beta<\alpha_F<\beta'} [d_{(n)}(\alpha\alpha',\beta\beta')d_{(m)}{}^*(\alpha\alpha',\beta\beta') - d_{(n)}(\alpha'\alpha,\beta'\beta)d_{(m)}{}^*(\alpha'\alpha,\beta'\beta)] = \delta_{mn}, \quad (10)$$

where α_F is the Fermi level. The completeness relations are also quite analogous to those given for the usual RPA, e.g., by Thouless,[5] or in I.

We now proceed to the study of the actual physical states of spherical nuclei, i.e., we introduce the total angular momentum, the isotopic spin, the parity, and the total nuclear spin. For the sake of simplicity, let us first consider a system of identical nucleons, i.e., without the isotopic spin complication, and employ a simple Wigner force

$$\hat{V} = \tfrac{1}{2}\sum_{J'M'} f_{J'}(\alpha\alpha',\beta\beta')(-)^{j_\alpha+j_\beta} \times \hat{A}_{J'M'}(\alpha\alpha')(-)^{M'}\hat{A}_{J'-M'}(\beta\beta'). \quad (11)$$

Here

$$f_{J'}(\alpha\alpha',\beta\beta') \equiv g[J']^{-\frac{3}{2}}(4\pi)^{-\frac{1}{2}}\{[j_\alpha][j_{\alpha'}][j_\beta][j_{\beta'}]\}^{\frac{1}{2}} \times (j_\alpha j_{\alpha'};-\tfrac{1}{2}\tfrac{1}{2}|J'0)(j_\beta j_{\beta'};-\tfrac{1}{2}\tfrac{1}{2}|J'0)v_{J'}(\alpha\alpha',\beta\beta'),$$

where g is a coupling constant, $[j]=2j+1$, $v_{J'}(\alpha\alpha',\beta\beta')$ is a radial matrix element, and the operator of a basic single-nucleon excitation is defined as[6]

$$\hat{A}_{JM}(\alpha\alpha') \equiv \sum_{m_\alpha}(-)^{j_\alpha-m_\alpha}(j_\alpha j_{\alpha'};-m_\alpha m_{\alpha'}|JM)\hat{\rho}_{\alpha\alpha'}. \quad (12)$$

The basic double excitation operators are defined as:

$$\hat{B}_{(J'J'')JM}(\alpha\alpha',\beta\beta') \equiv \sum_{M'M''}(J'J'';M'M''|JM) \times \hat{A}_{J'M'}(\alpha\alpha')\hat{A}_{J''M''}(\beta\beta'). \quad (13)$$

From Eqs. (7) and (9) we now can obtain the final coupled system of equations for the $\hat{A}$ and $\hat{B}$ operators for nuclear states of the total (integer) spin J, projection M

$$(E_\mu^0 - E_\nu^0 - E)\hat{A}_{JM}(\nu\mu) = (n_\mu - n_\nu)\sum_{\kappa\neq\kappa'}\tilde{f}_J(\mu\nu,\kappa\kappa')\hat{A}_{JM}(\kappa\kappa') + \sum_{\substack{\kappa\kappa'S \\ \text{all different}}}\sum_{J'J''}([J'][J''])^{\frac{1}{2}}W(J'j_\mu J''j_\nu;j_sJ) \times[\tilde{f}_{J''}(s\nu,\kappa\kappa')\hat{B}_{(J'J'')JM}(s\mu,\kappa\kappa') - \tilde{f}_{J'}(\mu s,\kappa\kappa')\hat{B}_{(J'J'')JM}(\kappa\kappa',\nu s)], \quad (14)$$

and

$$[\Delta E^0(\mu\mu';\nu\nu') - E]\hat{B}_{(J'J'')JM}(\nu\mu,\nu'\mu') = ([J'][J''])^{\frac{1}{2}}\sum_\kappa\{[n_\nu n_{\nu'} + n_{\mu'}(1-n_\nu-n_{\nu'})] \times W(J'j_\mu J''j_\kappa;j_\nu J)\tilde{f}_{J''}(\nu\kappa,\nu'\mu')\hat{A}_{JM}(\kappa\mu) + [n_\nu n_{\nu'} + n_\mu(1-n_\nu-n_{\nu'})] \times W(J'j_\kappa J''j_{\mu'};j_{\nu'}J)(-)^{J'+J''-J}\tilde{f}_{J'}(\nu'\kappa,\nu\mu) \times \hat{A}_{JM}(\kappa\mu') - [n_\mu n_{\mu'} + n_{\nu'}(1-n_\mu-n_{\mu'})] \times W(J'j_\nu J''j_\kappa;j_\mu J)(-)^{J'+J''-J}\tilde{f}_{J''}(\kappa\mu,\nu'\mu') \times \hat{A}_{JM}(\nu\kappa) - [n_\mu n_{\mu'} + n_\nu(1-n_\mu-n_{\mu'})] \times W(J'j_\kappa J''j_{\nu'};j_{\mu'}J)\tilde{f}_{J'}(\kappa\mu',\nu\mu)\hat{A}_{JM}(\nu'\kappa)\} + \text{coupling terms with the } \hat{B} \text{ operators}, \quad (15)$$

where $W(\cdots)$ is a Racah coefficient, and

$$\tilde{f}_J(\alpha\alpha',\beta\beta') \equiv (-)^{j_{\alpha'}+j_\beta}\{f_J(\alpha\alpha',\beta\beta') + \textstyle\sum_K (-)^{K-J}[K] \times W(j_{\alpha'}j_\beta j_\alpha j_{\beta'};KJ)(-)^{j_\alpha+j_{\alpha'}-j_\beta-j_{\beta'}}f_K(\beta\alpha',\alpha\beta')\}.$$

We omit here the explicit form of the coupling coefficients between the $\hat{B}$ operators as it is rather lengthy and complex. Among these coupling terms, there are terms involving $\hat{B}_{(J'''J'''')JM}(\alpha\alpha',\beta\beta')$ with $J'''\neq J'$, $J''''\neq J''$, in addition to the ones with $\hat{B}_{(J'J'')JM}(\alpha\alpha',\beta\beta')$.

One must be careful not to count the same terms twice for the case ($\nu'=\nu$, $\mu'=\mu$) in Eq. (15). In fact, in going over from the original Eqs. (9)–(15), we have introduced the unrestricted sums over the magnetic substates.

The nucleonic charge τ and a general spin and isotopic spin dependent two-body potential $V(1,2)$, as given by Eq. (8) of I, can now be introduced. Thus, we have two coupling constants g_T with $T=0$, 1 associated with the spin-independent part of $V(1,2)$ and two coupling constants g_T' corresponding to the part of $V(1,2)$ proportional to the operator $\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$. The quantity $f_J{}^{(T)}(\alpha\alpha',\beta\beta')$ associated with g_T is exactly of the form of our previous $f_J(\alpha\alpha',\beta\beta')$, and $g_J{}^{(T)}(\alpha\alpha',\beta\beta')$ associated with g_T' is defined in I.

We obtain the coupled system of equations for the operators $\hat{A}_{JM}(\alpha\alpha',\tau)$ and $\hat{B}_{(J'J'')JM}(\alpha\alpha',\tau;\beta\beta',\tau')$ quite analogous to that of Eqs. (14) and (15) with $\tilde{f}_J(\alpha\alpha',\beta\beta')$

[5] D. J. Thouless, Nuclear Phys. **22**, 78 (1961).

[6] The phase convention adopted here, different from that of I, ensures the hermiticity of the secular matrix for the forward-going graphs (see the coupling terms between the $\hat{A}$ and $\hat{B}$ operators).

replaced by

$$\tilde{f}_J(\alpha\alpha',\tau;\beta\beta',\tau')$$
$$=(-)^{j_{\alpha'}+j_\beta}\{[(f_J{}^{(1)}+g_J{}^{(1)})(\alpha\alpha',\beta\beta')\delta_{\tau'\tau}$$
$$+\tfrac{1}{2}(f_J{}^{(1)}+f_J{}^{(0)}+g_J{}^{(1)}+g_J{}^{(0)})(\alpha\alpha',\beta\beta')\delta_{\tau'-\tau}]$$
$$+\sum_K(-)^{K-J}[K]W(j_{\alpha'}j_\beta j_\alpha j_{\beta'};KJ)(-)^{j_\alpha+j_{\alpha'}-j_\beta-j_{\beta'}}$$
$$\times[(f_K{}^{(1)}+g_K{}^{(1)})(\beta\alpha',\alpha\beta')\delta_{\tau'\tau}$$
$$+\tfrac{1}{2}(f_K{}^{(1)}-f_K{}^{(0)}+g_K{}^{(1)}-g_K{}^{(0)})$$
$$\times(\beta\alpha',\alpha\beta')\delta_{\tau'-\tau}]\}. \quad (16)$$

One can also consider nuclear states of a definite total isotopic spin T by using the usual projection method as in I.

The equations simplify if one uses the harmonic oscillator wave functions and neglects the single particle spin-orbit coupling in $\hat{H}_0$. One can employ the Talmi method, and still use the j-j coupling scheme. Here it is convenient to write $V(1,2)$ in the popular form as a mixture of Wigner, Bartlett, Majorana, and Heisenberg forces:

$$V(1,2)=J(r)(w+bP^\sigma+mP^r+hP^rP^\sigma).$$

In this case we again obtain the system of Eqs. (14) and (15), where one must replace $-\tilde{f}_J(\alpha\alpha',\beta\beta')$ by $(S_J{}^d-\delta_{\tau'\tau}S_J{}^{\rm ex})(\alpha\alpha',\beta\beta')$, and where

$$S_J{}^d(\alpha\alpha',\beta\beta')$$
$$\equiv(-)^{j_{\alpha'}+j_\beta}\sum_{nn'lNL\lambda}[\lambda]\{[j_\alpha][j_{\alpha'}][j_\beta][j_{\beta'}]\}^{\frac{1}{2}}$$
$$\times\left\{(-)^{l_\alpha+l_{\alpha'}-\lambda}W(l_\alpha j_\alpha l_{\alpha'}j_{\alpha'};\tfrac{1}{2}J)W(l_\beta j_\beta l_{\beta'}j_{\beta'};\tfrac{1}{2}J)\right.$$
$$\times W(l_\alpha l_{\alpha'}l_\beta l_{\beta'};J\lambda)(w+(-)^l m)+(-)^{l_\beta+l_{\beta'}-\lambda}$$
$$\times\begin{Bmatrix} l_\alpha & j_\alpha & j_{\alpha'} & l_{\alpha'} \\ \frac{1}{2} & J & \frac{1}{2} & \lambda \\ l_{\beta'} & j_{\beta'} & j_\beta & l_\beta \end{Bmatrix}\left.(b+(-)^l h)\right\}$$
$$\times\langle nl,NL,\lambda|\alpha,\beta,\lambda\rangle\langle n'l,NL,\lambda|\alpha',\beta',\lambda\rangle$$
$$\times\langle nl\|J(r)\|n'l\rangle. \quad (17)$$

Here

$$\begin{Bmatrix} l_\alpha & j_\alpha & j_{\alpha'} & l_{\alpha'} \\ \frac{1}{2} & J & \frac{1}{2} & \lambda \\ l_{\beta'} & j_{\beta'} & j_\beta & l_\beta \end{Bmatrix}$$

is a $12-j$ symbol in the notation of Ord-Smith[7] and $\langle nl,NL,\lambda|\alpha,\beta,\lambda\rangle\equiv\langle nl,NL,\lambda|n_\alpha l_\alpha,n_\beta l_\beta,\lambda\rangle$ is a transformation bracket for the harmonic oscillator wave functions; such brackets have been extensively tabulated by Brody and Moshinsky.[8] $\langle nl\|J(r)\|n'l\rangle$ is a reduced radial matrix element. All the other symbols have been defined in I. The quantity $S_J{}^{\rm ex}(\alpha\alpha',\beta\beta')$ is identical in form to S^d, however, with w interchanged with h, and m with b.

The eigenvectors obtained from the solution of the secular problem with the matrix which is the transpose of the secular matrix of the system of Eqs. (14) and (15). The components satisfy the orthonormality relations quite analogous to those of Eq. (10) and the related completeness relations.

A simplified version of the above equations is obtained if one neglects the j splittings of $\{E_\alpha{}^0\}$ altogether, and uses the L-S coupling scheme. This simplified case is given in the Appendix.

3. 6.06-MEV STATE IN O^{16}

The first excited 6.06-Mev state in O^{16} has the assignment $J^\pi=0^+$, $T=0$, and decays to ground state by pair emission. The lifetime $\tau_{\rm exp}=7\times10^{-11}$ sec implies a rather small value of the $E0$ transition matrix element. This fact, and the very low energy of the state pose a well-known problem. The literature on the subject is rather extensive. Many authors have attempted to explain the properties of this state by doing the usual shell-model configuration mixing calculations[9,10] or by the usual RPA method, i.e., by the monopole breathing modes of the Sawada type.[11–13] None of these authors could quite succeed in bringing the energy of the state down to about the experimental value, and in simultaneously explaining the small $E0$ matrix element. In 1956, Elliott[14] pointed out that, in addition to the basic one nucleon configuration ($1s^{-1}2s$) and ($1p^{-1}2p$), one should consider the energetically equivalent basic two-nucleon configurations ($1p^{-2}2s^2$), ($1p^{-2}2s1d$), and ($1p^{-2}1d^2$). Our second RPA method appears to be particularly suitable for treating this problem.

We have performed numerical calculations by diagonalizing the secular matrix of the simplified system of equations, as given in the Appendix. Similarly, as in references 10–13, we have neglected the spin-orbit coupling in the single particle potential and used the energies averaged over the splittings. The LS coupling scheme is employed. The $V(1,2)$ used is with $b=h=0$. Out of all the possible coupling terms between the $\hat{B}$-operators, we have retained only the most important terms corresponding to the first and fourth double sum $\sum_{\kappa\kappa'}$ in Eq. (9), and we have neglected the exchange parts of the matrix elements in the coupling between the $\hat{A}$ and $\hat{B}$ operators. Although these

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approximations seem to be rather rough, they are not too unreasonable and should be sufficient for a semiquantitative analysis (cf. Appendix).

If we consider only the forward-going graphs, i.e., the single and double transitions "up across" the Fermi surface, our secular matrix is 7×7, and if also the backward-going graphs are included, it is 14×14. We have excluded the possible "mixed" double excitations, i.e., one "up across" and one "down across."

The greatest uncertainty in our numerical calculations is connected with the lack of self-consistency and the uncertainty in the single-particle excitation energies $E_{\alpha'}{}^0-E_\alpha{}^0$. These enter into the diagonal elements of the secular matrix and their magnitude is of crucial importance for the magnitude of the eigenvalues, i.e., energies relative to the ground state.

In particular, in our equations we have elements diagonal in the particle-hole pairs, i.e., corresponding to the "elastic scattering" of such pairs. Such terms are clearly of self-energy character, and, in fact, they are formally of the same type as the omitted "proper" self-energy terms of Eq. (9). It appears reasonable to use in $E_{\alpha'}{}^0-E_\alpha{}^0$ the "empirical" single particle energies $\{(E_\alpha{}^0)_{\text{exp}}\}$. However, in addition to the "empirical" particle-core and hole-core energies, we must include in each $E_{\alpha'}{}^0-E_\alpha{}^0$ the important particle-hole interaction energy. On the other hand, as our calculation is non-self-consistent, we do not know which part of the diagonal particle-hole matrix elements is already included in $\{(E_\alpha{}^0)_{\text{exp}}\}$. For the sake of a semiquantitative analysis, we have considered two cases: (a) only pure "empirical" single-particle energies are used in the diagonal elements of the secular matrix, and (b) some "average" particle-hole interaction energies are included. As the "average" energies, we assumed -10 Mev for the singly-excited configurations, and -15 Mev for the double excitations. These numbers seem to be taken rather arbitrarily. However, the resulting diagonal elements of the secular matrix are not very different from what one obtains from a calculation where one computes such diagonal elements from the kinetic energies, and *all* the possible self-energy terms with our model parameters. A similar calculation was done by Fallieros[13] for the case of the breathing modes. In Table I, we give the numerical values of the diagonal elements of our secular matrix for the cases (a) and (b) for the five basic configurations.

TABLE I. Diagonal elements of the secular matrix for the $J^\pi=0^+$, $T=0$ states in O^{16}: (a) with only the empirical single-particle energies[a]; (b) with the "average" particle-hole interaction energies included.

Configuration	$(1s^{-1}2s)$	$(1p^{-1}2p)$	$(1p^{-2}2s^2)$	$(1p^{-2}2s1d)$	$(1p^{-2}1d^2)$
Excitation energy (Mev) (a)	46.72	26.28	30.90	34.44	37.98
Excitation energy (Mev) (b)	36.72	16.28	15.90	19.44	22.98

[a] See reference 18.

The numerical computations were performed for the simple Serber force with the Gaussian radial shape: $w=m=0.5$, $J(r)=-V_0e^{-r^2/\alpha^2}$, $V_0=51.9$ Mev, $\alpha=1.732\times10^{-13}$ cm; the parameter of the harmonic oscillator wave functions used $\gamma^{-\frac{1}{2}}=1.68\times10^{-13}$ cm. This $V(1,2)$ is very similar to that used by Ferrell and Visscher.[11] The secular matrices were diagonalized with the aid of the IBM 704 computer of the Centro di Calcoli in Bologna.

The eigenvalues and eigenvectors for the 7×7 secular matrix are given in Table II. In Table II we have omitted the eigensolutions and the components corresponding to the two least important $\hat{B}_{(J'J')00}(1p1d,1p1d)$ operators with $J'=2$ and 3.

The lowest lying 7.55-Mev state in case (b) is to be compared with the 6.06-Mev observed level. We see that, due to the net attractive particle-hole interactions, the calculated energy of that state is decreased by 8.35 Mev relative to the smallest unperturbed excitation energy (11.89 Mev relative to $\Delta E^0(1p^{-2}2s1d)$—the most important component); the corresponding state in case (a) is shifted by 4.85 Mev relative to the smallest ΔE^0, and 13.01 Mev relative to $\Delta E^0(1p^{-2}2s1d)$.

Several examples have also been done which were intermediate between (a) and (b) and it was found that the properties of the lowest lying, and all the other states, are always the same. Our lowest lying state is a coherent superposition of all but one single-pair components and has a clearly collective character. The predominance of the two-pair components and the destructive interference between the two one-nucleon components, i.e., the out-of-phase vibration of the s and p shells ensures the smallness of the $E0$ matrix element $\langle M\rangle$. The rate of decay of the 6.06-Mev state by pair emission is given as[15,16]: $\tau^{-1}=0.97\times10^{61}|\langle M\rangle|^2$ sec^{-1}. The observed rate[16] $(\tau^{-1})_{\text{exp}}=1.4\times10^{10}$ sec^{-1} implies $|\langle M\rangle|=3.8\times10^{-26}$ cm^2. For our 7.55-Mev state

TABLE II. Five most important eigenvalues E and the corresponding eigenvectors of the 7×7 secular matrix for the $J^\pi=0^+$, $T=0$ modes in O^{16}.

E (Mev)	$(1s^{-1}2s)$	$(1p^{-1}2p)$	$(1p^{-2}2s^2)$	$(1p^{-2}2s1d)$	$(1p^{-2}1d^2)$
(a) Only empirical energies in the diagonal elements:					
60.60	−0.78	0.31	0.01	−0.53	0.08
38.89	−0.18	0.12	−0.15	0.19	−0.94
32.77	−0.18	0.07	−0.89	0.32	0.25
22.59	−0.53	−0.73	0.20	0.37	0.06
21.43	−0.19	0.58	0.38	0.67	0.18
(b) Particle-hole interaction energies included:					
49.31	−0.81	0.33	0.00	−0.48	0.06
24.11	−0.16	0.13	−0.17	0.24	−0.93
17.94	−0.17	0.06	−0.87	0.36	0.29
12.36	−0.42	−0.90	0.04	0.09	−0.03
7.55	−0.33	0.24	0.46	0.76	0.20

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we find $|\langle M\rangle| = 1.5\times10^{-26}$ cm^2. The corresponding $E0$ oscillator strength is only a fraction of 1%. This result is not unreasonable in view of the crudeness of our calculation.

For $T=0$ states there is always the problem of the possible admixtures of the spurious modes of the center-of-mass motion. In the case of excitations by two major shells, the elimination of all such possible impurities is a difficult matter even in the case of the harmonic oscillator model.[17] One such important spurious mode is the double excitation of the p-wave motion of the center of mass. The corresponding single excitation is generated by the operator $\hat{C}_{1M}\equiv(\frac{1}{6})^{\frac{1}{2}}\hat{A}_{1M}(1p2s)-(\frac{5}{6})^{\frac{1}{2}}\hat{A}_{1M}(1p1d)$; the double excitation is given by

$$\hat{S}=\bar{\alpha}\sum_M (11;M-M|00)\hat{C}_{1M}\hat{C}_{1-M}$$
$$=\tfrac{1}{6}\bar{\alpha}[\hat{B}_{(11)00}(1p2s,1p2s)-2(5)^{\frac{1}{2}}\hat{B}_{(11)00}(1p2s,1p1d)+5\hat{B}_{(11)00}(1p1d,1p1d)];$$

$\bar{\alpha}$ is a normalization constant. We can now calculate the overlap integrals of our modes with the $\hat{S}|\Psi_0\rangle$. For the 7.55-Mev state, this overlap is rather high, almost 28%, and for the second 12.36-Mev state, it is 7%.

The second excited state at 12.36 Mev is the usual monopole breathing mode and exhausts almost one-half of the $E0$ strength sum rule $\sum_n f_{0n}=1$. One can attempt to compare this state with the observed state at 11.25 Mev.

In order to know the effect of the backward-going graphs on the lowest-lying state, the corresponding 14×14 matrix was diagonalized. The following five energies corresponding to the five energies given in Table II are obtained: $E=48.77$, 24.09, 17.90, 8.50, and 6.61 Mev. We see that, due to the correlations in the ground state, the lowest E is still lowered by about 1 Mev in the direction of a better agreement with the experiment. A similar effect of the backward-going graphs has been noted by Gillet and Vinh Mau[18] for the 1^-, 3^-, and 2^+, $T=0$ states in C^{12} and O^{16}, as calculated with the usual RPA theory.

4. ALIGNED COUPLING SCHEME

In connection with the effect of the energy gap and the pairing force in even nuclei, a schematic extreme coupling scheme has been considered, especially by Mottelson.[19] In this so-called aligned coupling scheme one considers only pairs of single particle states with paired-off projections of the total angular momentum, i.e., pairs $(\nu\bar{m}, \nu-\bar{m})$ of nucleons of identical charge; here $\nu\equiv\{n_\nu l_\nu j_\nu\}$, $\bar{m}$ is the z projection of j_ν. Due to the effect of the energy gap, the lowest possible excitations correspond to lifting such pairs rather than breaking them.

Let us define the pair operators $b_\nu\equiv c_{\nu-\bar{m}}c_{\nu\bar{m}}$, and $b_\mu^\dagger\equiv c_{\mu m}^\dagger c_{\mu-m}^\dagger$. From Eq. (9) we can write the equations of motion for $b_\mu^\dagger b_\nu$ with all the surviving non-self-energy terms:

$$(2E_\mu^0-2E_\nu^0-E)b_\mu^\dagger b_\nu$$
$$=-\tfrac{1}{2}\sum_{\kappa m_\kappa}\{\langle\kappa m_\kappa\kappa-m_\kappa|U|\mu m\mu-m\rangle(1-2n_\mu)b_\kappa^\dagger b_\nu$$
$$+\langle\nu\bar{m}\nu-\bar{m}|U|\kappa m_\kappa\kappa-m_\kappa\rangle(1-2n_\nu)b_\mu^\dagger b_\kappa\}. \quad (18)$$

It is natural to use the following operators:

$$b_J(\nu)\equiv\sum_{\bar{m}}(j_\nu j_\nu;\bar{m}-\bar{m}|J0)b_\nu,$$
$$b_J^\dagger(\mu)\equiv\sum_m(j_\mu j_\mu;m-m|J0)b_\mu,$$
$$\hat{B}_J(\nu\mu)\equiv\sum_{J'J''}(J'J'';00|J0)b_{J'}^\dagger(\mu)b_{J''}(\nu).$$

In the simplified case of no spin-orbit coupling, we have both the projections of the orbital angular momentum and of the spin paired-off in the aligned coupling scheme. If we use the harmonic oscillator wave functions and a spin-independent $V(1,2)$, the system of Eq. (18) reduces to the especially simple form:

$$(2E_\mu^0-2E_\nu^0-E)b_{J'}^\dagger(\mu)b_{J''}(\nu)$$
$$=-\tfrac{1}{2}\sum_\kappa\{\langle\langle\kappa\kappa,J'|V|\mu\mu,J'\rangle\rangle(1-2n_\mu)b_{J'}^\dagger(\kappa)b_{J''}(\nu)$$
$$+\langle\langle\nu\nu,J''|V|\kappa\kappa,J''\rangle\rangle(1-2n_\nu)b_{J'}^\dagger(\mu)b_{J''}(\kappa)\}, \quad (19)$$

where, in the notation of Sec. 2 and of I:

$$\langle\langle\alpha\alpha',\lambda|V|\beta\beta',\lambda\rangle\rangle$$
$$\equiv\sum_{nn'lNL}\langle nl,NL,\lambda|\alpha,\alpha',\lambda\rangle\langle n'l,NL,\lambda|\beta,\beta',\lambda\rangle$$
$$\times\langle nl\|J(r)\|n'l\rangle[w+(-)^l m].$$

In the case of the $J^\pi=0^+$, $T=0$ states in O^{16}, the only non-self-energy coupling term corresponding to $J'=J''=0$ involves $\langle\langle 2s2s,0|V|1d1d,0\rangle\rangle$ which is a small number of the order of 1 Mev or so. Consequently, one cannot expect an explanation of the lowness of the 6.06-Mev state on the basis of this aligned coupling scheme, unless such lowness already results from a self-consistent calculation involving all the self-energy terms.

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APPENDIX. SIMPLIFIED SECOND RANDOM PHASE APPROXIMATION

If we neglect the single particle spin-orbit coupling, and average over the $j=l\pm\frac{1}{2}$ splittings of $\{E_\alpha{}^0\}$, we can conveniently use the L-S coupling scheme. In order to simplify the equations, we confine ourselves to a spin-independent potential $V(1,2)$, i.e., we set $b=h=0$. Furthermore, of all the coupling terms between the $\hat{B}$ operators, we retain only the most important terms corresponding to the first and the fourth double sums $\sum_{\kappa\kappa'}$ in Eq. (9). We also neglect the exchange parts of the V-matrix elements in the coefficients of coupling between the $\hat{A}$ and $\hat{B}$ operators.

With all the above approximations and with the use of the harmonic oscillator wave functions, the equations of the Second RPA for the case $T=0$, $S=0$, and the nuclear spin L, projection M take on the especially simple form:

$$(E_\mu{}^0-E_\nu{}^0-E)\hat{A}_{LM}(\nu\mu)$$
$$=(n_\mu-n_\nu)\sum_{\kappa\neq\kappa'}(-)^{l_\nu+l_{\kappa'}}F_L(\mu\nu,\kappa\kappa')\hat{A}_{LM}(\kappa\kappa')+\tfrac{1}{2}\sum_{\substack{\kappa\kappa' s\\ \text{all different}}}\sum_{L'L''}([L'][L'])^{\frac{1}{2}}W(L'l_\mu L''l_\nu;l_sL)[(-)^{l_\nu+l_{\kappa'}}F_{L''}{}'(s\nu,\kappa\kappa')$$
$$\times\hat{B}_{(L'L'')LM}(s\mu,\kappa\kappa')-(-)^{l_s+l_{\kappa'}}F_{L'}{}'(\mu s,\kappa\kappa')\hat{B}_{(L'L'')LM}(\kappa\kappa',\nu s)], \quad \text{(A1)}$$

$$(\Delta E^0(\mu\mu',\nu\nu')-E)\hat{B}_{(L'L'')LM}(\nu\mu,\nu'\mu')$$
$$=\tfrac{1}{2}([L'][L''])^{\frac{1}{2}}\sum_\kappa\{[n_\nu n_{\nu'}+n_{\mu'}(1-n_\nu-n_{\nu'})](-)^{l_\kappa+l_{\mu'}}W(L'l_\mu L''l_\kappa;l_\nu L)F_{L''}{}'(\nu\kappa,\nu'\mu')\hat{A}_{LM}(\kappa\mu)$$
$$+[n_\nu n_{\nu'}+n_\mu(1-n_\nu-n_{\nu'})](-)^{l_\kappa+l_\mu}(-)^{L'+L''-L}W(L'l_\kappa L''l_{\mu'};l_{\nu'}L)F_{L'}{}'(\nu'\kappa,\nu\mu)\hat{A}_{LM}(\kappa\mu')$$
$$-[n_\mu n_{\mu'}+n_{\nu'}(1-n_\mu-n_{\mu'})]W(L'l_\nu L''l_\kappa;l_\mu L)(-)^{l_\mu+l_{\mu'}}(-)^{L'+L''-L}F_{L'}{}'(\kappa\mu,\nu'\mu')\hat{A}_{LM}(\nu\kappa)$$
$$-[n_\mu n_{\mu'}+n_\nu(1-n_\mu-n_{\mu'})]W(L'l_\kappa L''l_{\nu'};l_{\mu'}L)(-)^{l_\mu+l_{\mu'}}F_{L'}{}'(\kappa\mu',\nu\mu)\hat{A}_{LM}(\nu'\kappa)\}-\sum_{\kappa\neq\kappa'}\{(n_\nu-n_\mu)(-)^{l_\nu-l_{\kappa'}}$$
$$\times F_{L'}(\mu\nu,\kappa\kappa')\hat{B}_{(L'L'')LM}(\kappa\kappa',\nu'\mu')+(n_{\nu'}-n_{\mu'})(-)^{l_{\nu'}-l_{\kappa'}}F_{L''}(\kappa\kappa',\mu'\nu')\hat{B}_{(L'L'')LM}(\nu\mu,\kappa\kappa')\}, \quad \text{(A2)}$$

where

$$F_L(F_L')(\alpha\alpha',\beta\beta')\equiv\sum_{nn'lN\lambda}(-)^\lambda[\lambda]W(l_\alpha l_{\alpha'}l_\beta l_{\beta'};L\lambda)\langle nl,NL,\lambda|\alpha,\beta,\lambda\rangle\langle n'l,NL,\lambda|\alpha',\beta',\lambda\rangle\langle nl\|J(r)\|n'l\rangle U_l(U_l'),$$
$$U_l=4w-m+(-)^l(4m-w),\quad U_l'=4w+(-)^l4m.$$

Here the basic operators are:

$$\hat{A}_{LM}(\alpha\alpha')\equiv\sum_{m_\alpha}(-)^{l_\alpha-m_\alpha}(l_\alpha l_{\alpha'};-m_\alpha m_{\omega'}|LM)$$
$$\times\hat{X}_{\alpha\alpha'}{}^{(S_{\alpha\alpha'}=0,T_{\alpha\alpha'}=0)}, \quad \text{(A3)}$$

$$\hat{X}_{\alpha\alpha'}{}^{(S_{\alpha\alpha'}=0,T_{\alpha\alpha'}=0)}\equiv\tfrac{1}{2}\sum_{\sigma_\alpha\sigma_{\alpha'}}\sum_{\tau_\alpha\tau_{\alpha'}}\delta_{\sigma_{\alpha'}\sigma_\alpha}\delta_{\tau_{\alpha'}\tau_\alpha}\hat{\rho}_{\alpha\alpha'}, \quad \text{(A4)}$$

and

$$\hat{B}_{(L'L'')LM}(\alpha\alpha',\beta\beta')$$
$$\equiv\sum_{M'M''}(L'L'';M'M''|LM)$$
$$\times\hat{A}_{L'M'}(\alpha\alpha')\hat{A}_{L''M''}(\beta\beta'). \quad \text{(A5)}$$

In Eq. (A2), as, previously, in Eq. (9), one must not count the same terms twice for ($\nu'=\nu$, $\mu'=\mu$).

The omitted coupling terms between the $\hat{B}$ operators involve three extra Racah coefficients each, and are generally much smaller. Among these there occur couplings with the $\hat{B}_{(L'''L'''')LM}$-operator with $L'''\neq L'$, $L''''\neq L''$.

With all our approximations, we have avoided the double excitation operators involving pairs with $S_{\alpha\alpha'}=1$ and/or $T_{\alpha\alpha'}=1$, i.e., terms with $\hat{X}_{\alpha\alpha'}{}^{(1,0)}$, $\hat{X}_{\alpha\alpha'}{}^{(0,1)}$, and $\hat{X}_{\alpha\alpha'}{}^{(1,1)}$.

The secular matrix of Eqs. (A1) and (A2) is Hermitian both for the forward-going and backward-going graphs taken separately. We exclude the "mixed" (up-down across the Fermi surface) double excitations.