Equations-of-Motion Method and the Extended Shell Model*

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This paper presents the equations-of-motion method as a useful and flexible tool in the study of nuclear spectroscopy. It is partly a review, but also it introduces a new and much more powerful equations-of-motion technique which supercedes the older linearization methods. The older methods worked with operator equations. To obtain closed expressions they had to be linearized in a rather arbitrary manner. The present approach works with the ground-state expectation of operator equations and thereby avoids all problems of linearization. Thus, like the Green's function method, the equations-of-motion method becomes potentially exact. It has many advantages over Green's function methods, however, among which are its greater compactness, simplicity, and the physical insight it yields.

The method is first applied to rederive the random phase approximation (RPA) and the quasi-particle RPA (QRPA) and to show precisely what terms they neglect. It is demonstrated that some of these terms have coherent phases. A higher RPA and QRPA are then derived to include these terms. The corrections have some interesting effects: notably, there is a reduction of the effective interaction strength and a stabilization of the nucleus against sudden phase transitions. The equations-of-motion method is also used to generalize, in a very simple and natural way, the Hartree–Fock (HF) and Hartree–Bogolyubov (HB) concepts of independent particles and quasi-particles to nonsimple ground states.

The equations-of-motion method is presented as a simple extension of the shell model to the treatment of excitationg of a correlated ground state. By concentrating on the quantities of direct physical interest, the complexity of workins with correlated wavefunctions is avoided.

I. INTRODUCTION

It is generally agreed that the nucleus is a rather complicated system. Nevertheless many very simple nuclear models have been extremely successful. This is not surprising, for even complicated systems have their simpler aspects. But frequently one finds that, while the general features of some data can be understood in simple terms, a more accurate description involves a considerable effort that is not always rewarded by substantially improved results. This does not necessarily mean that the effort is worthless, but it does mean that effort should be conserved by designing the approach to optimize the significant aspects of the problem. This is the philosophy underlying the equations-of-motion approach to nuclear spectroscopy.

As an example of an approach that is not optimized consider the shell-model calculation of the spectrum of a closed-shell nucleus. A first calculation would assume the ground state to be a determinant of independent-particle wave functions and would assume excited states to be particle–hole states. Such calculations, which are also known as Tamm–Dancoff calculations, have been very successful, but they are not sufficient. A notable deficiency is their inability to explain the extraordinary strength of some of the low-lying collective states, which sometimes more than exhausts the closed-shell (nonenergy-weighted) sum rule. To improve the situation, which necessarily involves enhancing the sum rule itself, one may try to compute a better ground state by allowing admixtures of two particle–hole excitations and better excited states also by including more complicated configurations. Unfortunately, the problem escalates so rapidly that it gets out of hand before significant improvement is achieved.

Now if the significant quantities of the problem are excitation energies and ground-state transition strengths, this is not an optimal procedure. These are relative quantities, concerning an energy difference and a transition density; they are not necessarily sensitive to the full complexities of the stationary-state wave functions.

A less oblique approach (in this respect) is the random phase approximation (RPA), which calculates these observable quantities directly, treating the stationary-state wave functions as of secondary importance. The several calculations that have been made with the RPA[1] indicate that, in cases where it is applicable, it gives a much better and more consistent description of nuclear spectra than comparable shell-model calculations. In particular, it satisfies sum rules and separates out spurious excited states (which otherwise are a problem).

But in spite of its successes the RPA is still criticized for its rather shaky foundations. The derivations of the RPA fall essentially into three classes:

(i) the Green's function method[2];
(ii) time-dependent Hartree–Fock (TDHF) theory[3];

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[1] V. Gillet, A. M. Green, and E. A. Sanderson, Nucl. Phys. **88**, 321 (1966); V. Gillet and E. A. Sanderson, *ibid.* **A91**, 292 (1967); see also the review article of A. M. Green, Rept. Progr. Phys. **28**, 113 (1965), for a list of earlier references.

[2] R. A. Ferrell and T. T. Quinn, Phys. Rev. **108**, 570 (1957); D. J. Thouless, Nucl. Phys. **22**, 78 (1961).

[3] R. A. Ferrell, Phys. Rev. **107**, 1631 (1957); J. Goldstone and K. Gottfried, Nuovo Cimento **13**, 849 (1959); D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961); M. Baranger, *1962 Cargèse Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963); D. J. Rowe, Nucl. Phys. **80**, 209 (1966).

(iii) the method of linearized equations of motion[4] (also known as the quasi-boson approximation).

But there are many variations on these methods, many of which are discussed in Lane's book.[5]

The Green's function method is usually considered the most rigorous. The method is to derive an approximate expression for the two-particle Green's function by summing a restricted class of bubble diagrams in a perturbation expansion. The first objection to this method is that it is inconsistent on energetic grounds: whereas the bubble diagrams are summed to all orders (just because they can be summed), other low-order diagrams are neglected. The argument that other diagrams contribute incoherently is not altogether convincing. The second objection is that summing only bubble diagrams violates the Pauli exclusion principle, since the diagrams that would compensate are neglected. Green's function methods are, of course, potentially exact and can correct these defects. The problem is that one is confronted with an infinity of diagrams, but little indication of their relative importance or their physical significance is given.

TDHF theory is physically appealing and is useful in relating the RPA and the phenomenological vibrational models[6]; but, as a derivation of the RPA, it has nothing to add to the linearized equations-of-motion method (to which it is equivalent).[7]

One variation of the method of linearized equations of motion is to approximate particle–hole (or two quasi-particle) pairs as bosons. Such an approximation clearly violates the Pauli principle and, when used to linearize the equations of motion, implies approximations equivalent to the Green's function method. This method has, in some circles, fallen into disrepute because it often tends to be a prescription rather than a derivation. Nevertheless, it is the most flexible method; as such, it has been used in different ways by different authors to extend the RPA to higher order in an attempt to correct its defects. We show in this paper, however, that the equations-of-motion method can also be put in a form which is potentially exact, but which is much simpler than the Green's function method.

Some of the first extensions were made by Sawicki[8] and by Tamura and Udagawa,[9] who generalized the two quasi-particle excitation operators to include four quasi-particles. These extensions are known as second RPA's.[10] They are undoubtedly an improvement on the RPA, but are still subject to the criticism (although to a lesser extent) that they involve a rather arbitrary linearization procedure. A similar (and essentially equivalent) second RPA was also derived by da Providencia,[11] based on an analogous extension of TDHF theory. His treatment has the virtue of establishing a connection with the Brueckner theory of the ground state. Improved linearization methods are also used by Do Dang and Klein[12] and coworkers in an attempt to understand the anharmonicities of vibrational spectra.

Other authors have tackled the problem from the quasi-boson point of view. The simplest method, due to Ikeda *et al.*,[13] was merely to renormalize the quasi-boson operators in a plausible (although rather arbitrary) manner to correct for violation of the Pauli principle. It was found that the interaction strength is effectively reduced in such a way as to increase the excitation energies of low-lying states and thereby stabilize the nucleus against phase transitions. More elaborate and very elegant methods have been developed by Belyaev and Zelevinsky,[14] Marumori and co-workers,[15] and, more recently, by da Providencia.[16] These methods recognize that quasi-particle pairs are not good bosons, but they suppose that *ideal bosons* do exist.[17] Thus a series expansion in *ideal bosons* is attempted, first for the quasi-particle pairs and then for the Hamiltonian itself. In this way one is left with an anharmonic oscillator Hamiltonian and a direct connection with phenomenological treatments. Our only criticism of this approach is that boson methods are only really appropriate for large numbers of particles with an even larger density of states. Without these conditions, which are not well satisfied for nuclei, series expansions in terms of *ideal bosons* tend to be slowly convergent.

The equations-of-motion method described in this paper is a new and a particularly simple one which shows promise of much greater flexibility than previous methods. It differs from the above treatments in certain fundamental respects. The equations of motion are not expressed as operator equations, but rather as the ground-state expectation of operator equations. Thus while the relation to other methods remains apparent, all arbitrariness of linearization procedures is avoided. Similarly, the necessity for ideal bosons is dispelled. The formal equations become exact closed

[4] K. Sawada, Phys. Rev. **106,** 372 (1957); M. Baranger, *ibid.* **120,** 957 (1960); J. Sawicki, Nucl. Phys. **23,** 285 (1961).

[5] A. M. Lane, *Nuclear Theory* (W. A. Benjamin, Inc., New York, 1964).

[6] D. J. Rowe, Nucl. Phys. **85,** 365 (1966).

[7] D. J. Rowe, Nucl. Phys. **80,** 209 (1966).

[8] J. Sawicki, Phys. Rev. **126,** 2231 (1962); see also H. Suhl and N. R. Werthamer, *ibid.* **122,** 359 (1961).

[9] T. Tamura and T. Udagawa, Nucl. Phys. **53,** 33 (1964).

[10] We reserve the term "higher RPA" to describe a higher particle-hole RPA without the inclusion of two particle–hole operators.

[11] J. da Providencia, Nucl. Phys. **61,** 87 (1965).

[12] G. Do Dang and A. Klein, Phys. Rev. **133,** B257 (1964); G. Do Dang *et al.*, Phys. Rev. Letters **17,** 709 (1966); G. Do Dang and A. Klein, Phys. Rev. **156,** 1159 (1967); R. M. Dreizler *et al.*, *ibid.* **156,** 1167 (1967).

[13] K. Ikeda, T. Udagawa, and H. Yamaura, Progr. Theoret. Phys. (Kyoto) **33,** 22 (1965).

[14] S. T. Belyaev and V. G. Zelevinsky, Nucl. Phys. **39,** 582 (1962).

[15] T. Marumori, M. Yamamura, and A. Tokunaga, Progr. Theoret. Phys. (Kyoto) **31,** 1009 (1964); T. Marumori *et al.*, *ibid.* **32,** 726 (1964).

[16] J. da Providencia (preprint).

[17] In some cases the ideal bosons are supposed to exist in another space, but with a one-to-one correspondence to the space of the nucleus.

expressions which do not violate the Pauli principle, which are fully consistent, and which are not subject to the early objections to the RPA. The method may be regarded as a straightforward extension of the shell model to admit the complexities of wave functions but (at the same time) to bypass them by concentrating on the quantities of direct physical interest.

Of course it is not expected that the equations can be solved exactly, but it is clearly an advantage that the formal statement of the method should be exact. Furthermore, the equations have been designed so that good approximations are possible. Generally speaking, the approximations that must be made are those of standard shell-model computations. Firstly, the vector space must be truncated, and, secondly, some assumptions must be made about the ground state. Here the extended shell model is better off than the conventional shell model because it absorbs most of the information needed directly from the Hamiltonian. As a consequence, the results imply a higher order of ground-state correlations than those fed in. This reflects the fact that the equations, according to our philosophy, are as insensitive as possible to the complexities of eigenstate wave functions.

The general equations of motion are derived in Sec. 2. Their formal properties are investigated in Sec. 3. It is found that the properties of the RPA equations, as described by Thouless,[18] are quite general and hold to all orders of approximation. The reader who is familiar with these properties (and is prepared to accept that they do generalize) may therefore omit this formal section. Sections 4–7 are devoted to the particle–hole approximations. The equations are derived in complete generality and solved first in the RPA. This approximation is shown to neglect important coherent contributions, due to violation of the Pauli principle, which are then included in a higher RPA. As a byproduct of deriving the general particle–hole equations, it is also shown, in Sec. 6, how the equations-of-motion method can be applied to generalize the HF definition of single-particle energies and wavefunctions, to non-HF ground states. Section 8 treats the two quasi-particle approximation in a similar manner. A discussion of the approximations is given in Sec. 9, together with some comments on the interpretation of the finite vector-space equations in terms of centroid energies. Concluding remarks are made in Sec. 10.

2. THE EQUATIONS OF MOTION

The equations of motion for a harmonic oscillator Hamtiltonian of frequency ω are

$$[H, O^\dagger]=\omega O^\dagger,$$
$$[H, O]=-\omega O, \tag{1}$$

where we put $\hbar=1$ and where O, $O^\dagger$ are boson operators satisfying the commutation relation

$$[O, O^\dagger]=1. \tag{2}$$

From the solution to these equations a set of eigenfunctions can be constructed, defined by

$$O\,|\,0\rangle=0,$$
$$O^\dagger\,|\,0\rangle=|\,1\rangle,$$
$$O^\dagger\,|\,n\rangle=(n+1)^{1/2}\,|\,n+1\rangle, \tag{3}$$

and with the eigenvalues

$$E_n=(n+\tfrac{1}{2})\omega. \tag{4}$$

It is apparent that the solution to Eqs. (1) and (2) is given, in Hilbert space, by

$$O^\dagger=\sum_{n=0}^{\infty}(n+1)^{1/2}\,|\,n+1\rangle\langle n\,|. \tag{5}$$

Let us now consider whether this approach can be adapted to a more general Hamiltonian, which will eventually be identified with the nuclear Hamiltonian. Suppose that our Hamiltonian is not completely harmonic but has a harmonic spectrum up to the mth level. By this we mean that

$$E_{n+1}-E_n=\omega, \qquad \text{all } n\leq m, \tag{6}$$

where ω is a constant independent of n. We now define the concept of the harmonic space as that region of Hilbert space spanned by the set of eigenvectors $n\leq m$. If the Hamiltonian is not in the least harmonic, then $m=0$ and the harmonic space is the one-dimensional space of the ground state. Certainly this is not much of a space, but it is in fact adequate.

Now if $O^\dagger$ is given the form

$$O^\dagger=\sum_{n=0}^{m}(n+1)^{1/2}\,|\,n+1\rangle\langle n\,|+\sum_{p,q>m}C_{pq}\,|\,p\rangle\langle q\,| \tag{7}$$

for arbitrary C_{pq}, it is apparent that Eqs. (1)–(3) are still satisfied, provided they are allowed to operate only within the harmonic space. In other words, we can write, quite generally,

$$[H, O^\dagger]=\omega O^\dagger+P,$$
$$[H, O]=-\omega O-P^\dagger, \tag{8}$$

and

$$[O, O^\dagger]=1+Q, \tag{9}$$

where

$$P\,|\,n\rangle=P^\dagger\,|\,n\rangle=Q\,|\,n\rangle=Q^\dagger\,|\,n\rangle=0, \qquad \text{all } n\leq m.$$

These equations can be put into a more tractable form. Premultiply the first equation of (8) by an arbitrary operator R and the second by $R^\dagger$; then take the expectation of the first plus the Hermitian conjugate of the second with respect to a wave function $|\,\phi\rangle$. Pro-

[18] D. J. Thouless, Nucl. Phys. **22**, 78 (1961).

vided $|\phi\rangle$ lies within the harmonic space, we obtain

$$\langle\phi|[R,[H,O^\dagger]]|\phi\rangle=\omega\langle\phi|[R,O^\dagger]|\phi\rangle, \quad \text{all } R. \tag{10}$$

Similarly

$$\langle\phi|[R,[H,O]]|\phi\rangle = -\omega\langle\phi|[R,O]|\phi\rangle, \quad \text{all } R. \tag{11}$$

The advantages of using the double commutator in these equations, rather than a simple product, are twofold. Firstly, the two equations are Hermitian conjugates, so that we need only consider one. Thus both $O^\dagger$ and O should emerge as solutions of one equation with energies $\pm\omega$, respectively. Secondly, the commutator of two operators is of lower particle rank than the product, and hence its matrix elements require less knowledge of the wave functions. As we shall see, these features are vital to the success of the method. We also have the pseudo-boson commutator

$$\langle\phi|[O,O^\dagger]|\phi\rangle=1. \tag{12}$$

The usefulness of this approach is that the solutions are independent of $|\phi\rangle$, which can lie anywhere within the harmonic space. Now strictly speaking, the nuclear Hamiltonian is not harmonic at all, which means that $|\phi\rangle$ must be restricted to the ground-state wave function $|0\rangle$. However, by setting up the equations in the general harmonic vector space, we have insured that they are as insensitive to the wave function as possible. Restricting $|\phi\rangle$ to be the ground state also ensures that the matrices that occur are Hermitian. As we show in the following section, many useful properties follow from this Hermiticity—in particular, the orthogonality relation

$$\langle 0|[O_\kappa,O_\lambda^\dagger]|0\rangle=\delta_{\kappa\lambda},$$

for different solutions $O_\kappa^\dagger$ and $O_\lambda^\dagger$. The corresponding equation for arbitrary $|\phi\rangle$ is not necessarily expected, even for a harmonic spectrum.[19]

Now, in general, the ground-state wave function is not too well known *a priori*, although we may have a good zero-order approximation to it in terms of Hartree–Fock theory, for example (or the shell model). We therefore retain the symbol $|\phi\rangle$ to distinguish such approximate ground states from the *exact* ground state, which should be self-consistent according to Eq. (3). To obtain better results it may be worthwhile to iterate the solution of the equations using (3) to define a better approximation $|\phi\rangle$ to $|0\rangle$. Such a procedure would be suggested, for example, if an uncorrelated wave function had been used for $|\phi\rangle$, but the solutions subsequently revealed the presence of large ground-state correlations. Since the equations are not very sensitive to $|\phi\rangle$, we may expect convergence to be rapid, except for certain pathological cases which we discuss later.

Unfortunately, Hermiticity of the equations is not guaranteed for an approximate ground-state wave function $|\phi\rangle$, and this is inconvenient. To regain the Hermitian properties we can generalize (10) to

$$\langle\phi|[R,H,O^\dagger]|\phi\rangle=\omega\langle\phi|[R,O^\dagger]|\phi\rangle, \text{ all } R, \tag{13}$$

where the double commutator $[R,H,O^\dagger]$ is defined

$$2[R,H,O^\dagger]=[R,[H,O^\dagger]]+[[R,H],O^\dagger]. \tag{14}$$

Equation (13) follows exactly from (10) in the limit where $|\phi\rangle$ is an eigenstate[20] when

$$\langle\phi|[H,[R,O^\dagger]]|\phi\rangle=0.$$

Suppose now we wish to find solutions $O_\kappa^\dagger$, ω_κ of (13) within some finite operator space spanned by the set of basis operators $\{\eta_\alpha^\dagger\}$. Since we also want solutions O_κ, $-\omega_\kappa$ to emerge, this set must include all adjoint operators $\eta_{\bar{\alpha}}^\dagger$ where

$$\eta_{\bar{\alpha}}^\dagger\equiv\eta_\alpha.$$

Thus we expand

$$O_\kappa^\dagger=\sum_\alpha X_\alpha(\kappa)\eta_\alpha^\dagger \tag{15}$$

and obtain from (13) the eigenvalue equations

$$\sum_\beta\langle\phi|[\eta_\alpha,H,\eta_\beta^\dagger]|\phi\rangle X_\beta(\kappa) = \omega_\kappa\sum_\beta\langle\phi|[\eta_\alpha,\eta_\beta^\dagger]|\phi\rangle X_\beta(\kappa) \tag{16}$$

or

$$\sum_\beta M_{\alpha\beta}X_\beta(\kappa)=\omega_\kappa\sum_\beta N_{\alpha\beta}X_\beta(\kappa) \tag{17}$$

with obvious notation.

These equations are very similar to the standard eigenstate equations for diagonalization of a Hamiltonian in a finite configuration space. Indeed, if we assume that $|\phi\rangle$ is already the *exact* ground state

$$H|\phi\rangle=E_0|\phi\rangle$$

and set up excited state configurations

$$|\alpha\rangle=\eta_\alpha^\dagger|\phi\rangle, \qquad \eta_\alpha|\phi\rangle=0, \qquad \text{all } \alpha>0,$$

[19] For example, $O_\kappa^\dagger$ and $O_\lambda^\dagger$ might be associated with different harmonics of the same normal mode. Thus, if $O_\kappa^\dagger$ has the form given by (7), then $O_\lambda^\dagger$ might be

$$O_\lambda^\dagger=\sum_{n/2=0}^{(m-1)/2}(\tfrac{1}{2}n+1)^{1/2}|n+2\rangle\langle n|+\sum_{pq>m}C_{pq}|p\rangle\langle q|$$

with frequency $\omega_\lambda=2\omega_\kappa$. Thus, unless $|\phi\rangle$ is an eigenstate, $\langle\phi|[O_\kappa,O_\lambda^\dagger]|\phi\rangle$ is not necessarily equal to $\delta_{\kappa\lambda}$. On truncation of the vector space, (e.g., to the space of single-particle operators). this possibility often disappears.

[20] Like the orthogonality relations, (13) does not necessarily hold exactly throughout the harmonic vector space. But this does not imply any approximation, since we now require $|\phi\rangle$ to be the ground state. It simply means that (13) is not quite as insensitive to $|\phi\rangle$ as we would have wished.

then (16) reduces to the set of equations of half the dimensionality:

$$\sum_{\beta>0}\langle\alpha\,|\,H\,|\,\beta\rangle X_\beta(\kappa)=(E_0+\omega_\kappa)\sum_{\beta>0}\langle\alpha\,|\,\beta\rangle X_\beta(\kappa),$$

all $\alpha>0$.

These are the general Tamm–Dancoff equations. They are inferior to (16) for the following important reason. The Hamiltonian matrix elements are the ground-state expectation of operators $\eta_\alpha H\eta_\beta{}^\dagger$ which are operators of a particle-rank which is two greater than the corresponding operators $[\eta_\alpha, H, \eta_\beta{}^\dagger]$ of the equations-of-motion method. Consequently, the Tamm–Dancoff method relies on considerably more detailed knowledge of the ground state. This results in the fact that, in contrast to Tamm–Dancoff, the equations of motion take ground-state correlations into account to a higher order than those (if any) contained in $|\,\phi\rangle$.

The price paid for this improvement is twofold. Firstly, the equations have double the dimensions and, secondly, the metric matrix $N_{\alpha\beta}$ ceases to be positive definite. Indeed, since the basis operators $\{\eta_\alpha{}^\dagger\}$ will not generally be orthonormal with respect to the correlated ground state, the metric matrix may not even be diagonal. This is not a problem formally (which we will discuss in a separate paper). It does add to the technical difficulties of solving the equations, but it adds little more than the conventional RPA.

3. FORMAL PROPERTIES OF THE EQUATIONS

It is shown in Sec. 5 that a first approximation to the equations of motion is the standard RPA. The formal properties of the RPA equations have been investigated by Thouless.[18] These properties, as we now demonstrate, are completely general.

3.1. Adjoint Pairs

In the exact solution of the formal equations we expect that solutions will appear in adjoint pairs corresponding to excitation creation- and destruction-operators, with energies $\pm\omega$, respectively. Let us examine whether or not this result also follows for an approximate ground-state wave function $|\,\phi\rangle$ and for a finite operator space. If $O_\kappa{}^\dagger$ is given by (15), its adjoint, which we write as

$$O_{\bar\kappa}{}^\dagger\equiv O_\kappa,$$

is given by

$$O_{\bar\kappa}{}^\dagger=\sum_\alpha X_\alpha{}^*(\kappa)\eta_{\bar\alpha}{}^\dagger=\sum_\alpha X_{\bar\alpha}{}^*(\kappa)\eta_\alpha{}^\dagger.$$

Thus we obtain

$$X_\alpha(\bar\kappa)=X_{\bar\alpha}{}^*(\kappa).$$

From the definitions [(16) and (17)] of $M_{\alpha\beta}$ and $N_{\alpha\beta}$, we also get

$$M_{\bar\alpha\bar\beta}=M_{\alpha\beta}{}^*,\qquad N_{\bar\alpha\bar\beta}=-N_{\alpha\beta}{}^*.$$

Taking the complex conjugate of (17), putting bars over the indices, and using the above symmetry relations gives

$$\sum_\beta M_{\alpha\beta}X_\beta(\bar\kappa)=-\omega_\kappa{}^*\sum_\beta N_{\alpha\beta}X_\beta(\bar\kappa).\qquad(18)$$

Thus, for *any* wave function $|\,\phi\rangle$, solutions always appear in adjoint pairs with energies ω_κ and $-\omega_\kappa{}^*$ *unless* ω_κ *vanishes*. If ω_κ vanishes, the corresponding solution (or pair of solutions) may be self-adjoint.

3.2. Stability conditions

Consider a small displacement ϵ of the wave function $|\,\phi\rangle$, given by the unitary transformation

$$|\,\chi\rangle=\exp(\epsilon F)\,|\,\phi\rangle$$

where F is an arbitrary anti-Hermitian operator. The energy expectation

$$\langle\chi\,|\,H\,|\,\chi\rangle=\langle\phi\,|\,H\,|\,\phi\rangle+\epsilon\langle\phi\,|\,[H,F]\,|\,\phi\rangle+\tfrac{1}{2}\epsilon^2\langle\phi\,|\,[F^\dagger,[H,F]]\,|\,\phi\rangle+\cdots$$

can be regarded as a multidimensional energy surface. The linear term in ϵ is its slope and the quadratic term its curvature along some line in this surface specified by the choice of F. If $|\,\phi\rangle$ were the exact ground state, its slope would be zero and its curvature positive in all directions (unless the ground state is degenerate, when it may vanish). For convergence of an iterative calculation of the ground state, as suggested in Sec. 2, it is not essential that the slope be zero for all F; otherwise $|\,\phi\rangle$ would already be an eigenstate. But it should be in the region of positive curvature surrounding the point on the energy surface corresponding to the ground state. We require therefore that $|\,\phi\rangle$ approximate the ground state sufficiently closely that

$$\langle\phi\,|\,[F^\dagger,[H,F]]\,|\,\phi\rangle=\sum_{\alpha\beta}F_\alpha{}^*M_{\alpha\beta}F_\beta\geq 0\qquad(19)$$

for all anti-Hermitian operators F, within the finite operator space considered. We shall refer to this inequality as *the stability condition*, by analogy with the stability condition for the HF state.[18]

Consider an eigenvector $Y(\lambda)$ of the matrix M:

$$\sum_\beta M_{\alpha\beta}Y_\beta(\lambda)=\lambda Y_\alpha(\lambda),\qquad\text{all }\alpha.$$

Since M is Hermitian, its eigenvalues λ are real. From the symmetry of M, there exists another eigenvector degenerate with $Y_\alpha(\lambda)$ given by

$$\sum_\beta M_{\alpha\beta}Y_{\bar\beta}{}^*(\lambda)=\lambda Y_{\bar\alpha}{}^*(\lambda),\qquad\text{all }\alpha.$$

This pair of degenerate eigenvectors can be recombined to form new eigenvectors whose elements are

$$Y_\alpha(\lambda)-Y_{\bar\alpha}{}^*(\lambda)\quad\text{or}\quad i(Y_\alpha(\lambda)+Y_{\bar\alpha}{}^*(\lambda)),$$

which correspond to anti-Hermitian operators and cannot both vanish. Thus, if M has any negative eigenvalue, it is possible to construct an anti-Hermitian operator F violating the stability condition. Therefore the stability condition is that M is positive definite:

$$\sum_{\beta} Y_{\alpha}^{*} M_{\alpha\beta} Y_{\beta} \geq 0 \tag{20}$$

for *all* Y.

Following Thouless,[18] we now show that, provided this stability condition is satisfied, all solutions of Eq. (16) have real energies. Suppose that there exists a solution $X(\kappa)$ with complex energy ω_{κ}. Then

$$\sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) M_{\alpha\beta} X_{\beta}(\kappa) = \omega_{\kappa} \sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) N_{\alpha\beta} X_{\beta}(\kappa). \tag{21}$$

The left-hand side is the expectation of a Hermitian positive-definite matrix, and so it is a real nonnegative number. The coefficient of ω_{κ} on the right-hand side is similarly real, and so, if ω_{κ} is complex, it must vanish. The expectation of a Hermitian matrix can only attain its minimum value for an eigenvector, which implies that $X(\kappa)$ is an eigenvector with eigenvalue zero. If this is so, ω_{κ} is also zero. Thus we conclude that, provided the stability condition is satisfied, ω_{κ} can never be complex.

This proof apparently breaks down if N has a zero eigenvalue. We show elsewhere that this can happen only if the vector space is overcomplete, which is automatically recognized and corrected in the solution of the equations.

3.3. Spurious Solutions

We have shown that complex energies should not occur. What about zero energies? Clearly any operator that commutes with the Hamiltonian will produce a zero-energy solution of Eq. (10). For example, the momentum operator P commutes with the Hamiltonian and hence

$$\langle \phi \mid [R, [H, P]] \mid \phi \rangle = 0, \qquad \text{all } R.$$

Other examples are the angular momentum operator and the number operator. Of course, the solution of Eq. (13) for an approximate ground state $\mid \phi \rangle$ and for a finite vector space only give solutions with energies approximately equal to zero.

These solutions are spurious in the sense that they do not correspond to real excitations of the nucleus. On the contrary, they represent operators which should be diagonal. They do correspond, however, to real degrees of freedom. It is a very satisfactory feature of this kind of approach that spurious excitations associated with these degrees of freedom should separate out and appear, at least formally, with zero energy. At the same time, the mere existence of spurious solutions raises problems of another kind which concern the derivation of the ground state. It is apparent that we should not require the correlated ground state $\mid 0 \rangle$ to be the vacuum of such operators, but rather an eigenstate. If $\mid \phi \rangle$ is not already an eigenfunction, it can be made so by projection. In practice, however, it appears that projection is not such a good idea for the following reason: Nearly all our understanding of nuclear structure is based on the belief that the nucleus, to some extent, resembles a system of independent particles. But if we insist that the nucleus have definite center-of-mass momentum, we apply a constraint on the particle coordinates which destroys all semblance of independent particle motion. The same happens if we demand definite angular momentum for deformed nuclei or definite particle number for superconducting nuclei. Now in the case of translational motion, the nucleus can be localized by the application of a field in the center-of-mass coordinate. Such a field cannot affect the intrinsic structure, since the center of mass and intrinsic motion are completely decoupled. But it regains the possibility of a nondivergent description of the nucleus in terms of an independent particle basis. We believe that something similar can be done for deformed and superconducting nuclei. But here there is an essential difference in that the intrinsic structure of deformed nuclei does depend, to some extent, on the rotational angular momentum, and the structure of superconducting nuclei does depend on the particle number. These problems and the derivation of the correlated ground state will be discussed in more detail elsewhere.

3.4. Orthogonality and Normalization

Consider two solutions $X(\kappa)$ and $X(\lambda)$ of Eq. (16). Since the matrices M and N are Hermitian,

$$\sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) M_{\alpha\beta} X_{\beta}(\lambda) = \omega_{\lambda} \sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) N_{\alpha\beta} X_{\beta}(\lambda),$$

$$= \omega_{\kappa}^{*} \sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) N_{\alpha\beta} X_{\beta}(\lambda).$$

Unless ω_{λ} and ω_{κ}^{*} are equal, therefore, both sides of this equation must vanish. If $\kappa = \lambda$, then, provided the stability condition (20) is satisfied, M is positive definite,

$$\omega_{\kappa} \sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) N_{\alpha\beta} X_{\beta}(\kappa) \geq 0$$

and ω_{κ}, ω_{λ} are real. This suggests orthogonality relations with the normalization

$$\sum_{\alpha\beta} X_{\alpha}^{*}(\kappa) N_{\alpha\beta} X_{\beta}(\lambda) = +\delta_{\kappa\lambda} \qquad \text{if } \omega_{\kappa} > 0,$$

$$= -\delta_{\kappa\lambda} \qquad \text{if } \omega_{\kappa} < 0. \tag{22}$$

Spurious solutions, with $\omega = 0$ and which correspond to Hermitian operators, are self-orthogonal.

For orthogonality of excited-state wave functions we require that

$$\langle\kappa\,|\,\lambda\rangle=\langle 0\,|\,[O_\kappa,\,O_\lambda{}^\dagger]\,|\,0\rangle=\delta_{\kappa\lambda},\qquad \omega_\kappa>0. \quad (23)$$

Equation (22) shows that

$$\langle\phi\,|\,[O_\kappa,\,O_\lambda{}^\dagger]\,|\,\phi\rangle=\delta_{\kappa\lambda},\qquad \omega_\kappa>0, \quad (24)$$

which gives us orthogonality of excited-state wave functions just to the extent that $|\,\phi\,\rangle$ is a good approximation to $|\,0\,\rangle$, in as much as (23) is sensitive to $|\,0\,\rangle$.

Clearly, if we iterate until self-consistency is achieved, i.e., until $|\,\phi\,\rangle$ becomes the vacuum of the O_κ operators, then exact orthogonality of wave functions will be achieved.

3.5. Closure Relations

If there are no spurious solutions, either because the corresponding operators have been removed from the operator space, because the degeneracy of the ground state has been lifted by the addition of a field to the Hamiltonian, or because the equations have been reduced by transformation to an angular momentum representation and we are considering a subspace without spurious solutions, then the usual arguments[18] can be applied to show that the solutions form a complete set.

Any arbitrary vector Y within this vector space can therefore be expanded:

$$Y=\sum_{\kappa>0}[a_\kappa X(\kappa)+a_{\bar\kappa}X(\bar\kappa)],$$

where

$$\begin{aligned}a_\kappa&=\sum_{\alpha\beta}X_\alpha{}^*(\kappa)N_{\alpha\beta}Y_\beta,\\ a_{\bar\kappa}&=-\sum_{\alpha\beta}X_\alpha{}^*(\bar\kappa)N_{\alpha\beta}Y_\beta\\ &=-\sum_{\alpha\beta}X_{\bar\alpha}(\kappa)N_{\alpha\beta}Y_\beta.\end{aligned}$$

Thus we obtain the closure relation

$$\sum_{\kappa>0}\sum_\beta[X_\alpha(\kappa)X_\beta{}^*(\kappa)-X_{\bar\alpha}{}^*(\kappa)X_{\bar\beta}(\kappa)]N_{\beta\gamma}=\delta_{\alpha\gamma}. \quad (25)$$

3.6. Matrix Elements and Sum Rules

The matrix element of some operator W between the ground and an excited state,

$$\langle\kappa\,|\,W\,|\,0\rangle=\langle 0\,|\,[O_\kappa,\,W]\,|\,0\rangle,$$

is given, to whatever approximation one is working, by

$$\begin{aligned}\langle\kappa\,|\,W\,|\,0\rangle&\cong\langle\phi\,|\,[O_\kappa,\,W]\,|\,\phi\rangle\\ &=\sum_{\alpha\beta}X_\alpha{}^*(\kappa)N_{\alpha\beta}W_\beta. \quad (26)\end{aligned}$$

The exact energy-weighted sum rule S_{EW} for a Hermitian operator W is defined by

$$\begin{aligned}S_{EW}&=\sum_\kappa\omega_\kappa\,|\,\langle\kappa\,|\,W\,|\,0\rangle\,|^2\\ &=\tfrac{1}{2}\langle 0\,|\,[W,[H,W]]\,|\,0\rangle. \quad (27)\end{aligned}$$

Now the double commutator in this ground-state matrix element is essentially a constant or a single-body operator for most transition operators W of interest. Consequently its expectation is particularly insensitive to the wave function. This, of course, is the value of the energy-weighted sum rule, as opposed to the nonenergy weighted. One therefore defines an energy-weighted sum by

$$\begin{aligned}S_{EW}&=\tfrac{1}{2}\langle\phi\,|\,[W,[H,W]]\,|\,\phi\rangle\\ &=\tfrac{1}{2}\langle\phi\,|\,[W,H,W]\,|\,\phi\rangle, \quad (28)\end{aligned}$$

which is either equal to S_{EW} or a very good approximation to it.

Consider the situation when W has angular momentum for which there are no spurious solutions. W can then be expanded:

$$W=\sum_{\kappa>0}(a_\kappa O_\kappa{}^\dagger+a_\kappa{}^*O_\kappa),$$

where

$$a_\kappa=\langle\phi\,|\,[O_\kappa,\,W]\,|\,\phi\rangle.$$

Inserting this expansion into (28) and using the orthogonality relations (24) gives

$$\begin{aligned}S_{EW}&=\tfrac{1}{2}\sum_{\kappa,\lambda>0}a_\kappa{}^*a_\lambda\{\omega_\lambda\langle\phi\,|\,[O_\kappa,\,O_\lambda{}^\dagger]\,|\,\phi\rangle\\ &\qquad-\omega_\kappa\langle\phi\,|\,[O_\lambda{}^\dagger,\,O_\kappa]\,|\,\phi\rangle\},\\ &=\sum_{\kappa>0}\omega_\kappa\,|\,a_\kappa\,|^2,\\ &=\sum_{\kappa>0}\omega_\kappa\,|\,\langle\phi\,|\,[O_\kappa,\,W]\,|\,\phi\rangle\,|^2. \quad (29)\end{aligned}$$

Thus the transition strengths of (26) exactly exhaust the energy-weighted sum S_{EW}.

If W has the angular momentum of a spurious state, a sum rule for intrinsic excitations can still be devised by subtracting from W that component which operates on the spurious coordinate. For example, the electric dipole operator

$$D=e\sum_i^{\text{protons}}Z_i$$

can also be written

$$D=\tfrac{1}{2}e\sum_i Z_i-\tfrac{1}{2}e\sum_i\tau_0(i)Z_i,$$

where the sum is now over all nucleons. The first term operates only on the center-of-mass coordinate and can therefore be subtracted to leave an intrinsic dipole operator. The above arguments now apply to show that the solutions of the equations of motion exactly exhaust

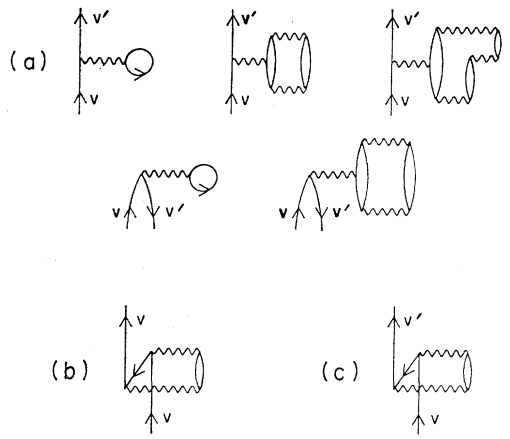

FIG. 1. (a) Some low-order self-energy insertions which are eliminated by the representation and single-particle energies $\mathcal{E}_\nu$ of Eq. (42). (b) Additional self-energies included in the single-particle energies $\mathcal{E}_\nu^{(\pm)}$ of Eq. (43). (c) Off-diagonal self-energy insertions neglected in the definition of $\mathcal{E}_\nu^{(\pm)}$ [Eq. (43)].

the energy-weighted sum rule for this intrinsic dipole operator.

4. PARTICLE–HOLE APPROXIMATION

A first approximation is to restrict the operators $O^\dagger$ to particle–hole form:

$$O^\dagger=\sum_{mi}(Y_{mi}a_m^\dagger a_i-Z_{mi}a_i^\dagger a_m). \tag{30}$$

Here (and throughout this paper) the subscripts m, n, p, and q are reserved for particle states (single-particle states above the Fermi energy) and i, j, k, and l are reserved for hole states (single-particle states below the Fermi energy).[21]

Inserting (30) into (16), we obtain the matrix equation

$$\begin{pmatrix}A & B\\ B^\dagger & A^*\end{pmatrix}\begin{pmatrix}Y\\ Z\end{pmatrix}=\omega\begin{pmatrix}U & 0\\ 0 & -U^*\end{pmatrix}\begin{pmatrix}Y\\ Z\end{pmatrix} \tag{31}$$

for the column vectors (Y_{mi}) and (Z_{mi}), where A and U are Hermitian and B is a symmetric matrix defined by

$$\begin{aligned}A_{minj}&=\langle\phi\mid[a_i^\dagger a_m,\ H,\ a_n^\dagger a_j]\mid\phi\rangle,\\ B_{minj}&=-\langle\phi\mid[a_i^\dagger a_m,\ H,\ a_j^\dagger a_n]\mid\phi\rangle,\\ U_{minj}&=\langle\phi\mid[a_i^\dagger a_m,\ a_n^\dagger a_j]\mid\phi\rangle.\end{aligned} \tag{32}$$

Given a well-behaved Hamiltonian, which we write in the general antisymmetrized form

$$H=\sum_{\nu\nu'}T_{\nu\nu'}a_\nu^\dagger a_{\nu'}+\tfrac{1}{4}\sum_{\mu\nu\mu'\nu'}V_{\mu\nu\mu'\nu'}a_\mu^\dagger a_\nu^\dagger a_{\nu'}a_{\mu'}, \tag{33}$$

and a wave function $\mid\phi\rangle$, the construction and solution of Eq. (31) is straightforward.

For particle–hole operators, the orthogonality relations (22) become

$$\begin{aligned}\sum_{minj}\{Y_{mi}^*(\kappa)U_{minj}Y_{nj}(\lambda)-Z_{mi}^*(\kappa)U_{minj}^*Z_{nj}(\lambda)\}&\\ =+\delta_{\kappa\lambda}\quad&\text{if }\omega_\kappa>0,\\ =-\delta_{\kappa\lambda}\quad&\text{if }\omega_\kappa<0.\end{aligned} \tag{34}$$

The closure relations (25) become

$$\begin{aligned}\sum_{\kappa>0}\sum_{pk}\{Y_{mi}(\kappa)\,Y_{pk}^*(\kappa)-Z_{mi}^*(\kappa)Z_{pk}(\kappa)\}U_{pknj}&=\delta_{mn}\delta_{ij},\\ \sum_{\kappa>0}\sum_{pk}\{Z_{mi}(\kappa)\,Y_{pk}^*(\kappa)-Y_{mi}^*(\kappa)Z_{pk}(\kappa)\}U_{pknj}&=0,\end{aligned} \tag{35}$$

and the transition matrix elements (26) become

$$\begin{aligned}\langle\kappa\mid W\mid 0\rangle=\sum_{minj}\{&Y_{mi}^*(\kappa)U_{minj}W_{nj}\\ &+Z_{mi}^*(\kappa)U_{minj}^*W_{jn}\}.\end{aligned} \tag{36}$$

5. RANDOM PHASE APPROXIMATION

Suppose we choose for $\mid\phi\rangle$ the particle–hole vacuum $\mid\ \rangle$. We find

$$A_{minj}=\delta_{ij}\langle\mid a_m[H,\ a_n^\dagger]\mid\rangle+\delta_{mn}\langle\mid a_i^\dagger[H,\ a_j]\mid\rangle+V_{mjin}.$$

The single-particle representation still remains to be specified. The obvious choice is the one which diagonalizes the single-particle matrix elements:

$$\begin{aligned}\langle\mid a_m[H,\ a_n^\dagger]\mid\rangle&=\delta_{mn}\mathcal{E}_m,\\ \langle\mid a_i^\dagger[H,\ a_j]\mid\rangle&=-\delta_{ij}\mathcal{E}_i.\end{aligned} \tag{37}$$

In fact this is the Hartree–Fock (HF) representation; the $\mathcal{E}_\nu$ are HF single-particle energies, and the particle–hole vacuum $\mid\ \rangle$ is the HF wave function.

In this representation we obtain finally

$$\begin{aligned}A_{minj}&=\delta_{mn}\delta_{ij}(\mathcal{E}_m-\mathcal{E}_i)+V_{mjin},\\ B_{minj}&=V_{mnij},\\ U_{minj}&=\delta_{mn}\delta_{ij},\end{aligned} \tag{38}$$

and (31) becomes the standard RPA equation.

6. GENERAL PARTICLE–HOLE EQUATIONS

It is well known that the RPA is inconsistent from the point of view that the HF wave function is not the vacuum of the RPA excitation operators:

$$O(\kappa)\mid\ \rangle\neq 0.$$

The corresponding statement in Green's function language is that the Pauli exclusion principle is violated. If ground-state correlations are large, this may introduce serious errors. Let us therefore examine the structure of the matrix elements (32) when $\mid\phi\rangle$ is the fully correlated ground state $\mid 0\rangle$.

[21] The term "Fermi energy" is used rather loosely here. It is to be understood as that energy such that, if all particles occupied the lowest-possible single-particle states, all states below the Fermi energy would be occupied and all states above it would be empty. Single-particle states and their energies can be defined in many ways. For the moment, we shall be completely general and delay their definition until the most appropriate definition becomes apparent.

6.1. Complete Equations

We find

$$\left.\begin{aligned} A_{minj} = {} & \langle 0 \mid a_i^\dagger [H, a_j] \mid 0\rangle \delta_{mn} - \langle\!| \{a_i^\dagger, [H, a_j]\} |\!\rangle \langle 0 \mid a_n^\dagger a_m \mid 0\rangle \\ & + \langle 0 \mid a_m [H, a_n^\dagger] \mid 0\rangle \delta_{ij} - \langle\!| \{a_m, [H, a_n^\dagger]\} |\!\rangle \langle 0 \mid a_j a_i^\dagger \mid 0\rangle \end{aligned}\right\} \text{I}$$

$$\left.\begin{aligned} & + V_{mjin} - \sum_\mu V_{\mu jin} \langle 0 \mid a_\mu^\dagger a_m \mid 0\rangle - \sum_\mu V_{m\mu in} \langle 0 \mid a_j a_\mu^\dagger \mid 0\rangle \\ & \quad - \sum_\mu V_{mj\mu n} \langle 0 \mid a_\mu a_i^\dagger \mid 0\rangle - \sum_\mu V_{mji\mu} \langle 0 \mid a_n^\dagger a_\mu \mid 0\rangle \end{aligned}\right\} \text{II} \quad (39)$$

$$\left.\begin{aligned} & + \sum_{\mu\nu} V_{m\mu\nu n} \langle 0 \mid :a_i^\dagger a_\mu^\dagger a_j a_\nu: \mid 0\rangle + \sum_{\mu\nu} V_{\mu ji\nu} \langle 0 \mid :a_n^\dagger a_\mu^\dagger a_m a_\nu: \mid 0\rangle \\ & + \tfrac{1}{2} \sum_{\mu\nu} V_{\mu\nu in} \langle 0 \mid :a_\mu^\dagger a_\nu^\dagger a_m a_j: \mid 0\rangle + \tfrac{1}{2} \sum_{\mu\nu} V_{mj\mu\nu} \langle 0 \mid :a_i^\dagger a_n^\dagger a_\mu a_\nu: \mid 0\rangle \end{aligned}\right\} \text{III}$$

$$\begin{aligned} B_{minj} = {} & \langle\!| \{a_m, [H, a_j^\dagger]\} |\!\rangle \langle 0 \mid a_n a_i^\dagger \mid 0\rangle + \langle\!| \{a_i^\dagger, [H, a_n]\} |\!\rangle \langle 0 \mid a_j^\dagger a_m \mid 0\rangle\} \qquad \text{I} \end{aligned}$$

$$\left.\begin{aligned} & + V_{mnij} - \sum_\mu V_{\mu nij} \langle 0 \mid a_\mu^\dagger a_m \mid 0\rangle - \sum_\mu V_{m\mu ij} \langle 0 \mid a_\mu^\dagger a_n \mid 0\rangle \\ & \quad - \sum_\mu V_{mn\mu j} \langle 0 \mid a_\mu a_i^\dagger \mid 0\rangle - \sum_\mu V_{mni\mu} \langle 0 \mid a_\mu a_j^\dagger \mid 0\rangle \end{aligned}\right\} \text{II} \quad (40)$$

$$\left.\begin{aligned} & + \sum_{\mu\nu} V_{m\mu\nu j} \langle 0 \mid :a_i^\dagger a_\mu^\dagger a_\nu a_n: \mid 0\rangle + \sum_{\mu\nu} V_{\mu ni\nu} \langle 0 \mid :a_j^\dagger a_\mu^\dagger a_\nu a_m: \mid 0\rangle \\ & + \tfrac{1}{2} \sum_{\mu\nu} V_{mn\mu\nu} \langle 0 \mid :a_j^\dagger a_i^\dagger a_\mu a_\nu: \mid 0\rangle + \tfrac{1}{2} \sum_{\mu\nu} V_{\mu\nu ij} \langle 0 \mid :a_\nu^\dagger a_\mu^\dagger a_m a_n: \mid 0\rangle \end{aligned}\right\} \text{III}$$

$$U_{minj} = \delta_{mn} \langle 0 \mid a_i^\dagger a_j \mid 0\rangle - \delta_{ij} \langle 0 \mid a_n^\dagger a_m \mid 0\rangle, \qquad (41)$$

where the operators enclosed by dotted brackets ($: \cdots :$) are to be arranged in normal order with respect to the particle–hole vacuum $\mid\ \rangle$.

6.2. Single-Particle Terms I

The equations look frightful, but are simplified considerably by a suitable choice of single-particle basis. A desirable choice would be one which diagonalizes all the single-particle matrix elements labeled I in (39) and (40), but it is not clear how one would achieve this exactly. A natural basis is one which diagonalizes

$$\begin{aligned} \langle 0 \mid \{a_\nu, [H, a_{\nu'}^\dagger]\} \mid 0\rangle &= \langle 0 \mid \{[a_\nu, H], a_{\nu'}^\dagger\} \mid 0\rangle, \\ &= T_{\nu\nu'} + \sum_{\mu\mu'} V_{\mu\nu\mu'\nu'} \langle 0 \mid a_\mu^\dagger a_{\mu'} \mid 0\rangle \\ &= \mathcal{E}_\nu \delta_{\nu\nu'}. \end{aligned} \qquad (42)$$

This is a generalization of the HF basis in which the self-consistent field is replaced by a single-particle field calculated for the true rather than the HF density. In diagrammatic language these self-energies correspond to the elimination of all self-energy insertions of the type shown in Fig. 1(a).

A very reasonable approximation now is to assume that this representation also diagonalizes all the single-particle matrix elements I.[22] Angular momentum conservation guarantees this, of course, in the majority of cases. Thus we define single-particle energies $\mathcal{E}^{(\pm)}$:

$$\begin{aligned} \langle 0 \mid a_m [H, a_n^\dagger] \mid 0\rangle &\cong \delta_{mn} \langle 0 \mid a_m [H, a_m^\dagger] \mid 0\rangle \\ &\equiv \delta_{mn} \mathcal{E}_m^{(+)} (1 - p_m), \\ \langle 0 \mid a_i^\dagger [H, a_j] \mid 0\rangle &\cong \delta_{ij} \langle 0 \mid a_i^\dagger [H, a_i] \mid 0\rangle \\ &\equiv -\delta_{ij} \mathcal{E}_i^{(-)} (1 - h_i), \end{aligned} \qquad (43)$$

where

$$\begin{aligned} p_m &= \langle 0 \mid a_m^\dagger a_m \mid 0\rangle, \\ h_i &= \langle 0 \mid a_i a_i^\dagger \mid 0\rangle. \end{aligned} \qquad (44)$$

p_m is the number of particles already occupying the particle state m, and h_i is the number of holes occupying the hole state i. These single-particle energies include self-energy diagrams of the type shown in Fig. 1(b), [in addition to those of 1 (a)] but neglect off-diagonal diagrams of type 1 (c).

The remaining single-particle terms are an order of magnitude smaller and can be approximated a little more crudely. Rather than introduce a third single-particle energy we therefore approximate[23]

$$\begin{aligned} \langle\!| \{a_i^\dagger, [H, a_j]\} |\!\rangle &\cong -\delta_{ij} \mathcal{E}_i, \\ \langle\!| \{a_m, [H, a_n^\dagger]\} |\!\rangle &\cong \delta_{mn} \mathcal{E}_m. \end{aligned} \qquad (45)$$

[22] This assumption underlies the whole of the shell model; without its fulfillment to a high degree of accuracy, it would be hard to understand the persistence of shell structure.

[23] It is observed in HF calculations [see K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. **84**, 545 (1966)] that the single-particle energies converge much more rapidly than the self-consistent field. This indicates that the single-particle energies are insensitive to the field. Thus, if the ground state is described at all well by HF theory, the above simplification is hardly an approximation at all.

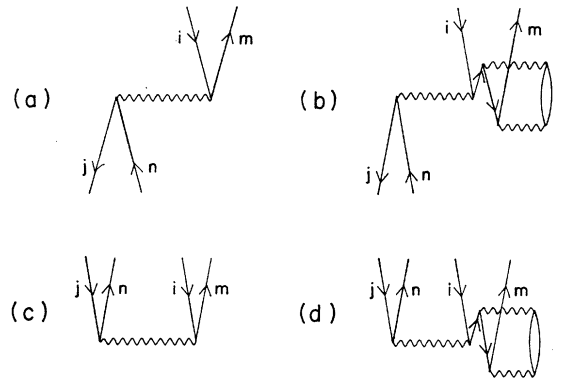

FIG. 2. Some low-order diagrams contributing to the particle-hole interaction terms II of Eqs. (39) and (40): (a) V_{mjin}; (b) Low-order Pauli correction to A_{minj}; (c) V_{mnij}; (d) Low-order Pauli correction to B_{minj}.

The sum of the single-particle terms I of A_{minj} then becomes

$$\delta_{mn}\delta_{ij}[\mathcal{E}_m^{(+)}(1-p_m)-\mathcal{E}_m h_i-\mathcal{E}_i^{(-)}(1-h_i)+\mathcal{E}_i p_m]. \quad (46)$$

The terms I of B_{minj} vanish.

The single-particle energies $\mathcal{E}_\nu$, $\mathcal{E}_m^{(+)}$, and $\mathcal{E}_i^{(-)}$ are experimentally observable quantities: $\mathcal{E}_\nu$ is the centroid for the total strength of the single-particle state ν, as evidenced in stripping and pick-up reactions; $\mathcal{E}_m^{(+)}$ is the centroid of just the stripping strength of the particle state m; $\mathcal{E}_i^{(-)}$ is the centroid of just the pick-up strength of the hole state i.

With these assumptions, the metric matrix (41) becomes

$$U_{minj}=\delta_{mn}\delta_{ij}(1-p_m-h_i). \quad (47)$$

The fact that this matrix becomes diagonal is extremely useful because it can be inverted very easily to convert (31) to standard RPA form.

6.3. Particle–Hole Interaction Terms II and III

Under the above assumptions, the interaction terms II of (39) and (4), which depend only on the single-particle density of the ground state, are given for A_{minj} by

$$V_{mjin}(1-p_m-p_n-h_i-h_j) \quad (48)$$

and for B_{minj} by

$$V_{mnij}(1-p_m-p_n-h_i-h_j). \quad (49)$$

Some of the low-order diagrams contributing to these terms are shown in Fig. 2.

The correlation terms III are not simplified by the choice of particle basis. Some of the lowest-order diagrams, which are summed in these terms, are illustrated in Fig. 3.

Some low-order diagrams which are conspicuously absent are those of the type shown in Fig. 4. These diagrams represent a coupling of a one particle–hole phonon to a two- (or more) phonon state. Such a coupling will cause a splitting of the one-phonon strength, but it cannot shift its centroid energy, which is predicted exactly by the equations-of-motion method (see Sec. 9.2). To account for the energy shift of specific states due to coupling to states outside of the space, one can always renormalize the interaction in the usual manner. A formal statement of how this is achieved for equations of RPA form is given by da Providencia.[11]

7. HIGHER RPA

If we neglect the correlation terms and the difference between $\mathcal{E}_\nu$ and $\mathcal{E}_\nu^{(\pm)}$ in the Pauli correction terms of (46), then the equations simplify considerably. We obtain

$$A_{minj}=\delta_{mn}\delta_{ij}(\mathcal{E}_m^{(+)}-\mathcal{E}_i^{(-)})(1-p_m-h_i) + V_{mjin}(1-p_m-h_i-p_n-h_j),$$

$$B_{minj}=V_{mnij}(1-p_m-h_i-p_n-h_j),$$

$$U_{minj}=\delta_{mn}\delta_{ij}(1-p_m-h_i).$$

Since U is a diagonal matrix, it is readily inverted and (31) can be written

$$\begin{pmatrix} U^{-1/2} & 0 \\ 0 & U^{-1/2} \end{pmatrix}\begin{pmatrix} A & B \\ B^\dagger & A^* \end{pmatrix}\begin{pmatrix} U^{-1/2} & 0 \\ 0 & U^{-1/2} \end{pmatrix}\begin{pmatrix} U^{1/2} & 0 \\ 0 & U^{1/2} \end{pmatrix}\begin{pmatrix} Y \\ Z \end{pmatrix}=\omega\begin{pmatrix} U^{1/2} & 0 \\ 0 & U^{1/2} \end{pmatrix}\begin{pmatrix} Y \\ -Z \end{pmatrix}.$$

In more compact form, this becomes

$$\begin{pmatrix} \mathfrak{A} & \mathfrak{B} \\ \mathfrak{B}^\dagger & \mathfrak{A}^* \end{pmatrix}\begin{pmatrix} \mathcal{Y} \\ \mathcal{Z} \end{pmatrix}=\omega\begin{pmatrix} \mathcal{Y} \\ -\mathcal{Z} \end{pmatrix}, \quad (50)$$

where

$$\mathcal{Y}_{mi}=(1-p_m-h_i)^{1/2}Y_{mi},$$

$$\mathcal{Z}_{mi}=(1-p_m-h_i)^{1/2}Z_{mi},$$

$$\mathfrak{A}_{minj}=\delta_{mn}\delta_{ij}(\mathcal{E}_m^{(+)}-\mathcal{E}_i^{(-)})+(1-p_m-h_i)^{1/2}V_{mjin}(1-p_n-h_j)^{1/2},$$

$$\mathfrak{B}_{minj}=(1-p_m-h_i)^{1/2}V_{mnij}(1-p_n-h_j)^{1/2}, \quad (51)$$

and we have neglected some terms quadratic in the p's and h's.

These equations are of the same form as those of the RPA (38), differing only by a renormalization of the two-body interaction.

Transition matrix elements are given by

$$\langle \kappa \mid W \mid 0 \rangle = \sum_{mi} [W_{mi}(1-p_m-h_i)^{1/2} \mathcal{Y}_{mi}^*(\kappa) + W_{im}(1-p_m-h_i)^{1/2} \mathcal{Z}_{mi}^*(\kappa)], \quad (52)$$

which (again) is the RPA result, but which is now given for a renormalized transition operator.

These results are almost identical to those obtained by an extended linearized equation-of-motion prescription. The small difference may, however, be very important. In this method, the equations of motion

$$[H, a^\dagger a] \sim a^\dagger a + a^\dagger a^\dagger a a$$

are linearized by replacing pairs of particle creation- and destruction-operators by their *correlated ground-state* expectation values.[24] The results differ from ours in that the single-particle energies involved are $\mathcal{E}_\nu$ rather than $\mathcal{E}_\nu^{(\pm)}$, but otherwise they are identical.

The correlation diagrams of Fig. 3 occur first at the same order as the Pauli correction diagrams for the forward-going graphs [Fig. 2(b)] and actually at a lower order for the backward-going graphs [Fig. 2(d)]. Therefore they cannot be neglected on energetic grounds. However, it is supposed that they contribute with random phases and consequently are unimportant. But it is abundantly clear that the Pauli violation corrections, which we now include, do contribute coherently and do effect a reduction of the effective interaction strength.

Whether or not the approximation of random phases for the correlation terms is justified is an important

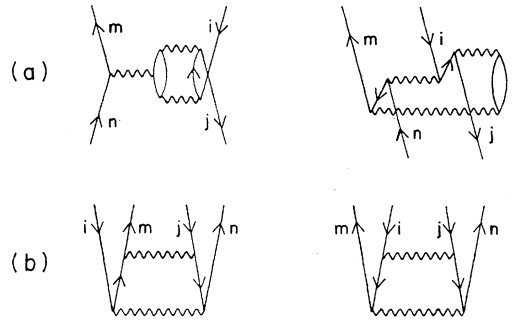

FIG. 3. Some of the lowest-order diagrams contributing to the correlation terms III in Eqs. (39) and (40) of (a) A_{minj} and (b) B_{minj}.

[24] This approach has been used by Ikeda *et al.* (see Ref. 13) in the two quasi-particle approximation for a "pairing $+P_2$" interaction, but the method is general.

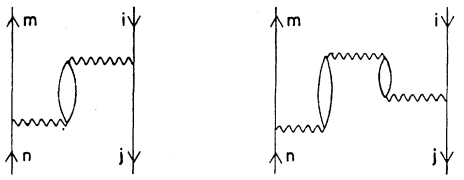

FIG. 4. Some low-order diagrams which do not contribute to the particle–hole equations.

question that should be decided by computation. The important point is that we now have closed expressions which makes their computation feasible. The only remaining problem is how to derive the correlated ground state—or at least its one- and two-particle densities. Suggested methods for doing this will be discussed in a separate paper.

8. TWO QUASI-PARTICLE APPROXIMATION

8.1. General Equations

Whatever wave functions $\mid \phi \rangle$ one uses as an approximation to the ground state, the particle–hole treatment can only make sense if ground-state correlations are not too large. Otherwise the distinction between particle and hole states becomes artificial. In particular, if ground-state correlations are of the superconducting type, the particle–hole vacuum could be almost orthogonal to the correlated ground state. In such a case, a two quasi-particle approximation is more appropriate for the excitation operators:

$$O^\dagger = \sum_{\mu\nu} (Y_{\mu\nu}\alpha_\mu^\dagger \alpha_\nu^\dagger + Z_{\mu\nu}\alpha_\mu \alpha_\nu). \quad (53)$$

The quasi-particles are defined by the Bogolyubov–Valatin transformation

$$\alpha_\nu^\dagger = U_\nu a_\nu^\dagger - V_\nu a_{\bar\nu},$$
$$\alpha_{\bar\nu}^\dagger = U_\nu a_{\bar\nu}^\dagger + V_\nu a_\nu, \quad (54)$$

where U_ν and V_ν are positive real numbers which remain to be defined, but which are subject to the normalization

$$U_\nu^2 + V_\nu^2 = 1. \quad (55)$$

A barred index $\bar\nu$ refers to a single-particle state which is the time-reverse of ν.

Substituting the above expression (53) into the equations of motion (15) and (16), we derive equations identical in form to those of the particle–hole equations (31), but with submatrices:

$$A_{\mu\nu\mu'\nu'} = \langle \phi \mid [\alpha_\nu \alpha_\mu, H, \alpha_{\mu'}^\dagger \alpha_{\nu'}^\dagger] \mid \phi \rangle,$$
$$B_{\mu\nu\mu'\nu'} = \langle \phi \mid [\alpha_\nu \alpha_\mu, H, \alpha_{\mu'} \alpha_{\nu'}] \mid \phi \rangle,$$
$$U_{\mu\nu\mu'\nu'} = \langle \phi \mid [\alpha_\nu \alpha_\mu, \alpha_{\mu'}^\dagger \alpha_{\nu'}^\dagger] \mid \phi \rangle. \quad (56)$$

These may be expanded:

$$A_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})[(1+\hat{p}_{\mu\nu}\hat{p}_{\mu'\nu'})(\langle\phi\mid\alpha_\nu[H,\alpha_{\nu'}{}^\dagger]\mid\phi\rangle\delta_{\mu\mu'}$$
$$-\langle\mid\{\alpha_\nu,[H,\alpha_{\nu'}{}^\dagger]\}\mid\rangle\langle\phi\mid\alpha_{\mu'}{}^\dagger\alpha_\mu\mid\phi\rangle)+\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}$$
$$-\tfrac{1}{2}(1-\hat{p}_{\mu\nu})\langle\phi\mid[\alpha_\mu,\{[H,\alpha_{\mu'}{}^\dagger],\alpha_{\nu'}{}^\dagger\}]\alpha_\nu\mid\phi\rangle$$
$$-\tfrac{1}{2}(1-\hat{p}_{\mu'\nu'})\langle\phi\mid\alpha_{\nu'}{}^\dagger[\alpha_\nu,\{\alpha_\mu,[H,\alpha_{\mu'}{}^\dagger]\}]\mid\phi\rangle$$
$$-(1+\hat{p}_{\mu\nu}\hat{p}_{\mu'\nu'})\langle\phi\mid:\alpha_{\mu'}{}^\dagger\{\alpha_\nu,[H,\alpha_{\nu'}{}^\dagger]\}\alpha_\mu:\mid\phi\rangle],\tag{57}$$

$$B_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})[(1+\hat{p}_{\mu\nu}\hat{p}_{\mu'\nu'})\langle\mid\{\alpha_\mu,[H,\alpha_{\mu'}]\}\mid\rangle\langle\phi\mid\alpha_\nu\alpha_{\nu'}\mid\phi\rangle$$
$$+\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{B})}$$
$$+\tfrac{1}{2}(1-\hat{p}_{\mu\nu})\langle\phi\mid[\alpha_\mu,\{[H,\alpha_{\mu'}],\alpha_{\nu'}\}]\alpha_\nu\mid\phi\rangle$$
$$+\tfrac{1}{2}(1-\hat{p}_{\mu'\nu'})\langle\phi\mid[\alpha_\nu,\{\alpha_\mu,[H,\alpha_{\mu'}]\}]\alpha_{\nu'}\mid\phi\rangle$$
$$+(1+\hat{p}_{\mu\nu}\hat{p}_{\mu'\nu'})\langle\phi\mid:\{\alpha_\mu,[H,\alpha_{\mu'}]\}\alpha_\nu\alpha_{\nu'}:\mid\phi\rangle],\tag{58}$$

$$U_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})[\delta_{\mu\mu'}\delta_{\nu\nu'}-\delta_{\mu\mu'}\langle\phi\mid\alpha_\nu{}^\dagger\alpha_\nu\mid\phi\rangle-\delta_{\nu\nu'}\langle\phi\mid\alpha_{\mu'}{}^\dagger\alpha_\mu\mid\phi\rangle],\tag{59}$$

where $\hat{p}_{\mu\nu}$ is an operator which permutes the indices μ, ν. $\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}$ is defined by

$$\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}=\tfrac{1}{2}\{\alpha_\nu,[\alpha_\mu,\{[H,\alpha_{\mu'}{}^\dagger],\alpha_{\nu'}{}^\dagger\}]\}\tag{60}$$

and is the quasi-particle generalization of a forward-going particle–hole graph [Fig. 2(a)]. $\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{B})}$ is defined by

$$\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{B})}=-\tfrac{1}{2}\{\alpha_\nu,[\alpha_\mu,\{[H,\alpha_{\mu'}],\alpha_{\nu'}\}]\}\tag{61}$$

and is the quasi-particle generalization of a backward-going particle–hole graph [Fig. 2(c)].

8.2. Quasi-Particle Random Phase Approximation (QRPA)

Suppose we choose for $\mid\phi\rangle$ the quasi-particle vacuum $\mid\ \rangle$ given by

$$\mid\ \rangle=\prod_{\nu>0}(U_\nu+V_\nu a_\nu{}^\dagger a_{\bar{\nu}}{}^\dagger)\mid-\rangle,\tag{62}$$

where $\mid-\rangle$ is the bare vacuum. We find that

$$A_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})[(1+\hat{p}_{\mu\nu}\hat{p}_{\mu'\nu'})\langle\mid\alpha_\nu[H,\alpha_{\nu'}{}^\dagger]\mid\rangle\delta_{\mu\mu'}$$
$$+\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}].$$

To evaluate this expression, the particle basis ν and the parameters U_ν, V_ν must be specified. This we do in accord with Hartree–Bogolyubov theory, but we use the equations-of-motion method, which is more in keeping with the present development. The method is simple and has the advantage that it is readily generalized to a correlated ground state. Since this method will be described more fully elsewhere, here we merely note the salient expressions.

The single-particle basis is chosen as the one which diagonalizes[25]

$$\langle\mid\{a_\nu,[H,a_{\nu'}{}^\dagger]\}\mid\rangle=\delta_{\nu\nu'}(\mathcal{E}_\nu-\lambda).\tag{63}$$

[25] Since we are utilizing quasi-particles which do not conserve particle number, it is appropriate to modify the Hamiltonian in the usual manner: $H\to H-\lambda\eta$, where λ is the chemical potential and n is the number operator.

The coefficients U_ν and V_ν are defined by the requirement that

$$\langle\mid\{\alpha_{\bar{\nu}}{}^\dagger,[H,\alpha_{\nu'}{}^\dagger]\}\mid\rangle$$
$$=\delta_{\nu\nu'}[(U_\nu{}^2-V_\nu{}^2)\Delta_\nu-2U_\nu V_\nu(\mathcal{E}_\nu-\lambda)]=0,\tag{64}$$

where Δ_ν is the gap parameter defined by

$$\langle\mid\{a_{\bar{\nu}},[H,a_{\nu'}]\}\mid\rangle=\langle\mid\{a_\nu{}^\dagger,[H,a_{\bar{\nu}'}{}^\dagger]\}\mid\rangle=\delta_{\nu\nu'}\Delta_\nu.\tag{65}$$

Explicitly,

$$\Delta_\nu=\tfrac{1}{2}\sum_\mu V_{\bar{\mu}\mu\bar{\nu}\nu}\langle\mid a_{\bar{\mu}}{}^\dagger a_\mu{}^\dagger\mid\rangle=-\tfrac{1}{2}\sum_\mu V_{\bar{\mu}\mu\bar{\nu}\nu}U_\mu V_\mu.\tag{66}$$

These equations, together with the normalization (55) and the number equation

$$\langle\mid n\mid\rangle=A,\tag{67}$$

define the quasi-particles completely. The quasi-particle energy E_ν, defined by

$$\langle\mid\{\alpha_\nu,[H,\alpha_{\nu'}{}^\dagger]\}\mid\rangle=\delta_{\nu\nu'}\langle\mid\{\alpha_\nu,[H,\alpha_\nu{}^\dagger]\}\mid\rangle=\delta_{\nu\nu'}E_\nu,\tag{68}$$

after some manipulation of the above equations, is given by

$$E_\nu=(U_\nu{}^2-V_\nu{}^2)(\mathcal{E}_\nu-\lambda)+2U_\nu V_\nu\Delta_\nu,$$
$$=\{(\mathcal{E}_\nu-\lambda)^2+\Delta_\nu{}^2\}^{1/2}.\tag{69}$$

With this choice of quasi-particle basis, the submatrices of the QRPA become

$$A_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})[\delta_{\mu\mu'}\delta_{\nu\nu'}(E_\mu+E_\nu)+\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}],$$
$$B_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})\mathcal{U}_{\mu\nu\mu'\nu'}{}^{(\mathrm{B})},$$
$$U_{\mu\nu\mu'\nu'}=(1-\hat{p}_{\mu\nu})\delta_{\mu\mu'}\delta_{\nu\nu'}.\tag{70}$$

8.3. Higher QRPA

The QRPA can be taken to a higher order just as the particle-hole RPA. For $\mid\phi\rangle$ we take a correlated ground-

state wave function $|0\rangle$ containing the vacuum plus admixtures of quasi-particle excitations.[26] Now the equations defining the particle basis and the transformation to quasi-particles generalize to a correlated wave function without any change in form. They become

$$\langle 0 \mid \{a_\nu, [H, a_{\nu'}{}^\dagger]\} \mid 0\rangle = \delta_{\nu\nu'}(\mathcal{E}_\nu - \lambda), \tag{71}$$

$$\langle 0 \mid \{\alpha_\nu{}^\dagger, [H, \alpha_{\bar{\nu}'}{}^\dagger]\} \mid 0\rangle = \delta_{\nu\nu'}[(U_\nu{}^2 - V_\nu{}^2)\Delta_\nu - 2U_\nu V_\nu(\mathcal{E}_\nu - \lambda)] = 0, \tag{72}$$

where

$$\Delta_\nu = \langle 0 \mid \{a_{\bar{\nu}}, [H, a_\nu]\} \mid 0\rangle = \tfrac{1}{2}\sum_\mu V_{\bar{\mu}\mu\bar{\nu}\nu}\langle 0 \mid a_{\bar{\mu}}{}^\dagger a_\mu{}^\dagger \mid 0\rangle. \tag{73}$$

The expression (69) for the quasi-particle energy E_ν, now defined by

$$\langle 0 \mid \{\alpha_\nu, [H, \alpha_{\nu'}{}^\dagger]\} \mid 0\rangle = \delta_{\nu\nu'}E_\nu, \tag{74}$$

remains unchanged.

The quasi-particle energy E_ν becomes the combined centroid for creation and destruction of a quasi-particle. However, in Eqs. (57)–(59), only the centroid energy for creation of a quasi-particle appears. Thus we define

$$\langle 0 \mid \alpha_\nu[H, \alpha_{\nu'}{}^\dagger] \mid 0\rangle \cong \delta_{\nu\nu'}\langle 0 \mid \alpha_\nu[H, \alpha_\nu{}^\dagger] \mid 0\rangle = \delta_{\nu\nu'}E_\nu{}^{(+)}(1 - N_\nu),$$

where N_ν is the number of quasi-particles occupying the state ν in the correlated ground state:

$$N_\nu = \langle 0 \mid \alpha_\nu{}^\dagger\alpha_\nu \mid 0\rangle. \tag{75}$$

It is doubtful whether, in practice, $E_\nu{}^{(+)}$ will differ significantly from E_ν.

If we now make the assumption of random phases for the correlation terms of (57) and (58) and follow exactly the same steps as in the derivation of the higher RPA, we again obtain equations of RPA form with

$$\begin{aligned}
\mathcal{Y}_{\mu\nu} &= (1 - N_\mu - N_\nu)^{1/2}Y_{\mu\nu},\\
\mathcal{Z}_{\mu\nu} &= (1 - N_\mu - N_\nu)^{1/2}Z_{\mu\nu},\\
\mathcal{A}_{\mu\nu\mu'\nu'} &= (1 - \hat{p}_{\mu\nu})[\delta_{\mu\mu'}\delta_{\nu\nu'}(E_\mu{}^{(+)} + E_\nu{}^{(+)}) + (1 - N_\mu - N_\nu)^{1/2}\mathcal{V}_{\mu\nu\mu'\nu'}{}^{(\mathrm{F})}(1 - N_{\mu'} - N_{\nu'})^{1/2}],\\
\mathcal{B}_{\mu\nu\mu'\nu'} &= (1 - \hat{p}_{\mu\nu})(1 - N_\mu - N_\nu)^{1/2}\mathcal{V}_{\mu\nu\mu'\nu'}{}^{(\mathrm{B})} \times (1 - N_{\mu'} - N_{\nu'})^{1/2},\\
\mathcal{U}_{\mu\nu\mu'\nu'} &= (1 - \hat{p}_{\mu\nu})\delta_{\mu\mu'}\delta_{\nu\nu'}.
\end{aligned} \tag{76}$$

[26] In the quasi-particle treatment, we do not suppose $|0\rangle$ to be the exact ground state with definite particle number for the reasons stated in Sec. 3.3. Rather, it is considered a good wave function if its A-particle components approximate the A-particle ground states. As a result, the quasi-particle equations-of-motion yield spectra which are averages over a few nuclei in the neighborhood of the nucleus in question. This is the penalty one must pay for the simplicity of quasi-particle methods.

9. DISCUSSION OF THE APPROXIMATIONS

The approximations that must be made in order to solve the equations of motion are of two types: approximations for the ground-state wave function and approximations of the truncation of the vector space. These we discuss separately.

9.1. Approximations for the Ground State

For the particle–hole (two quasi-particle) equations, the only input data required of the ground state are its one- and two-particle densities. In the RPA (QRPA) these are approximated by HF (HB) values. By extending these approximations to a higher order, we have shown that they neglect important coherent contributions which are particularly associated with corrections to the one-particle densities or diagrams of the types shown in Figs. 1 and 2. The inclusion of these contributions in the higher RPA is manifested in two ways. Firstly, the HF particle–hole energy is replaced by $(\mathcal{E}_m{}^{(+)} - \mathcal{E}_i{}^{(-)})$, which inevitably is larger. This replacement is advantageous because the $\mathcal{E}^{(\pm)}$ (rather than HF energies) are observable centroid energies.[27] Secondly, the effective interaction strength is reduced. Both corrections increase the energy of low-lying excitations for a given Hamiltonian.

Without detailed calculation it is not easy to predict the consequence of including the remaining neglected terms [namely, the correlation terms associated with corrections to the two-particle densities or diagrams of the type shown in Fig. 3]. It is hoped that the corrections will be small due to a random phase cancellation.

9.2. Truncation of the Vector Space

We now assume that the ground-state wave function is exact, and we consider the effect of truncating the vector space. The first observation is that the $O_\kappa{}^\dagger|0\rangle$ cease to be exact eigenstates and the $O_\kappa|0\rangle$ may not completely vanish. We then must consider the significance of the energy ω_κ of the equation

$$\langle 0 \mid [O_\kappa, H, O_\lambda{}^\dagger] \mid 0\rangle = \delta_{\kappa\lambda}\omega_\kappa.$$

Expanding in terms of exact eigenstates $|\alpha\rangle$, we find

$$\omega_\kappa = \sum_\alpha (E_\alpha - E_0)\{|\langle\alpha \mid O_\kappa{}^\dagger \mid 0\rangle|^2 + |\langle\alpha \mid O_\kappa \mid 0\rangle|^2\}. \tag{77}$$

Thus ω_κ is the centroid energy for the $O_\kappa{}^\dagger$, O_κ strength. This is an exact and very significant result, for it tells us just what to expect when the vector space is enlarged. If the original truncation was reasonable, the bulk of the strength would reside in a single eigenstate close in energy to the centroid. As the vector space is enlarged, the strength of the original solution becomes

[27] If, for lack of experimental information, one takes the energies of only the lowest states with single-particle strength rather than the centroid of all such states, then the particle–hole energy is inevitably underestimated.

split among a number of solutions which, in the limit of an infinite space, become the eigenstates. It is apparent therefore that *enlarging the vector space can only lower the energy* of the lower solutions.

Similarly, if we wish to take into account the coupling to vectors outside of the space by the use of an effective interaction, it is clear that, for the lowest states, *all such effective interactions must be attractive.* For example, if the original vector space included only $1\hbar\omega$ particle–hole (two quasi-particle) excitations, then the effective interaction associated with coupling to $3\hbar\omega$ excitations, two-particle–two-hole excitations, etc., (e.g., diagrams of Fig. 4) can only be attractive.

10. CONCLUDING REMARKS

The higher RPA goes a long way towards the inclusion of superconducting effects without giving up number conservation (as does the QRPA). If we assume that HB theory accurately describes single-particle energies

$$\mathcal{E}_m^{(+)}-\lambda=E_m, \qquad \mathcal{E}_i^{(-)}-\lambda=-E_i$$

and single-particle occupancies

$$p_m=V_m^2, \qquad h_i=U_i^2,$$

but that nevertheless the Fermi surface is sufficiently sharp to justify the neglect of quadratic terms in p_m and h_i, then the QRPA and the higher RPA become equivalent. In fact, such a situation is almost certainly nonexistent, for under these circumstances a superconducting solution is unlikely to exist. Nevertheless, it is very satisfactory that the equations continue into the domain of each other in this way.

It is well known that, in standard RPA theory, the excitation energy of the "collective" state falls as the interaction strength is increased; eventually it vanishes and starts to become imaginary. This (as Thouless[18] has shown) indicates the instability of the HF wave function and the occurrence of a phase transition. The calculations of Ikeda *et al.*[13] indicate that, for the higher RPA, this no longer happens. We differ from Ikeda *et al.*, however, in the interpretation of this result. It does not mean that phase transitions cannot occur; that is unrealistic. It means, rather, that phase transitions are not sudden and that the correlated ground state slowly makes the transition, leaving excited states always at positive, real energies. In the difficult region of a phase transition, the particle–hole or two quasi-particle truncation is almost certainly inadequate, but the elimination of imaginary roots is surely an essential feature of any realistic calculation.[28]

In this paper we have tried to indicate some of the usefulness of the equations-of-motion approach. But its potentiality has not yet been fully explored. Because of its simplicity and formal exactness, it has a flexibility which holds considerable promise for its successful application to further problems of nuclear spectroscopy.

[28] *Note added in proof.* Since the completion of this manuscript, the significance of imaginary roots and the meaning of a phase transition have been more fully investigated in terms of general variational equations [D. J. Rowe, Nucl. Phys. (to be published)].