Nuclear Ground-State Correlations and Boson Expansions*

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It is well known that the second-order ground-state correlation energy calculated in the usual random-phase approximation (RPA) is off by a factor of 2. It has also been noted that there is a factor-of-2 discrepancy in the correlation corrections to the Hartree-Fock occupation probabilities. The reason for these phenomena is traced to the treatment of the exchange terms in the interaction matrix element. An illustration based on a simple single multipole interaction shows that the factor of 2 arises from a coherent sum of small higher-order terms. Results based on the consideration of one or a few eigenmodes at a time are seen to be free of this difficulty. The correlation energy, occupation-probability corrections, and equations of motion are reexamined in the Beliaev-Zelevinsky boson expansion, as an illustration of clearly defined higher-order treatments.

I. INTRODUCTION

LET us set ourselves the problem of calculating the ground-state nuclear correlation energy by looking at the zero-point energy obtained in the random-phase approximation (RPA). It has been pointed out[1] that if one proceeds straightforwardly, using the usual antisymmetrized form of the two-body interaction matrix elements, the result is in error by a factor of 2. It has also been noted[2] that the RPA overestimates correlation corrections to the Hartree-Fock occupation probabilities; thus, the 2-particle–2-hole component of the RPA ground state is too large by a factor of 2. These are serious errors in any case. They are especially serious if one believes that the RPA is the lowest order of some expansion, since on the face of it, a factor of 2 does not seem to be the result of higher-order errors. The appearance of the factor of 2 can be traced to the use of the antisymmetrized interaction matrix element, and if a nonantisymmetrized interaction matrix element is used the correlation energy is correct to the extent that exchange effects may be neglected. On the other hand, the effects of antisymmetrized rather than nonantisymmetrized matrix elements make only small differences in the RPA equations of motion. This latter behavior is compatible with the general idea of higher orders causing small errors in the lowest order. It is the purpose of this paper to clear up this apparent paradox.

II. RANDOM-PHASE APPROXIMATION

We begin by reviewing the difficulties we have mentioned. The Hamiltonian is taken[3] to have the general form of a sum of a one-body and a two-body interaction:

$$H=\sum T_{ab}\eta_a^\dagger\eta_b+\tfrac{1}{2}\sum V_{ij,kl}\eta_i^\dagger\eta_j^\dagger\eta_l\eta_k. \quad (2.1)$$

It is presumed that a Hartree-Fock, rather than a Hartree-Fock-Bogoliubov, treatment is a sufficient starting point, although nothing important changes if this complexity is added. It is convenient to explicitly introduce the Hartree-Fock particle-hole notation:

occupied orbitals, α, $\beta\cdots$

$$1,\cdots N \qquad \eta_\alpha=b_\alpha^\dagger, \qquad \eta_\alpha^\dagger=b_\alpha,$$

empty orbitals, m, n $\cdots$

$$N+1,\cdots \qquad \eta_m=a_m, \qquad \eta_m^\dagger=a_m^\dagger.$$

The Hartree-Fock state is denoted by $|0\rangle$, which is the vacuum for both the particle and hole operators: $a_i|0\rangle=b_\alpha|0\rangle=0$. The Hamiltonian then takes the form

$$\begin{aligned}H=E_{\rm HF}&+\sum\epsilon_m a_m^\dagger a_m-\sum\epsilon_\alpha b_\alpha^\dagger b_\alpha\\&+\sum_{\alpha\beta,mn}(V_{\alpha n,m\beta}-V_{\alpha n,\beta m})a_n^\dagger b_\beta^\dagger b_\alpha a_m\\&+\tfrac{1}{2}\sum_{\alpha\beta mn}(V_{mn,\alpha\beta}a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger+V_{\alpha\beta,mn}b_\beta a_n b_\alpha a_m)\\&+(\text{terms with 3-particle–1-hole, 3-hole–1-particle,}\\&\qquad\text{4-particle–4-hole operators}). \quad (2.2)\end{aligned}$$

This can also be written with the two-body interaction matrix elements explicitly antisymmetrized:

$$\begin{aligned}H=E_{\rm HF}&+\sum_m\epsilon_m a_m^\dagger a_m-\sum_\alpha\epsilon_\alpha b_\alpha^\dagger b_\alpha\\&+\sum_{\alpha\beta,mn}(V_{\alpha n,m\beta}-V_{\alpha n,bm})a_n^\dagger b_\beta^\dagger b_\alpha a_m\\&+\tfrac{1}{4}\sum(V_{mn,\alpha\beta}-V_{mn,\beta\alpha})a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger\\&+\tfrac{1}{4}\sum(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})b_\beta a_n b_\alpha a_m+\cdots. \quad (2.3)\end{aligned}$$

It will be sufficient for our purpose to calculate in second-order perturbation theory. The ground-state

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[1] N. Fukuda, F. Iwamoto, and K. Sawada, Phys. Rev. **135**, 705 (1964).
[2] D. J. Rowe, Phys. Rev. **175**, 1283 (1968); R. E. Johnson, R. M. Dreizler, and A. Klein (report of work prior to publication).
[3] Use is made of the notation and forms employed by E. R. Marshalek and J. Weneser, Ann. Phys. (N.Y.) **53**, 569 (1969).

correlation energy is

$$E_{\text{corr}}{}^{(2)}=\sum_I[\langle 0\mid \tfrac{1}{4}\sum(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})b_\alpha b_\beta a_n a_m\mid I\rangle\langle I\mid \tfrac{1}{4}\sum(V_{m'n',\alpha'\beta'}-V_{m'n',\beta'\alpha'})a_m{}^{\dagger\prime}a_n{}^{\dagger\prime}b_\beta{}^{\dagger\prime}b_\alpha{}^{\dagger\prime}\mid 0\rangle/(E_0-E_I)]$$
$$=\tfrac{1}{4}\sum_{\alpha\beta,mn}[(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})(V_{mn,\alpha\beta}-V_{mn,\beta\alpha})/(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n)]$$
$$=\tfrac{1}{2}\sum_{\alpha\beta,mn}[V_{\alpha\beta,mn}V_{mn,\alpha\beta}/(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n)]-\tfrac{1}{2}\sum[V_{\beta\alpha,mn}V_{mn,\alpha\beta}/(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n)]. \quad (2.4)$$

To examine the occupation-number question, we calculate the expectation value of the quantity $(a_p{}^\dagger a_p)$, again using perturbation theory. The second-order value is straightforwardly seen to be

$$\langle a_p{}^\dagger a_p\rangle_{\text{corr}}{}^{(2)}=\langle\psi^{(1)}\mid a_p{}^\dagger a_p\mid\psi^{(1)}\rangle, \quad (2.5)$$

where

$$\psi^{(1)}=\sum_I[1/(E_0-E_I)]\mid I\rangle\times\langle I\mid\sum_{\alpha\beta mn}\tfrac{1}{2}V_{mn,\alpha\beta}a_m{}^\dagger b_\alpha{}^\dagger a_n{}^\dagger b_\beta{}^\dagger\mid 0\rangle. \quad (2.6)$$

Then

$$\langle a_p{}^\dagger a_p\rangle_{\text{corr}}{}^{(2)}=\sum_{\alpha\beta m}\frac{V_{\alpha\beta,mp}(V_{mp,\alpha\beta}-V_{mp,\beta\alpha})}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}. \quad (2.7)$$

We can now compare the "exact" answers with those given by the RPA.

The usual form of the RPA is obtained by going to a boson approximation, in which H is replaced by a boson Hamiltonian according to the prescription

$$H\to H_B,$$
$$a_m{}^\dagger b_\alpha{}^\dagger\to B_{m\alpha}{}^\dagger,\qquad b_\alpha a_m\to B_{m\alpha},$$
$$b_\alpha{}^\dagger b_\beta\to\sum_m B_{m\alpha}{}^\dagger B_{m\beta},$$
$$a_m{}^\dagger a_n\to\sum_\alpha B_{m\alpha}{}^\dagger B_{n\alpha}, \quad (2.8a)$$

or, more precisely,

$$H_B=E_{\text{HF}}+\sum_{mn\alpha\beta}\langle 0\mid[[b_\alpha a_m,H],a_n{}^\dagger b_\beta{}^\dagger]\mid 0\rangle B_{m\alpha}{}^\dagger B_{n\beta}$$
$$+\tfrac{1}{2}\sum_{mn\alpha\beta}\langle 0\mid[b_\beta a_n,[b_\alpha a_m,H]]\mid 0\rangle B_{m\alpha}{}^\dagger B_{n\beta}{}^\dagger$$
$$+\tfrac{1}{2}\sum_{mn\alpha\beta}\langle 0\mid[a_n{}^\dagger b_\beta{}^\dagger,[a_m{}^\dagger b_\alpha{}^\dagger,H]]\mid 0\rangle B_{n\beta}B_{m\alpha}, \quad (2.8b)$$

$$H_B=E_{\text{HF}}+\sum_{m\alpha}(\epsilon_m-\epsilon_\alpha)B_{m\alpha}{}^\dagger B_{m\alpha}$$
$$+\sum_{mn\alpha\beta}(V_{\alpha n,m\beta}-V_{\alpha n,\beta m})B_{n\beta}{}^\dagger B_{m\alpha}$$
$$+\tfrac{1}{2}\sum_{mn\alpha\beta}(V_{mn,\alpha\beta}-V_{mn,\beta\alpha})B_{m\alpha}{}^\dagger B_{n\beta}{}^\dagger$$
$$+\tfrac{1}{2}\sum_{mn\alpha\beta}(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})B_{n\beta}B_{m\alpha}. \quad (2.9)$$

The $B_{m\alpha}$ are understood to obey exact boson commutation rules:

$$[B_{m\alpha},B_{n\beta}{}^\dagger]=\delta_{m,n}\delta_{\alpha,\beta},\qquad \text{all others}=0. \quad (2.10)$$

The Hartree-Fock vacuum state $\mid 0\rangle$ goes into the boson vacuum state $\mid 0\rangle$:

$$B_{m\alpha}\mid 0\rangle=0. \quad (2.11)$$

The RPA just described has the very great advantage that, within the approximation, exact equations of motion are preserved. Thus, from the defining equation for H_B and the analogous one for any one-body operator F,

$$F_B=\langle 0\mid F\mid 0\rangle+\langle 0\mid[b_\alpha a_m,F]\mid 0\rangle B_{m\alpha}{}^\dagger$$
$$+\langle 0\mid[F,b_\alpha{}^\dagger a_m{}^\dagger]\mid 0\rangle B_{m\alpha}, \quad (2.12)$$

it immediately follows that[3]

$$[H_B,F_B]=[H,F]_B. \quad (2.13)$$

In particular, if the Hermitian one-body operator J is a constant of the motion,

$$[H,J]=0, \quad (2.14a)$$

then J_B is also a constant of the motion with respect to H_B,

$$[H_B,J_B]=0. \quad (2.14b)$$

We write out this last in expanded form for future use:

$$\sum_{p\gamma}B_{p\gamma}{}^\dagger\Big((\epsilon_p-\epsilon_\gamma)J_{p\gamma}+\sum_{m\alpha}(V_{p\alpha,\gamma m}-V_{p\alpha,m\gamma})J_{m\alpha}$$
$$-\sum(V_{pm,\gamma\alpha}-V_{pm,\alpha\gamma})J_{\alpha m}\Big)-\text{H.c.}=0. \quad (2.14c)$$

It can be directly verified that the quantity in the bold parenthesis does, in fact, vanish.[4]

We can again calculate the correlation energy in second-order perturbation theory:

$$[E_{\text{corr}}{}^{(2)}]_{\text{RPA}}=\sum_I[\langle 0\mid\tfrac{1}{2}\sum(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})B_{n\beta}B_{m\alpha}\mid I\rangle\langle I\mid\tfrac{1}{2}\sum(V_{mn,\alpha\beta}-V_{mn,\beta\alpha})B_{m\alpha}{}^\dagger B_{n\beta}\mid 0\rangle/(E_0-E_I)]$$
$$=\tfrac{1}{2}\sum_{mn,\alpha\beta}[(V_{\alpha\beta,mn}-V_{\beta\alpha,mn})(V_{mn,\alpha\beta}-V_{mn,\beta\alpha})/(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n)]. \quad (2.15)$$

[4] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).

Comparison of (2.4) and (2.15) present us with the factor-of-2 discrepancy. A similar calculation can be carried through for the occupation probabilities. Again we have to evaluate the expectation of $(a_p^\dagger a_p)$. Following the RPA prescription (2.8),

$$[\langle a_p^\dagger a_p\rangle]_{\mathrm{RPA}}=\langle \sum_\alpha B_{p\alpha}^\dagger B_{p\alpha}\rangle, \tag{2.16}$$

the second-order of perturbation theory leads to

$$[\langle a_p^\dagger a_p\rangle_{\mathrm{corr}}{}^{(2)}]_{\mathrm{RPA}}=\langle\psi_{\mathrm{RPA}}{}^{(1)}\mid \sum_\alpha B_{p\alpha}^\dagger B_{p\alpha}\mid \psi_{\mathrm{RPA}}{}^{(1)}\rangle, \tag{2.17}$$

and

$$\begin{aligned}[\langle a_p^\dagger a_p\rangle_{\mathrm{corr}}{}^{(2)}]_{\mathrm{RPA}}&=\sum_{m,\alpha\beta}\frac{(V_{\alpha\beta,mp}-V_{\alpha\beta,pm})(V_{mp,\alpha\beta}-V_{mp,\beta\alpha})}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}\\&=2\sum_{m,\alpha\beta}\frac{V_{\alpha\beta,mp}(V_{mp,\alpha\beta}-V_{mp,\beta\alpha})}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}.\end{aligned} \tag{2.18}$$

Comparison of result (2.18) with that of (2.7) again demonstrates a factor-of-2 discrepancy.

The paradox is that there is a factor-of-2 discrepancy in the ground-state correlation energy and occupation probabilities, but nothing like this in the equations of motion. The explanation is revealed by taking a very simple interaction as an illustration.

III. CLARIFYING SIMPLE ILLUSTRATION

Let us simplify the two-body interaction by taking a single multipole:

$$\begin{aligned}V_{ab,cd}&=\chi(-1)^{j_b+j_c-m_b-m_c}\\&\quad\times F(j_cj_a;j_dj_b)C(j_cm_c;j_a-m_a\mid JM)\\&\quad\times C(j_dm_d;j_b-m_b\mid J-M),\\F(j_cj_a;j_dj_b)&=F(j_dj_b;j_cj_a)(-1)^{j_a+j_b+j_c+j_d}\\&=F(j_aj_c;j_bj_a)(-1)^{j_a+j_b+j_c+j_d}.\end{aligned} \tag{3.1a}$$

The exchange term $V_{ab,dc}$ has, naturally, an analogous form with a and d coupled to J instead of a and c. We can, of course, rewrite it so that a and c are coupled together:

$$\begin{aligned}V_{ab,dc}&=\chi F(j_aj_a;j_cj_b)(-1)^{j_b+j_c-m_b-m_c}\\&\quad\times\sum_{J'}S_{J'}C(j_cm_c;j_a-m_a\mid J'M')\\&\quad\times C(j_dm_d;j_b-m_b\mid J'-M'),\\S_{J'}&\equiv S_{J'}(j_cj_a;j_dj_b)\\&\equiv(2J+1)\begin{Bmatrix}j_d & j_b & J'\\ j_c & j_a & J\end{Bmatrix}(-)^{j_d+j_c+J+J'}.\end{aligned} \tag{3.1b}$$

The interaction is now spread over many multipoles; if J is small, as in a quadrupole-quadrupole interaction, and j_a, j_b, j_c, j_d are large (say of order j), then each term in the sum (3.1b) is of the order of the direct term (3.1a) multiplied by $S_{J'}$, a small number, of the order $1/(2j+1)^{1/2}$.

This multipole form is introduced most easily into the Hamiltonian if we change the boson notation and use the combinations

$$\begin{aligned}&B(j_mj_\alpha;JM)\\&=\sum_{m_m,m_\alpha}B_{m\alpha}C(j_mm_m;j_\alpha-m_\alpha\mid JM)(-1)^{j_\alpha-m_\alpha},\end{aligned} \tag{3.2a}$$

which also obey boson commutation rules.

$$\begin{aligned}&[B(j_mj_\alpha;JM),B^\dagger(j_nj_\beta,J'M')]\\&\qquad=\delta_{JJ'}\delta_{MM'}\delta_{j_m,j_n}\delta_{j_\alpha j_\beta}[1+\delta_{J,0}].\end{aligned} \tag{3.2b}$$

Then, H_B in Eq. (2.9) becomes

$$\begin{aligned}H_B=E_{\mathrm{HF}}&+\sum_{m\alpha}\sum_{J'M'}(\epsilon_m-\epsilon_\alpha)B^\dagger(j_mj_\alpha;J'M')B(j_mj_\alpha;J'M')+\chi\sum_{mn\alpha\beta M}F(j_\beta j_n;j_mj_\alpha)B^\dagger(j_nj_\beta;JM)B(j_mj_\alpha;JM)\\&-\chi\sum_{J'M'}\sum_{mn\alpha\beta}F(j_\beta j_\alpha;j_mj_n)S_{J'}B^\dagger(j_nj_\beta;J'M')B(j_mj_\alpha;J'M')\\&+\tfrac{1}{2}\chi\sum_{mn\alpha\beta M}F(j_\alpha j_m;j_\beta j_n)(-1)^{j_\beta+j_n}B^\dagger(j_mj_\alpha;JM)B^\dagger(j_nj_\beta;J-M)\\&-\tfrac{1}{2}\chi\sum_{J'M'}\sum_{mn\alpha\beta}F(j_\alpha j_n;j_\beta j_m)S_{J'}(-1)^{j_\beta+j_n}B^\dagger(j_mj_\alpha;J'M')B^\dagger(j_nj_\beta;J'-M')\\&+\tfrac{1}{2}\chi\sum_{mn\alpha\beta M}F(j_mj_\alpha;j_nj_\beta)(-1)^{j_m-j_\alpha}B(j_nj_\beta;J-M)B(j_mj_\alpha;JM)\\&-\tfrac{1}{2}\chi\sum_{J'M'}\sum_{mn\alpha\beta}F(j_mj_\beta;j_nj_\alpha)S_{J'}(-1)^{j_m+j_\alpha}B(j_nj_\beta;J'-M')B(j_mj_\alpha;J'M').\end{aligned} \tag{3.3}$$

The exchange terms appear as small (but many) terms, each with the characteristic $S_{J'}$ factor.

The point is that they are small and of the same order as the higher-order terms of the boson expansion, as we shall illustrate in Sec. IV with a specific expansion formalism—that of Beliaev and Zelevinsky.[5] If one adopts this expansionist view, then, to be consistent, all the exchange terms (those involving $S_{J'}$) must be dropped. What is the effect on the second-order correlation energy of each of the two alternatives: keeping the exchange terms as written or dropping them completely?

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

The second-order correlation energy is easily calculated from (3.3):

$$[E_{\text{corr}}^{(2)}]_{\text{RPA}}=\tfrac{1}{2}\chi^2(2J+1)\sum_{mn,\alpha\beta}\frac{F^2(j_m j_\alpha;j_n j_\beta)}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}+\tfrac{1}{2}\chi^2(2J+1)\sum_{mn\alpha\beta}\frac{F^2(j_m j_\alpha;j_n j_\beta)}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}\sum_{J'}S_{J'}{}^2(j_n j_\alpha;j_m j_\beta)$$

$$-\chi^2(2J+1)\sum_{mn\alpha\beta}\frac{F(j_m j_\alpha;j_n j_\beta)F(j_m j_\beta;j_n j_\alpha)}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}S_J(j_n j_\beta;j_m j_\alpha). \quad (3.4)$$

The origins of the three sets of terms is readily apparent. Dropping the exchange, $S_{J'}$, terms from the Hamiltonian (3.3) would correspondingly drop the second and third terms from the second-order correlation energy (3.4). As has been noted, for large j values the $S_{J'}$ are each small. Therefore, the last set of terms in (3.4) is indeed small. Similarly, the contribution of each J' in the second set is also small, but the sum is not. In fact, from the obvious sum rule

$$\sum_{J'}S_{J'}{}^2(j_n j_\alpha;j_m j_\beta)=1,$$

we see that keeping this set of terms just doubles the contribution of the nonexchange, the first set of terms in (3.4). This is the source of the factor-of-2 difficulty that we are considering, since the exact value of $E_{\text{corr}}^{(2)}$ [Eq. (2.4)] obtained by inserting the chosen interaction (3.1) is

$$E_{\text{corr}}^{(2)}=\tfrac{1}{2}\chi^2(2J+1)\sum_{mn,\alpha\beta}\frac{F^2(j_m j_\alpha;j_n j_\beta)}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}$$

$$-\tfrac{1}{2}\chi^2(2J+1)\sum_{mn\alpha\beta}\frac{F(j_m j_\alpha;j_n j_\beta)F(j_m j_\beta;j_n j_\alpha)}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}\times S_J(j_n j_\beta;j_m j_\alpha). \quad (3.5)$$

Suppose we discarded the exchange ($S_{J'}$) terms in (3.3), as required by consistency. Then the second-order correlation energy would be (3.4) with each $S_{J'}$ put equal to zero. This would have agreed with the exact answer, excepting only the last term in (3.5). That is a truly small exchange term.

The calculation for $[\langle a_p{}^\dagger a_p\rangle_{\text{corr}}{}^{(2)}]_{\text{RPA}}$ goes through similarly. Instead of considering the number of particles with fixed j_p and m_p, it is convenient to consider the number of particles with a given j_p independently of m_p. The occupation number operator for a given j_p is

$$\sum_{m_p}a_p{}^\dagger a_p=\sum_{m_p}\sum_{\alpha}B_{p\alpha}{}^\dagger B_{p\alpha}$$

$$=\sum_{JMj_\alpha}B^\dagger(j_p j_\alpha;JM)B(j_p j_\alpha;JM).$$

One then obtains

$$\sum_{m_p}[\langle a_p{}^\dagger a_p\rangle_{\text{corr}}{}^{(2)}]_{\text{RPA}}$$

$$=\chi^2(2J+1)\sum_{m,\alpha\beta}\frac{F^2(j_m j_\alpha;j_p j_\beta)}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}$$

$$+\chi^2(2J+1)\sum_{m,\alpha\beta}\frac{F^2(j_m j_\alpha;j_p j_\beta)}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}\times\sum_{J'}S_{J'}{}^2(j_p j_\alpha;j_m j_\beta)$$

$$-2\chi^2(2J+1)\sum_{m,\alpha\beta}\frac{F(j_m j_\alpha;j_p j_\beta)F(j_m j_\beta;j_p j_\alpha)}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}\times S_J(j_p j_\beta;j_m j_\alpha). \quad (3.6)$$

The exact answer is

$$\sum_{m_p}\langle a_p{}^\dagger a_p\rangle_{\text{corr}}{}^{(2)}$$

$$=\chi^2(2J+1)\sum_{m,\alpha\beta}\frac{F^2(j_m j_\alpha;j_p j_\beta)}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}$$

$$-\chi^2(2J+1)\sum\frac{F(j_m j_\alpha;j_p j_\beta)F(j_m j_\beta;j_p j_\alpha)}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}\times S_J(j_p j_\beta;j_m j_\alpha). \quad (3.7)$$

The conclusions are just the same as those gathered from the correlation energy; the factor of 2 arises here also from the coherent sum over the small exchange terms.

The factor-of-2 difficulty has been seen, then, to arise from keeping higher-order terms—each small but adding up to an amount just equal to the lowest order. We can now also see why there is no trouble in the equations of motion. These are the equations given by forming the commutator

$$[H_B, B(j_n j_\alpha;\tilde{J}M)] \quad (3.8)$$

for some definite low values of $\tilde{J}M$. Then, *only one* term out of the set of exchange terms is selected with the weighting $S_{\tilde{J}}$. As we have seen, this is of higher order. The point is that there is no coherent sum that transforms higher-order terms into a lower order. Similarly, on diagonalizing the Hamiltonian into the

form

$$H_B=\sum\omega_\mu\theta_\mu^\dagger\theta_\mu+E_{\rm HF}+(E_{\rm corr})_{\rm RPA},$$
$$\theta_\mu=\text{linear combination of } B,\ B^\dagger,$$

each of the eigenenergies ω_μ will have a small higher-order term appended. The only coherent sum of such terms will, however, occur in $(E_{\rm corr})_{\rm RPA}$. There is then no trouble with the use of individual ω_μ, as we can ignore higher-order errors.

In this simple illustration we have used a one-multipole interaction, but clearly the same conclusions would hold if there were a sum of multipoles of low rank or even an infinite sum that did not weight the higher ranks too much.

In summary, we can see that the correct procedure is either to consistently stay in lowest order and discard each of the exchange terms or instead to take the higher orders into account consistently. If in an application only the lowest order is used, it is then necessary to take the discard alternative. Higher orders of the RPA are a controversial subject, but in Sec. IV, for illustrative purposes, we outline how the discussion would go for the Beliaev-Zelevinsky expansion method.[5]

IV. ILLUSTRATION OF HIGHER ORDERS IN THE BELIAEV-ZELEVINSKY EXPANSION

We begin by outlining the steps of the Beliaev-Zelevinsky expansion.[5] The prescription (see Appendix) for the various pairs of operators is

$$a_p^\dagger a_q=\sum_\gamma B_{p\gamma}^\dagger B_{q\gamma},$$
$$b_\alpha^\dagger b_\beta=\sum_p B_{p\alpha}^\dagger B_{p\beta},$$
$$b_\alpha a_m=B_{m\alpha}-\tfrac{1}{2}\sum_{p,\gamma}B_{p\gamma}^\dagger B_{p\alpha}B_{m\gamma}+\cdots. \quad (4.1)$$

It is designed to insure the correctness of the commutation relations between the quadratic pairs $a_p^\dagger a_q$, $b_\alpha a_m$, $b_\alpha^\dagger b_\beta$ up to the order considered. The orders of the expansion are in increasing powers of bosons and, more importantly, in sums over intermediate states; when combined with the interaction matrix elements these extra intermediate-state sums spread a given multipole interaction over a large number of multipoles. As in the discussion of exchange terms in the previous sections, this introduces a smallness parameter $S_J\sim1/(2j+1)^{1/2}$.

Using the expansion prescription for the Hamiltonian, the one-particle terms become

$$\sum_m\epsilon_m a_m^\dagger a_m-\sum_\alpha\epsilon_\alpha b_\alpha^\dagger b_\alpha\rightarrow\sum_{m,\alpha}(\epsilon_m-\epsilon_\alpha)B_{m\alpha}^\dagger B_{m\alpha}^\dagger. \quad (4.2)$$

The potential terms are more complicated. Assuming that in the interaction matrix element $V_{\alpha n,m\beta}$ only α and m are importantly coupled [in the sense of (3.1)] to low rank moments, the expansion of

$$V_{\alpha n,m\beta}a_n^\dagger b_\beta^\dagger b_\alpha a_m \quad (4.3a)$$

is given by

$$V_{\alpha n,m\beta}(a_n^\dagger b_\beta^\dagger)(b_\alpha a_m)$$
$$\rightarrow V_{\alpha n,m\beta}[B_{n\beta}^\dagger-\tfrac{1}{2}\sum B_{p\beta}^\dagger B_{n\gamma}^\dagger B_{p\gamma}+\cdots]$$
$$\times[B_{m\alpha}-\tfrac{1}{2}\sum_{q,\delta}B_{q\delta}^\dagger B_{m\delta}B_{q\alpha}+\cdots]$$
$$=V_{\alpha n,m\beta}[B_{n\beta}^\dagger\,B_{m\alpha}+\text{higher orders}]. \quad (4.3b)$$

The higher orders contain higher powers of the boson operators, but it can be seen that even when rewritten in normal form they do not contribute to the quadratic term. Then,

$$V_{\alpha n,m\beta}a_n^\dagger b_\beta^\dagger b_\alpha a_m\rightarrow V_{\alpha n,m\beta}B_{n\beta}^\dagger\,B_{m\alpha}$$
$$+(\text{higher orders involving higher powers of boson operators written in normal order}). \quad (4.3c)$$

The exchange version of (4.3) is characteristically different:

$$V_{\alpha n,\beta m}a_n^\dagger b_\beta^\dagger b_\alpha a_m=V_{\alpha n,\beta m}(a_n^\dagger a_m)(b_\beta^\dagger b_\alpha)$$
$$\rightarrow V_{\alpha n,\beta m}[(B_{n\gamma}^\dagger B_{m\gamma})+\cdots][(B_{p\beta}^\dagger B_{p\alpha})+\cdots], \quad (4.4a)$$

and, on rewriting in normal order,

$$=V_{\alpha n,\beta m}B_{n\beta}^\dagger B_{m\alpha}+(\text{higher orders involving powers of boson operators written in normal order}). \quad (4.4b)$$

The quadratic term is really a higher-order term as far as smallness is concerned, and should, in principle, be taken together with such higher orders in a calculation of a physical quantity.

The other interaction terms go in the same way. Thus,

$$V_{mn,\alpha\beta}a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger=V_{mn,\alpha\beta}(a_m^\dagger b_\alpha^\dagger)(a_n^\dagger b_\beta^\dagger)$$
$$\rightarrow V_{mn,\alpha\beta}[B_{m\alpha}^\dagger-\tfrac{1}{2}\sum B_{p\alpha}^\dagger B_{m\gamma}^\dagger B_{p\gamma}+\cdots]$$
$$\times[B_{n\beta}^\dagger-\tfrac{1}{2}\sum B_{q\beta}^\dagger B_{n\delta}^\dagger B_{q\delta}+\cdots]. \quad (4.5a)$$

If we keep only the zeroth- and first-order terms, this can be written as

$$V_{mn,\alpha\beta}a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger\rightarrow V_{mn,\alpha\beta}[B_{m\alpha}^\dagger B_{n\beta}^\dagger-\tfrac{1}{2}B_{n\alpha}^\dagger B_{m\beta}^\dagger]$$
$$+(\text{higher orders involving higher powers of boson operators written in normal order.}) \quad (4.5b)$$

Again a quadratic term that is really of first order appears, adding to the zeroth-order quadratic term.

It is worth noting that this Beliaev-Zelevinsky expansion has its drawbacks. In spite of the appearance of expansion in a smallness parameter, there are coherent sums that gravely alter the apparent speed of convergence. Thus if we were to continue the expansion

through just the next order (see Appendix),

$$a_m^\dagger b_\alpha^\dagger = B_{m\alpha}^\dagger - \tfrac{1}{2}\sum_{p\gamma} B_{p\alpha}^\dagger B_{m\gamma}^\dagger B_{p\gamma} - \tfrac{1}{8}\{B_{m\alpha}^\dagger(\sum_{p\gamma} B_{p\gamma}^\dagger B_{p\gamma}) + \sum_{pq\gamma\delta} B_{p\alpha}^\dagger B_{m\gamma}^\dagger B_{q\delta}^\dagger B_{p\delta} B_{q\gamma}\}.$$

The combination $a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger$ can be written, on rearrangement, as

$$a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger = B_{m\alpha}^\dagger B_{n\beta}^\dagger - \tfrac{1}{2}B_{m\beta}^\dagger B_{n\alpha}^\dagger - \tfrac{1}{8}B_{m\alpha}^\dagger B_{n\beta}^\dagger + (\text{higher powers of bosons written in normal order}) = (0\text{th order}) + (1\text{st order}) + (2\text{nd order}).$$

The new quadratic term is only numerically smaller than its predecessers. For certain matrix elements the contribution of these higher-order terms can be important. In using the expansion to obtain the contribution to physically important quantities, orders must be kept together.

Finally, then, the boson Hamiltonian that results from this expansion prescription, keeping to zeroth- and first-order terms, is

$$H_{\text{B-Z}} = E_{\text{HF}} + \sum_{m,\alpha}(\epsilon_m - \epsilon_\alpha) B_{m\alpha}^\dagger B_{m\alpha} + \sum (V_{\alpha n,m\beta} - V_{\alpha n,\beta m}) B_{n\beta}^\dagger B_{m\alpha} + \tfrac{1}{2}\sum (V_{mn,\alpha\beta} - \tfrac{1}{2}V_{mn,\beta\alpha}) B_{m\alpha}^\dagger B_{n\beta}^\dagger + \tfrac{1}{2}\sum (V_{\alpha\beta,mn} - \tfrac{1}{2}V_{\beta\alpha,mn}) B_{n\beta} B_{m\alpha} + (\text{higher powers of boson operators in normal order}). \quad (4.6)$$

This is, of course, very similar to (2.9), but is importantly different in the appearance of the factor $\frac{1}{2}$ in the $B_{m\alpha}^\dagger B_{n\beta}^\dagger$, $B_{n\beta}B_{m\alpha}$ terms.

We can again compute the second-order correlation energy with this new formulation. We collect terms according to the order of expansion.

$$[E_{\text{corr}}^{(2)}]_{\text{B-Z}} = \left\{\tfrac{1}{2}\sum_{\alpha\beta,mn} \frac{V_{\alpha\beta,mn}V_{mn,\alpha\beta}}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}\right\} + \left\{-\tfrac{1}{2}\sum_{\alpha\beta,mn} \frac{V_{\beta\alpha,mn}V_{mn,\alpha\beta}}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}\right\}. \quad (4.7)$$

The first bracket of (4.7) is the zeroth-order term $\frac{1}{2}\sum V_{mn\alpha\beta}B_{m\alpha}^\dagger B_{n\beta}^\dagger$ taken with the other zeroth term $\frac{1}{2}\sum V_{\alpha\beta,mn}B_{n\beta}B_{m\alpha}$. The second bracket is the cross term between the zeroth order, $\frac{1}{2}\sum V_{mn,\alpha\beta}B_{m\alpha}^\dagger B_{n\beta}^\dagger$, and the first order $(-\frac{1}{4})\sum V_{\beta\alpha,mn}B_{n\beta}B_{m\alpha}$ and the cross term between $(-\frac{1}{4})\sum V_{mn,\beta\alpha}B_{m\alpha}^\dagger B_{n\beta}^\dagger$ and $\frac{1}{2}\sum V_{\alpha\beta,mn}B_{n\beta}B_{m\alpha}$. We cannot keep higher terms without involving the nonquadratic boson terms. The expression (4.7) for $(E_{\text{corr}}^{(2)})_{\text{B-Z}}$ is seen to agree with the second form (2.4) of the exact result. The occupation-probability problem can be handled similarly. Keeping zeroth-order and cross terms between zeroth and first order, we have

$$[\langle a_p^\dagger a_p\rangle^{(2)}]_{\text{B-Z}} = \sum_{m\alpha\beta}\frac{V_{\alpha\beta,mp}V_{mp,\alpha\beta}}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2} - \sum \frac{V_{\alpha\beta,mp}(\frac{1}{2}V_{mp,\beta\alpha}) + (\frac{1}{2}V_{\alpha\beta,pm})V_{mp,\alpha\beta}}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2} = \sum_{m\alpha\beta}\frac{V_{\alpha\beta,mp}(V_{mp,\alpha\beta}-V_{mp,\beta\alpha})}{(\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_p)^2}. \quad (4.8)$$

We can also ask about the preservation of the commutation laws expressing the existence of constants of the motion or conservation laws:

$$[H, J] = 0. \quad (4.9)$$

For the one-body operator,

$$J = \sum_{ab} J_{ab}\eta_a^\dagger\eta_b \quad (4.10)$$

$$= \sum J_{\alpha\alpha} + \sum_{m\alpha}(J_{m\alpha}a_m^\dagger b_\alpha^\dagger + J_{\alpha m}b_\alpha a_m) + \sum_{mn} J_{mn}a_m^\dagger a_n - \sum_{\alpha\beta} J_{\alpha\beta}b_\beta^\dagger b_\alpha, \quad (4.11)$$

and the Beliaev-Zelevinsky boson expansion in zeroth and first order can be seen from the above rules to be

$$J = \sum J_{\alpha\alpha} + \sum_{m\alpha} J_{m\alpha}\{B_{m\alpha}^\dagger - \tfrac{1}{2}\sum_{q\gamma} B_{m\gamma}^\dagger B_{q\alpha}^\dagger B_{q\gamma} + \cdots\} + \sum_{m\alpha} J_{\alpha m}\{B_{m\alpha} - \tfrac{1}{2}\sum_{q\gamma} B_{q\gamma}^\dagger B_{q\alpha} B_{m\gamma} + \cdots\} + \sum_{mn} J_{mn}\sum_a B_{m\alpha}^\dagger B_{n\alpha} - \sum_{\alpha\beta} J_{\alpha\beta}\sum_m B_{m\beta}^\dagger B_{m\alpha} + \cdots. \quad (4.12)$$

The relation $[H, J]=0$ must clearly hold since the boson expansion is fixed to maintain the commutation rules. It is, however, interesting to work out the *one-boson* part of this to see how it comes out. We therefore write out $\langle 0 \mid B_{p\gamma}[H, J] \mid 0\rangle$:

$$\langle 0 \mid B_{p\gamma}[H, J] \mid 0\rangle = (\epsilon_p - \epsilon_\gamma)J_{p\gamma} + \sum_{m\alpha}(V_{p\alpha,\gamma m} - V_{p\alpha,m\gamma})J_{m\alpha} - \sum_{m\alpha} V_{pm,\gamma\alpha}J_{\alpha m} + \tfrac{1}{2}\sum_{m\alpha} V_{pm,\alpha\gamma}J_{\alpha m} + \tfrac{1}{2}\sum_{m\alpha} V_{mp,\gamma\alpha}J_{\alpha m}. \quad (4.13)$$

We have already seen in Eq. (2.14c) that this is zero. The origin of the last two terms is especially interesting since it is characteristic of the difference between the usual RPA form and the Beliaev-Zelevinsky expansion. The last term comes from the first-order term in J with the zeroth-order term in H, the next-to-last term comes from the zeroth order in J, the first order in H. They contribute equally, and combine to give just the exchange term obtained in (2.14c), but not in quite the same way.

If one would try to diagonalize the *two-boson* part of H_{B-Z}, $H_{B-Z}(2)$, [as given by Eq. (4.6)] one would arrive at equations of the RPA type which, however, have some undesirable aspects. For instance, in this version of the RPA, the spurious states do not come at zero energy. Further, although a sum of rule of the form

$$\sum_{\mu=\text{one-boson states}} \omega_\mu(0 \mid D \mid \mu)(\mu \mid D \mid 0) = \tfrac{1}{2}\langle 0 \mid [D,[H_{B-Z}(2), D]] \mid 0\rangle \quad (4.14)$$

still holds, it does so only if it is understood that D is linear in the boson operators, not a one-body operator. The difference comes about because of the first-order three-boson parts of the expansion of a one-body operator. However, in practice, transition operators and generators of symmetry operations are one-body operators, so the above sum rule is not useful as it stands. Fortunately, a canonical transformation can put things in better form, removing these undesirable aspects of the new version of the RPA.

We will comment first on the problem of translation and Galilean invariance. For the total momentum P and for the c.m. coordinate X we have the following expansions:

$$\begin{aligned} P &= P^{(0)}+P^{(1/2)}+P^{(1)}, \\ X &= X^{(0)}+X^{(1/2)}+X^{(1)}, \\ P^{(0)} &= \sum_{m\alpha}(P_{m\alpha}B_{m\alpha}^{\dagger}+P_{\alpha m}B_{\alpha m}), \\ P^{(1/2)} &= \sum_{mn\alpha} P_{mn}B_{m\alpha}^{\dagger}B_{n\alpha} - \sum_{\alpha\beta m} P_{\alpha\beta}B_{m\beta}^{\dagger}B_{m\alpha}, \\ P^{(1)} &= -\tfrac{1}{2}\sum_{m\alpha n\beta}(P_{m\alpha}B_{m\beta}^{\dagger}B_{n\alpha}^{\dagger}B_{n\beta}+P_{\alpha m}B_{n\beta}^{\dagger}B_{n\alpha}B_{m\beta}), \end{aligned} \quad (4.15)$$

with similar expressions for $X^{(0)}$, $X^{(1/2)}$, and $X^{(1)}$. We have assumed that $\sum_\alpha P_{\alpha\alpha}=0$. It is an important property of the Beliaev-Zelevinsky expansion that the commutation rule

$$[P, X] = -\mathrm{i} \quad (4.16)$$

implies the following set of commutation relations:

$$\begin{aligned} &[P^{(0)}, X^{(0)}] = -i, \\ &[P^{(0)}, X^{(1/2)}]+[P^{(1/2)}, X^{(0)}] = 0, \\ &[P^{(0)}, X^{(1)}]+[P^{(1)}, X^{(0)}]+[P^{(1/2)}, X^{(1/2)}] = 0. \end{aligned} \quad (4.17)$$

These relations are enough to insure the existence of a canonical transformation $\exp iS = \exp i(S^{(1/2)}+S^{(1)}+\cdots)$, which removes from P and X the terms containing more than one boson, so that the transforms of P and X are pure bosons. We will have

$$\begin{aligned} \tilde{P} &= e^{iS}Pe^{-iS} = P^{(0)}, \\ \tilde{X} &= e^{iS}Pe^{-iS} = X^{(0)}, \end{aligned} \quad (4.18)$$

provided the operators $S^{(1/2)}$ and $S^{(1)}$ are solutions of the following equations:

$$\begin{aligned} &i[S^{(1/2)}, X^{(0)}]+X^{(1/2)} = 0, \\ &i[S^{(1/2)}, P^{(0)}]+P^{(1/2)} = 0, \\ &i[S^{(1)}, X^{(0)}]+X^{(1)}+i[S^{(1/2)}, X^{(1/2)}] - \tfrac{1}{2}[S^{(1/2)}, [S^{(1/2)}, X^{(0)}]] = 0, \\ &i[S^{(1)}, P^{(0)}]+P^{(1)}+i[S^{(1/2)}, P^{(1/2)}] - \tfrac{1}{2}[S^{(1/2)}, [S^{(1/2)}, P^{(0)}]] = 0. \end{aligned} \quad (4.19)$$

Now, from the translation and Galilean invariance properties of the *whole* H_{B-Z}, we have

$$[H_{B-Z}, P] = 0, \quad (4.20a)$$

$$[H_{B-Z}, X] = -iP/M. \quad (4.20b)$$

Since our boson expansion preserves the commutation relations of fermion pairs to the desired order, these equations will follow from the symmetries of the original Hamiltonian. As far as one-boson components are concerned, these equations may be connected with the usual RPA results by techniques similar to those leading to Eq. (4.13), where the first-order term in H_{B-Z} and the first-order term in J combine to produce the final result.

The canonical transformation simplifies these results. From Eqs. (4.20a) and (4.20b), it follows then for the transform $\tilde{H}_{B-Z} = (\exp iS) H_{B-Z} \exp(-iS)$,

$$[\tilde{H}_{B-Z}, P^{(0)}] = 0, \quad (4.21a)$$

$$[\tilde{H}_{B-Z}, X^{(0)}] = -iP^{(0)}/M. \quad (4.21b)$$

In particular, these equations hold for just the two-boson part of $\tilde{H}_{B-Z}$. This can be seen by considering the one-boson part of (4.21) and noting that since $P^{(0)}$, $X^{(0)}$ are one-boson operators, only the two-boson part of $\tilde{H}_{B-Z}$ contributes. In other words, the two-boson part of $\tilde{H}_{B-Z}$, $\tilde{H}_{B-Z}(2)$, is itself translation- and Galilean-invariant, and its use leads to the correct mass. The canonical transformation $\exp iS$ actually transforms the original expansion into a new expansion, leading to a harmonic Hamiltonian with some of the properties of the RPA Hamiltonian (spurious states at zero energy, correct mass, etc.). From the present discussion it becomes clear that Eq. (4.14) may also hold for a one-body operator D provided it commutes with P and X, because then it is possible to transform D into a pure boson.

Let us now consider the RPA Hamiltonian H_B [see Eq. (2.9)]. We can easily derive

$$[H_B, P^{(0)}] = 0, \quad (4.22a)$$

$$[H_B, X^{(0)}] = -iP^{(0)}/M. \quad (4.22b)$$

Here, Eq. (4.22a) is for translations the analog of Eq. (2.14b) for rotations. (Note that $P^{(0)}=P_B$, $X^{(0)}=X_B$.) The connection with the expansion method is straightforward–analogous to Eq. (4.13). First we work with

the untransformed expansion of H_{B-Z}. Since P, X are one-body operators, the contribution of the cross term between the first order in P, X, zeroth order in H_{B-Z} is just equal to the cross term between zeroth order in P, X, first order in H_{B-Z}, and the sum can be seen to be equal to the exchange term from H_B. Thus, both the usual RPA and the expansion give the correct mass. Next consider the transformed equations involving $\tilde{H}_{B-Z}$, (4.21). From the similarity between Eqs. (4.21) and (4.22) we may ask if the two-boson part of $\tilde{H}_{B-Z}$, $\tilde{H}_{B-Z}(2)$, is not identical with H_B. The answer is that it is not. The difference between $\tilde{H}_{B-Z}(2)$ and H_B commutes with $X^{(0)}$ and $P^{(0)}$, but it does not commute with most bosons. In general, the eigenmodes of H_B differ from the the eigenmodes of $\tilde{H}_{B-Z}(2)$ by higher-order contributions.

We have seen that both the usual RPA and the expansion method give the same, correct mass. What of the moment of inertia? The Thouless-Valatin[4,6] value follows from equations very similar to (4.22):

$$\begin{aligned}&[H_B, J_B]=0,\\ &[H_B, \Phi_B]=-iJ_B/\mathcal{I},\\ &[J_B, \Phi_B]=-i.\end{aligned} \tag{4.23}$$

However, we cannot proceed with J, Φ as we did with P, X, since we do not know about the higher orders of Φ and so cannot assume that Φ is a one-body operator. Then, we are not guaranteed, as we were for the mass equation, that the exchange terms from H_B and from the expansion methods are exactly equal. Therefore, the moment of inertia deduced from $\tilde{H}_{B-Z}(2)$ can differ by high-order terms from the moment of inertia as given by the Thouless-Valatin formula.

V. SUMMARY

We have thus exposed the relation between the usual RPA and the expansion-based procedures. The relation is very close and, except for some unfortunate coherences, gives much the same results. In general, the differences amount to adding a higher-order quantity to a lower-order result. This holds if we work with one eigenmode at a time or, equivalently, with low-lying excitations. It unfortunately breaks down in the ground-state correlation energy because of the coherent addition over the zero-point energies of all the eigenmodes. There is a similar coherent sum in the correlation effects on the occupation probabilities. The discussion above indicates how, in a given calculation, one can tell whether such a coherence occurs and what to do about it.

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APPENDIX

In this Appendix, we wish to explicitly derive the expression for the second-order term in the Beliaev-Zelevinsky expansion.[5] First of all, we remark that commutation relations of the kind

$$[a_m^\dagger a_n, a_p^\dagger a_q]=a_m^\dagger a_q\delta_{np}-a_p^\dagger a_n\delta_{mq} \tag{A1}$$

are preserved to all orders by the prescription of Eq. (2.5),

$$\begin{aligned}b_\alpha^\dagger b_\beta&=\sum_m B_{m\alpha}^\dagger B_{m\beta},\\ a_m^\dagger a_n&=\sum_\alpha B_{m\alpha}^\dagger B_{n\alpha}.\end{aligned} \tag{A2}$$

It is therefore enough to include higher-order terms in the expansion for $b_\alpha a_m$; we then write

$$b_\alpha a_m=B_{m\alpha}-\tfrac{1}{2}\sum_{\gamma p} B_{p\gamma}^\dagger B_{p\alpha}B_{m\gamma}-\chi_{m\alpha}, \tag{A3}$$

where $\chi_{m\alpha}$ is to be regarded as a second-order quantity. For the commutation relation

$$[b_\alpha a_m, a_n^\dagger b_\beta^\dagger]=\delta_{\alpha\beta}\delta_{mn}-a_n^\dagger a_m\delta_{\alpha\beta}-b_\beta^\dagger b_\alpha\delta_{mn} \tag{A4}$$

to be satisfied up to second order, the quantities $\chi_{m\alpha}$ must be such that

$$\begin{aligned}&[\chi_{m\alpha}, B_{n\beta}^\dagger]+[B_{m\alpha}, \chi_{n\beta}^\dagger]\\ &\quad=-\tfrac{1}{4}[\sum_{\gamma p} B_{p\gamma}^\dagger B_{p\alpha}B_{m\gamma}, \sum_{q\delta} B_{q\beta}^\dagger B_{n\delta}^\dagger B_{q\delta}].\end{aligned} \tag{A5}$$

When we compute the commutator in the right-hand side of Eq. (A5), we find

$$\begin{aligned}&[\sum B_{p\gamma}^\dagger B_{p\alpha}B_{m\gamma}, \sum B_{q\beta}^\dagger B_{n\delta}^\dagger B_{q\delta}]\\ &\quad=\sum B_{p\beta}^\dagger B_{p\alpha}B_{n\delta}^\dagger B_{m\delta}+\delta_{\alpha\beta}\sum B_{p\gamma}^\dagger B_{n\delta}^\dagger B_{p\delta}B_{m\gamma}\\ &\qquad+\delta_{mn}\sum B_{p\gamma}^\dagger B_{p\alpha}B_{q\beta}^\dagger B_{q\gamma}\\ &\quad=B_{n\beta}^\dagger B_{m\alpha}+\delta_{mn}\delta_{\alpha\beta}\sum B_{p\gamma}^\dagger B_{p\gamma}\\ &\qquad+\delta_{\alpha\beta}\sum B_{p\gamma}^\dagger B_{n\delta}^\dagger B_{p\delta}B_{m\gamma}+\delta_{mn}\sum B_{p\gamma}^\dagger B_{q\beta}^\dagger B_{p\alpha}B_{q\gamma}\\ &\qquad+\sum B_{p\beta}^\dagger B_{n\gamma}^\dagger B_{p\alpha}B_{m\gamma},\end{aligned}$$

i.e., the commutator contains terms which, effectively, are of lower order. However, these terms obviously have their origin in coherent sums of many high-order terms, and, for consistency, should be regarded of high order. Equation (A5) is easily solved for χ, and one finally obtains

$$\begin{aligned}b_\alpha a_m&=B_{m\alpha}-\tfrac{1}{2}\sum_{p\gamma} B_{p\gamma}^\dagger B_{p\beta}B_{m\gamma}\\ &\quad-\tfrac{1}{8}\{\sum_{p\gamma} B_{p\gamma}^\dagger B_{p\gamma}B_{m\alpha}+\sum_{p\gamma q\delta} B_{q\gamma}^\dagger B_{p\delta}^\dagger B_{p\alpha}B_{m\gamma}B_{q\delta}\}.\end{aligned} \tag{A6}$$

It appears that this expansion converges very poorly. It may be, however, that the expansion will converge better for physically interesting quantities. We give here an example of how this may happen. To order ν in the expansion we may write

$$a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger=x_\nu B_{m\alpha}^\dagger B_{n\beta}^\dagger-y_\nu B_{m\beta}^\dagger B_{n\alpha}^\dagger$$
$$+(\text{higher powers of boson operators in normal order}).$$

We have already obtained the following values: $x_0=1$, $y_0=0$; $x_1=1$, $y_1=\frac{1}{2}$; $x_2=\frac{7}{8}$, $y_2=\frac{1}{2}$. We will now show that

$$\lim_{\nu=\infty} x_\nu = \lim_{\nu=\infty} y_\nu = 1/(2)^{1/2},$$

which indicates a poor convergence.

To prove this, we note that the products

$$\langle 0 \mid (b_\beta a_n)(b_\alpha a_m)(a_m^\dagger b_\alpha^\dagger)(a_n^\dagger b_\beta^\dagger) \mid 0\rangle = 1$$

and

$$\langle 0 \mid (b_\beta a_m)(b_\alpha a_n)(a_m^\dagger b_\alpha^\dagger)(a_n^\dagger b_\beta^\dagger) \mid 0\rangle = -1$$

may be calculated with the help of the commutation relations for the particle-hole operators. However, those scalar products may also be calculated by making use of the expansions for $(a_m^\dagger b_\alpha^\dagger)(a_n^\dagger b_\beta^\dagger)$ and $(a_m^\dagger b_\beta^\dagger)(a_n^\dagger b_\alpha^\dagger)$. One then finds

$$x_\infty^2 + y_\infty^2 = 1,$$
$$2x_\infty y_\infty = 1,$$

so that

$$x_\infty = y_\infty = 1/(2)^{1/2}.$$

As an example of the speed of convergence for a physically interesting quantity, we consider the second-order energy. Disregarding consistency, we obtain

$$E_\nu^{(2)} = \tfrac{1}{2}(x_\nu^2+y_\nu^2) \sum_{\alpha\beta mn} \frac{V_{\alpha\beta,mn}V_{mn,\alpha\beta}}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n} - \tfrac{1}{2}(2x_\nu y_\nu) \sum_{\alpha\beta mn} \frac{V_{\alpha\beta,mn}V_{mn,\beta\alpha}}{\epsilon_\alpha+\epsilon_\beta-\epsilon_m-\epsilon_n}$$

and it happens that even for $\nu=2$ both $(x_\nu^2+y_\nu^2)$ and $2x_\nu y_\nu$ are already quite near 1, although the equality is only attained for $\nu=\infty$. We remark finally that the relation

$$a_m^\dagger b_\alpha^\dagger a_n^\dagger b_\beta^\dagger \mid 0\rangle = [1/(2)^{1/2}](B_{m\alpha}^\dagger B_{n\beta}^\dagger - B_{m\beta}^\dagger B_{n\alpha}^\dagger) \mid 0\rangle,$$

arising in an infinite order Beliaev-Zelevinsky expansion, is contained in Marumori's prescription[7] for mapping a many-fermion Hilbert space into a many-boson Hilbert space.

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Excitation of $T=1$ Particle-Hole States in C^{12} by Inelastic Electron Scattering*

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The $T=1$ single-particle-hole states of C^{12} are considered on the basis of the harmonic-oscillator shell model in the particle-hole formalism developed by Lewis and Walecka. Configuration mixing is included via a Serber-Yukawa residual interaction. Resulting mixed states lying close in energy are grouped together into complexes whose inelastic-electron-scattering form factors are then compared with recent experimental data. This comparison is done mainly at large momentum transfers and large scattering angles, where the transverse excitations (and consequently the $T=1$ states) dominate, and where the excitation spectrum contains only a few strongly excited features (to be related here to collective single-particle-hole states). By working at high momentum transfer, the contributions from transitions of high multipolarity can be strongly enhanced. Here all possible $T=1$ single-particle-hole states of all allowed angular momenta are considered in a basis including single-particle states up to the $2s$-$1d$ shell. A simple square-well shell model is used to account for the quasielastic cross section in the giant-resonance region. All of the gross features of the experimental excitation spectrum for excitation energies between 14 and 30 MeV can be accounted for on the basis of this simple model.

I. INTRODUCTION

INELASTIC electron scattering provides a powerful means for obtaining information about the charge and current distributions of nuclei. For an excitation at a given energy loss, data taken as a function of three-momentum transfer, in principle, provide the Fourier transforms of the charge and current distributions, i.e., provide the inelastic form factors. In practice, some model for the nucleus is generally used to provide the nuclear four-current and the resulting model form factors are compared with experiment.[1,2] By working at large electron scattering angles, where the strongly angle-dependent $\tan^2(\frac{1}{2}\theta)$ factor in the cross section becomes large, states excited by transverse multipoles can be enhanced over longitudinal excitations. The transition operators for electron scattering contain isoscalar and isovector terms and consequently allow only states of $T=0$ and $T=1$, respectively, to be

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