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Methods for Calculating Ground-State Correlations of Vibrational Nuclei

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A general method for studying ground-state correlations is described. It is shown that the usual random-phase approximation overestimates depletion of the uncorrelated state by a factor of 2, in agreement with a result found by Rowe, using the number-operator method. The correctness of the latter method is then independently verified. A precise division of the ground-state correlations into collective and noncollective parts is shown for a simple model, but it is argued that the division is not valid in general.

I. INTRODUCTION

In a recent paper, Rowe[1] has examined a number of approximation methods in the theory of vibrational nuclei for their predictions of ground-state correlations; in particular, he has studied single-particle occupation probabilities and ground-state energies. The former is of special importance in efforts to improve the description of excited states in the random-phase approximation (RPA). In this context, several of the most favored proposals were tested on a simplified model in a succeeding paper by Parikh and Rowe.[2]

In the present paper, we restrict our discussion to the occupation probabilities or equivalent quantities, supplementing the above-mentioned paper on three counts:

(i) We point out the existence in the literature of a completely general intermediate-coupling method for computing ground-state correlations, namely, the self-consistent core-particle coupling method (CPC).[3,4] In Sec. II, we show that in the weak-coupling limit it agrees with the result found by Rowe by a number-operator method and therefore disagrees with the conventional RPA result, which overcounts by a factor of 2.

(ii) A sharpened derivation of the number-operator method is given, completely equivalent, however, to that developed in Ref. 1.

(iii) Rowe has suggested—in a puzzling remark—that the usual RPA formula for ground-state correlations may be approximately correct if one takes into account only the most collective states of the RPA. Though we remain skeptical about the general validity of this suggestion, we show in Sec. IV that it is correct for the model discussed in Ref. 2.

II. INTERMEDIATE-COUPLING METHOD FOR GROUND-STATE CORRELATIONS

We limit our considerations to variations about a Hartree-Fock (HF) limit. Let i refer to orbitals occupied in the HF state, m to those unoccupied. We seek the occupation probabilities

$$n(i)=\langle 0\,|\,\mathcal{A}_i^\dagger\mathcal{A}_i\,|\,0\rangle=1-\langle 0\,|\,\mathcal{A}_i\mathcal{A}_i^\dagger\,|\,0\rangle$$
$$=1+\delta n(i), \quad (1)$$

$$n(m)=\langle 0\,|\,\mathcal{A}_m^\dagger\mathcal{A}_m\,|\,0\rangle=\delta n(m). \quad (2)$$

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[1] D. J. Rowe, Phys. Rev. **175**, 1283 (1968).
[2] J. C. Parikh and D. J Rowe, Phys. Rev. **175**, 1293 (1968).
[3] A. K. Kerman and A. Klein, Phys. Rev. **132**, 1326 (1963).
[4] G. Do Dang, G. J. Dreiss, R. M. Dreizler, A. Klein, and Chi Shiang Wu, Nucl. Phys. **A114**, 481 (1968).

From number conservation, we have for the correlations

$$\sum_i \delta n(i) + \sum_m \delta n(m) = 0. \tag{3}$$

In the general intermediate-coupling method,[3,4] we construct a complete theory of the quantities

$$\langle Jh \mid \mathcal{A}_\alpha \mid I \rangle = \psi_{Jh}(\alpha I), \tag{4}$$

$$\langle I \mid \mathcal{A}_\alpha \mid Jp \rangle = \Phi_{Jp}(\alpha I), \tag{5}$$

where α is an arbitrary orbital, the $\mid I \rangle$ are the various states of the even core, and $\mid Jh \rangle$ and $\mid Jp \rangle$ are states of the lighter and heavier neighbors, respectively. We have, e.g.,

$$n(i) = \sum_{Jh} \langle 0 \mid \mathcal{A}_i^\dagger \mid Jh \rangle \langle Jh \mid \mathcal{A}_i \mid 0 \rangle = \sum_{Jh} \mid \psi_{Jh}(i0) \mid^2, \tag{6}$$

and, similarly,

$$1 - n(m) = \sum_{Jp} \mid \Phi_{Jp}(m0) \mid^2. \tag{7}$$

Since the amplitudes in (6) and (7) are constructed so as to satisfy the Pauli principle, the generality of these formulas can be averred. We simply allude to several instances of application of the general method.[5,6]

Further discussion is confined to the weak-coupling limit, which is the domain of the RPA. In this limit the states $\mid Jh \rangle$ are pictured as vibration-hole coupled states, the $\mid Jp \rangle$ as vibration-particle states. The quasiboson operators which create the RPA states $\mid J \rangle$ are written

$$B_J^\dagger = \sum_{mi} [Y_{mi}(J) \mathcal{A}_m^\dagger \mathcal{A}_i - Z_{mi}^*(J) \mathcal{A}_i^\dagger \mathcal{A}_m], \tag{8}$$

$$B_J \mid 0 \rangle = 0, \tag{9}$$

and

$$\sum_{mi} [\mid Y_{mi}(J) \mid^2 - \mid Z_{mi}(J) \mid^2] = 1. \tag{10}$$

The Y are the particle-hole amplitudes and the Z are the ground-state correlation amplitudes. The discussion which follows is valid only if the first sum in (10) dominates, so that one is not too near a nuclear "phase transition."

We evaluate the quantity $\delta n(i) = -\langle 0 \mid \mathcal{A}_i \mathcal{A}_i^\dagger \mid 0 \rangle$ in two ways by expanding in two different intermediate sets of states. First we consider the uncoupled particle-hole basis, and in particular the $2p$-$1h$ subspace

$$\mid mm'i' \rangle = \mathcal{A}_m^\dagger \mathcal{A}_{m'}^\dagger \mathcal{A}_{i'} \mid \mathrm{HF} \rangle. \tag{11}$$

[5] G. Do Dang, R. M. Dreizler, A. Klein, and C. S. Wu, Phys. Rev. **172**, 1022 (1968).

[6] G. J. Dreiss, Ph.D. thesis, University of Pennsylvania, 1968 (unpublished).

This contributes

$$\begin{aligned}
\delta n(i) &= -\tfrac{1}{2} \sum_{mm'i'} \langle 0 \mid \mathcal{A}_i \mathcal{A}_m^\dagger \mathcal{A}_{m'}^\dagger \mathcal{A}_{i'} \mid \mathrm{HF} \rangle \times \langle \mathrm{HF} \mid \mathcal{A}_{i'}^\dagger \mathcal{A}_{m'} \mathcal{A}_m \mathcal{A}_i^\dagger \mid 0 \rangle \\
&= -\tfrac{1}{2} \sum_{mm'i'} \sum_{JJ'} \langle 0 \mid \mathcal{A}_m^\dagger \mathcal{A}_i \mid J \rangle \langle J \mid \mathcal{A}_{m'}^\dagger \mathcal{A}_{i'} \mid \mathrm{HF} \rangle \times \langle \mathrm{HF} \mid \mathcal{A}_{i'}^\dagger \mathcal{A}_{m'} \mid J' \rangle \langle J' \mid \mathcal{A}_i^\dagger \mathcal{A}_m \mid 0 \rangle \\
&= -\tfrac{1}{2} \sum_{mm'i'} \sum_{JJ'} Z_{mi}(J') Z_{mi}^*(J) \times \langle J \mid \mathcal{A}_{m'}^\dagger \mathcal{A}_{i'} \mid \mathrm{HF} \rangle \langle \mathrm{HF} \mid \mathcal{A}_{i'}^\dagger \mathcal{A}_{m'} \mid J' \rangle.
\end{aligned} \tag{12}$$

The factor $\frac{1}{2}$ occurs because we sum without restriction on m, m'. Since this quantity is already $O(Z^2)$, we may introduce an approximation in the remaining matrix element, e.g., replacing $\mid \mathrm{HF} \rangle$ by $\mid 0 \rangle$. We then have

$$\sum_{m'i'} \langle J \mid \mathcal{A}_{m'}^\dagger \mathcal{A}_{i'} \mid 0 \rangle \langle 0 \mid \mathcal{A}_{i'}^\dagger \mathcal{A}_{m'} \mid J' \rangle = \sum_{m'i'} Y_{m'i'}^*(J) Y_{m'i'}(J') \cong \delta_{JJ'}, \tag{13}$$

and thus

$$\delta n(i) = -\tfrac{1}{2} \sum_{mJ} \mid Z_{mi}(J) \mid^2, \tag{14}$$

which agrees with the result given by the number-operator method, and perhaps indicates more clearly the origin of the factor of $\frac{1}{2}$ compared to a more naively computed RPA result.

Alternatively, we can (more quickly) reach result (14) if we replace the set (11) by the set

$$\mid mJ \rangle = \mathcal{A}_m^\dagger B_J^\dagger \mid 0 \rangle, \tag{15}$$

but, in obvious analogy with (12), include a factor $\frac{1}{2}$ when we sum over m and J. Thus

$$\delta n(i) = -\tfrac{1}{2} \sum_{mJ} \langle 0 \mid \mathcal{A}_m^\dagger \mathcal{A}_i B_J^\dagger \mid 0 \rangle \langle 0 \mid B_J \mathcal{A}_i^\dagger \mathcal{A}_m \mid 0 \rangle = -\tfrac{1}{2} \sum_{mJ} \mid Z_{mi}(J) \mid^2, \tag{16}$$

with the help of (9) and (10). In the present instance, the factor $\frac{1}{2}$ is no longer exact, but has the same standing as approximation (13).

In considering the application of (14) or (16), of course some RPA states are more collective than others. But as long as the series in $\sum \mid Z \mid^2$, of which these expressions are the first terms, converges, there is no basis for making a decisive distinction, in the application of these formulas, between more collective and less collective states. Some further remarks on this point will be found in Sec. IV.

It is rather more cumbersome in the present instance to derive (14) directly from (6); it can be done, but we shall omit the demonstration. Instead, we shall reconsider the number-operator method.

III. NUMBER-OPERATOR METHOD

We consider briefly a derivation of the number-operator method, equivalent to that given by Rowe, but differently phrased and ordered so as to bring into as sharp focus as possible the essential elements. We need one tool and one assumption. The former is the statement of number conservation in the form

$$\sum_p \langle A \mid \alpha_p{}^\dagger \alpha_p \mid B\rangle - \sum_i \langle A \mid \alpha_i \alpha_i{}^\dagger \mid B\rangle = \nu\langle A \mid B\rangle, \quad (17)$$

where $|A\rangle$ and $|B\rangle$ are any states of $N+\nu$ particles and $N=\sum_i$. The assumption is that the ground state is restricted to a linear combination of the HF state and of $2p$-$2h$ states. Thus we have

$$\langle 0 \mid \alpha_{i_1}\alpha_{i_2}\alpha_{i_3}\alpha_{i''}{}^\dagger \alpha_{i'}{}^\dagger \alpha_i{}^\dagger \mid 0\rangle = 0, \quad (18)$$

and similar statements.

Using (17) and (18), we derive the identity

$$\sum_{ii'} \langle 0 \mid \alpha_{p_1}{}^\dagger \alpha_{p_2}{}^\dagger \alpha_i \alpha_{i'} \alpha_{i'}{}^\dagger \alpha_i{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle$$
$$= \sum_i \langle 0 \mid \alpha_{p_1}{}^\dagger \alpha_{p_2}{}^\dagger \alpha_i \alpha_i{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle$$
$$= 2\langle 0 \mid \alpha_{p_1}{}^\dagger \alpha_{p_2}{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle. \quad (19)$$

Equation (19) is but a single example of numerous identities using the exact relation (17) and the approximate set of relations (18) by means of which all nonvanishing ground-state correlations can be expressed linearly in terms of the convenient sets

$$\langle 0 \mid \alpha_{p_1}{}^\dagger \alpha_{p_2}{}^\dagger \alpha_{i_1} \alpha_{i_2} \alpha_{i'}{}^\dagger \alpha_i{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle$$

and

$$\langle 0 \mid \alpha_{p_1}{}^\dagger \alpha_{i_1} \alpha_i{}^\dagger \alpha_p \mid 0\rangle,$$

which are both $O(Z^2)$, as shown by Rowe. Combining (19) with the relation [requiring (17) only]

$$\sum_{p'} \langle 0 \mid \alpha_p{}^\dagger \alpha_{p'}{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle$$
$$= \sum_i \langle 0 \mid \alpha_p{}^\dagger \alpha_i \alpha_i{}^\dagger \alpha_p \mid 0\rangle - \langle 0 \mid \alpha_p{}^\dagger \alpha_p \mid 0\rangle, \quad (20)$$

we have

$$\langle 0 \mid \alpha_p{}^\dagger \alpha_p \mid 0\rangle = \sum_i \langle 0 \mid \alpha_p{}^\dagger \alpha_i \alpha_i{}^\dagger \alpha_p \mid 0\rangle$$
$$\tfrac{1}{2} \sum_{ii'p'} \langle 0 \mid \alpha_p{}^\dagger \alpha_{p'}{}^\dagger \alpha_i \alpha_{i'} \alpha_{i'}{}^\dagger \alpha_i{}^\dagger \alpha_{p'} \alpha_p \mid 0\rangle, \quad (21)$$

from which we can derive once more the results of the Sec. II.[1]

It is also clear how to extend the above arguments in a controllable way if one is interested in going to higher-order RPA.

IV. FACTOR OF 2

As pointed out by Rowe, the conventional RPA calculation of ground-state correlations yields twice the value given by the number-operator method. In Sec. II, we have verified the formula given by the latter, emphasizing at the same time that for its validity we must require that no RPA state get *too* collective. This is, however, a condition for the validity of the RPA itself.

Rowe has attempted to justify *both* results by introducing a distinction between collective and noncollective RPA states. Though we doubt that this distinction has any general quantitative validity for the computation of ground-state correlations, we use this section to point out that his remarks are justified for the model of Lipkin, Meshkov, and Glick.[2,7] In this model, N particles are distributed between two single-particle levels $(p\sigma)$ of equal degeneracy, $p=1\cdots N$, and σ $(=\pm)$ distinguishes the upper from the lower level. The particles interact via a monopole force. The Hamiltonian is

$$H=\epsilon J_z+\tfrac{1}{2}V(J_+{}^2+J_-{}^2), \quad (22)$$

where

$$J_z=\tfrac{1}{2}\sum_\sigma \sigma \alpha_{p\sigma}{}^\dagger \alpha_{p\sigma},$$
$$J_+=(J_-)^\dagger=\sum_p \alpha_{p+}{}^\dagger \alpha_{p-} \quad (23)$$

are the generators of $SU(2)$. The ground state of (22) belongs to the representation characterized by

$$J^2=\tfrac{1}{2}N(\tfrac{1}{2}N+1)=\tfrac{1}{2}\{J_+,J_-\}+J_z{}^2. \quad (24)$$

As we shall see below, the study of ground-state correlations for this model may be based entirely upon (24).[8]

In this theory, the only *collective* RPA state, the first excited state of the representation (24), can be studied in terms of the matrix elements $\langle 1 \mid J_\pm \mid 0\rangle$ connecting it to the ground state. Improvement over RPA results depends on accurate values for

$$\langle 0 \mid J_z \mid 0\rangle \equiv J_z{}^{(0)} = -\tfrac{1}{2}N+\delta J_z{}^{(0)},$$

where

$$\delta J_z{}^{(0)}=\sum_p \langle 0 \mid \alpha_{p+}{}^\dagger \alpha_{p+} \mid 0\rangle. \quad (25)$$

From (24), the angular momentum algebra, and an intermediate-state expansion, we easily obtain

$$J_z{}^{(0)}-(J_z{}^{(0)})^2=-\tfrac{1}{2}N-\tfrac{1}{4}N^2+\sum_{n\neq 0} |\langle n \mid J_- \mid 0\rangle|^2$$
$$+\sum_{n\neq 0} |\langle n \mid J_z \mid 0\rangle|^2$$
$$\cong -\tfrac{1}{2}N-\tfrac{1}{4}N^2+|\langle 1 \mid J_- \mid 0\rangle|^2, \quad (26)$$

[7] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965).

[8] A separate discussion of the use of Casimir operators of appropriate symmetry groups as an expression of the Pauli principle is in preparation.

which serves as a convenient alternative to the general prescription of the previous sections.

In the leading order, (26) simplifies to

$$\delta J_z^{(0)}=N^{-1}\,|\,\langle 1\,|\,J_-\,|\,0\rangle\,|^2. \tag{27}$$

This can be evaluated by writing

$$|\,1\rangle=B^\dagger\,|\,0\rangle,\qquad B\,|\,0\rangle=0, \tag{28}$$

$$B^\dagger=N^{-1/2}[YJ_+-ZJ_-], \tag{29}$$

$$Y^2-Z^2=1. \tag{30}$$

Thus we have

$$\delta J_z^{(0)}=Z^2. \tag{31}$$

Let us contrast this with the general prescription which follows from (25) and the previous sections, namely,

$$\delta J_z^{(0)}=\sum_p\langle 0\,|\,\mathcal{A}_{p+}{}^\dagger\mathcal{A}_{p+}\,|\,0\rangle$$
$$=\tfrac{1}{2}\sum_{p'p\lambda}|\,Z_{p'+p-}(\lambda)\,|^2. \tag{32}$$

We have N^2 states $|\,\lambda\rangle$ which contribute to (32), since there are N^2 particle-hole states, all degenerate at excitation energy ϵ in the limit as V in Eq. (22) approaches 0. Of these, only one linear combination $J_+\,|\,\mathrm{HF}\rangle$ belongs to the ground-state band and goes over to the state $|\,1\rangle$ as we turn on V. For this state [cf. (29)]

$$Z_{p'+p-}=\delta_{p'p}ZN^{-1/2}, \tag{33}$$

and it therefore contributes $\frac{1}{2}Z^2$ to (32). The other N^2-1 noncollective states contribute the remaining $\frac{1}{2}Z^2$. Thus if we multiplied (32) by 2 and kept only the contribution of the collective state, we would still be correct, according to (31).

For good measure, we shall verify our conclusion directly from Eq. (20), which, in the present instance, reads

$$\delta J_z^{(0)}=\sum_{pp'}\langle 0\,|\,\mathcal{A}_{p+}{}^\dagger\mathcal{A}_{p'-}\mathcal{A}_{p'-}{}^\dagger\mathcal{A}_{p+}\,|\,0\rangle$$
$$-\sum_{pp'}\langle 0\,|\,\mathcal{A}_{p+}{}^\dagger\mathcal{A}_{p'+}{}^\dagger\mathcal{A}_{p'+}\mathcal{A}_{p+}\,|\,0\rangle. \tag{34}$$

We evaluate this directly by writing

$$|\,0\rangle\cong|\,\mathrm{HF}\rangle+\alpha J_+J_+\,|\,\mathrm{HF}\rangle, \tag{35}$$

omitting a change in over-all normalization, since only the term proportional to α^2 contributes to (34). We find

$$\delta J_z^{(0)}=2N^2\alpha^2-N^2\alpha^2=N^2\alpha^2. \tag{36}$$

The identity to the previous result is verified by computing

$$|\,\langle 1\,|\,J_-\,|\,0\rangle\,|^2=Z^2N=\langle 0\,|\,J_+J_-\,|\,0\rangle=N^3\alpha^2. \tag{37}$$

In conclusion, however, we repeat that we know of no justification for extending this result to any other model. In particular, appropriate revision of recent numerical discussions of ground-state correlations for closed-shell nuclei[9,10] would appear to be in order.

[9] G. E. Brown and C. W. Wong, Nucl. Phys. **A100**, 241 (1967).
[10] D. Agassi, V. Gillert, and A. Lumbroso, Nucl. Phys. **A130**, 129 (1969).

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Absence of Recoil Doppler Broadening of the 3367-keV Transition Following the Reaction ^{9}Be(n_{th}, γ)^{10}Be

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The 3367-keV ground-state γ-ray transition from the reaction ^{9}Be(n_{th},γ)^{10}Be shows no Doppler broadening from recoil imparted by emission of γ rays populating this level. This result is consistent with the known lifetime of this level, which is larger than the estimated slowing-down time of the recoil nucleus in the sample medium.

RECENTLY, the broadening of secondary transitions in cascades of γ rays emitted following thermal-neutron capture in light nuclei has been observed with the aid of high-resolution Ge(Li) spectrometers.[1,2] This broadening is caused by emission of

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[1] E. C. Campbell, J. A. Harvey, and G. G. Slaughter, Bull. Am. Phys. Soc. **13**, 1423 (1968).
[2] K. J. Wetzel, Phys. Rev. **181**, 1465 (1969).