Investigation of Ground-State Correlations for a Model Hamiltonian of the Nucleus*

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The importance of ground-state correlations in the spectroscopy of a finite many-particle system, such as the nucleus, is investigated for the model Hamiltonian of Lipkin, Meshkov, and Glick. In particular, we have investigated their effect on the solution of the equations of motion for excitation energies, transition matrix elements, and the correlation energy of the ground state. Methods are studied for calculating the correlations needed to make the necessary corrections to the equations of motion. Also studied is the behavior, with increase of interaction strength, of the phase transition from the spherical to the strongly deformed intrinsic states, in the projected Hartree-Fock scheme.

1. INTRODUCTION

IT has been suggested[1] that ground-state correlations may have a very important influence on the systematics of nuclear spectroscopy. To take an extreme example, one has only to contrast the ground state of a highly deformed nucleus with that of a so-called "spherical" nucleus. The dramatic difference in the spectra of the two nuclei is well known and can be attributed directly to the character of their ground states. However, we are not concerned here so much with the comparatively well-understood rotational correlations of strongly deformed nuclei as with the shape-fluctuation correlations of spherical and transition nuclei. In particular, we are interested in the effect of correlations on vibrational spectra. The present model investigation may thus be considered as a preliminary survey for the difficult problem of the spectroscopy of transition nuclei.

A major objective is to study the effect of ground-state correlations on the solution of the formally exact equations of motion that have been proposed[2] for nuclear excitations. The simplest approximate solution is to restrict the excitation operators to 1-particle-hole operators and to replace the correlated ground state in the equations of motion by the uncorrelated particle-hole vacuum. In this approximation one regains the well-known random-phase approximation (RPA). It has been argued,[2] however, that the use of correlated densities in the equations of motion can introduce important coherent corrections to the RPA. This we investigate in terms of a simple model Hamiltonian, which can be solved exactly for comparison. The corrections are found to be sizeable and when included give much improved results.

In view of the difficulty of evaluating correlated two-particle densities in a realistic problem, a higher (renormalized) RPA has been suggested[1,2] in which uncorrelated Hartree-Fock (HF) single-particle energies and densities are replaced by renormalized quantities, defined for the correlated ground state, but specific two-body correlations are ignored under the assumption that they contribute with random phases. Such a renormalized RPA comes quite close, although not exactly, to what one already does in most practical RPA calculations, when one takes single-particle energies from experiment and chooses an effective interaction to fit the data. The present calculations indicate that, for the model problem, the renormalized RPA is extraordinarily good, even for interactions so strong that the HF ground state is about to undergo a phase transition.

Now to use the renormalized RPA equations in a general nuclear problem, we need a reliable method for calculating the one-particle densities of the correlated ground state. Various methods were discussed in the preceding paper[1] (hereafter referred to as I). Here we apply these methods to the model problem and compare the results with exact calculations. Again the (*renormalized RPA*)+(*renormalized quasiboson*) *approximation* gives extraordinarily good results.

Of particular interest is the *projection method*, in which a correlated ground state is projected from a deformed determinant. This determinant, which is determined variationally after projection, in general looks very different from the HF determinant, obtained by variation before projection. The projection method is of special interest because it relates, in a continuous manner, the vibrational correlations of the so-called "spherical" nuclei to the rotational correlations of the strongly deformed nuclei. Thus it holds particular promise for the nuclei in the transition region, where it is not clear whether the structure is predominantly rotational or vibrational. Indeed it is not certain that the distinction is altogether meaningful. Thus it is interesting to follow the deformation of the intrinsic state as a function of interaction strength to see whether the transition from the spherical to the deformed limit takes place smoothly or suddenly. For the model problem we find the unexpected result that a sudden phase transition, in the deformation, does occur

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[1] D. J. Rowe, preceding paper, Phys. Rev. **175**, 1283 (1968), referred to in text as I.
[2] D. J. Rowe, Rev. Mod. Phys. **40**, 153 (1968); Nucl. Phys. **A107**, 99 (1968).

for sufficiently large particle number. The deformation before the phase transition is not zero, however, as in the HF description.

The model Hamiltonian employed is that invented by Lipkin, Meshkov, and Glick[3] and used by them to investigate various many-body approaches. In particular, these authors have investigated equation-of-motion methods with various linearization prescriptions. Their equations of motion differ from ours, which avoid the linearization problem and reveal more clearly the approximations and the next corrections. Even so, our renormalized RPA equations are closely related to their improved linearization methods. In testing our methods, designed for more realistic problems, we have tried to avoid duplicating the work of these authors as much as possible. In fact, there is little overlap. They have investigated various approximations for calculating excitation energies as a function of particle number, for a few fixed values of the interaction strength. We, on the other hand, have investigated different methods for calculating excitation energies, transition matrix elements, ground-state correlations, and the ground-state energy, as a function of interaction strength, for a few fixed numbers of particles. In particular, we have emphasized the intermediate interaction regions in the neighborhood of the HF phase transition. The model is reviewed briefly in Sec. 2. The general applications of 1-particle-hole equations of motion to derive excitation energies, transition matrix elements, and the correlated ground state have been reviewed in I. In Secs. 3–5 the methods are applied to the model problem. The projection method is applied in Sec. 6.

2. MODEL

The model has been discussed in some detail by its inventors[3] so that we shall here only review its essential constituents. It is supposed that the system is composed of N fermions occupying two energy levels, each having an N-fold degeneracy. Each state has a quantum number σ which has the value $+1$ in the upper level and -1 in the lower level, and a quantum number p distinguishing the degenerate states within a level. The system is described by the Hamiltonian

$$H=\tfrac{1}{2}\epsilon\sum_{p\sigma}\sigma a_{p\sigma}^{\dagger}a_{p\sigma}+\tfrac{1}{2}V\sum_{pp'\sigma}a_{p\sigma}^{\dagger}a_{p'\sigma}^{\dagger}a_{p'-\sigma}a_{p-\sigma}, \quad (1)$$

which has the property that the interaction scatters particles only between upper and lower states having the same value of p. The model does not attribute any particular physical significance to the quantum numbers p and σ. For convenience, however, we consider σ as a parity quantum number. The virtue of the Hamiltonian (1) is that it can be written

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

where J_z, J_+, J_- are quasispin operators

$$J_z=\tfrac{1}{2}\sum_{p\sigma}\sigma a_{p\sigma}^{\dagger}a_{p\sigma},$$
$$J_+=\sum_{p}a_{p+1}^{\dagger}a_{p-1}, \quad (3)$$
$$J_-=\sum_{p}a_{p-1}^{\dagger}a_{p+1}$$

obeying the usual angular momentum commutation relations. It follows, therefore, that J^2 is a constant of motion and that its eigenvalue for the ground state of the N-particle system is $j(j+1)$, where $j=\frac{1}{2}N$.

In this paper we shall be concerned only with the ground and first excited states of H. It has been shown[3] that these belong to a common multiplet, $j=\frac{1}{2}N$. In the limit $V=0$, the ground state is simply the state $|j, m=-j\rangle$ and the first excited state $|j, m=-j+1\rangle$. As the interaction is turned on, the members of the multiplet mix and m is lost as a good quantum quantum. However, it can be seen from inspection of the Hamiltonian (2) that the total parity of the system is conserved: J_+ and J_- are odd-parity operators and J_z is even. Thus components of even m do not mix with odd m.

The diagonalization of the Hamiltonian (2) is straightforward and has been carried out by the authors for $N=8$ and 20 as a function of the interaction strength; the relevant parameter is NV/ϵ. The parameters of interest, for which we compare the predictions of various approximate methods, are the following: the excitation energy $(E_1-E_0)/\epsilon$ of the first excited state in units of ϵ; the transition matrix elements $\langle 1|(J_++J_-)|0\rangle$ between ground and first excited state; the single-particle density parameter

$$N_+\equiv\langle 0|\sum_{p}a_{p+1}^{\dagger}a_{p+1}|0\rangle, \quad (4)$$

which is the number of particles occupying the upper single-particle level; and finally the correlation energy (i.e., the energy difference of the correlated and uncorrelated ground states).

3. RANDOM-PHASE APPROXIMATION

It is convenient in the RPA to write the excited state creation operator

$$O^{\dagger}=(YJ_+-ZJ_-)/\langle\,|[J_-,J_+]|\,\rangle^{1/2}, \quad (5)$$

where $|\,\rangle$ is the HF (Hartree-Fock) ground state

$$|\,\rangle=|j, m=-j\rangle=|\tfrac{1}{2}N, -\tfrac{1}{2}N\rangle. \quad (6)$$

The reason for the denominator in (5) is to maintain

[3] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965); N. Meshkov, A. J. Glick, and H. J. Lipkin, *ibid.* **62**, 199 (1965); A. J. Glick, H. J. Lipkin, and N. Meshkov, *ibid.* **62**, 211 (1965); D. Agassi, H. J. Lipkin, and N. Meshkov, *ibid.* **86**, 321 (1966).

the usual RPA normalization

$$\langle\,|[O,O^\dagger]|\,\rangle = Y^2 - Z^2 = 1. \tag{7}$$

With this normalization the coefficients Y and Z are completely defined by the RPA matrix equation

$$\begin{pmatrix} A-\omega & B \\ B & A+\omega \end{pmatrix}\begin{pmatrix} Y \\ Z \end{pmatrix} = 0, \tag{8}$$

where ω is the excitation energy $(E_1 - E_0)$ and

$$\begin{aligned} A &= \langle\,|[J_-,H,J_+]|\,\rangle / \langle\,|[J_-,J_+]|\,\rangle &&= \epsilon, \\ B &= -\langle\,|[J_-,H,J_-]|\,\rangle / \langle\,|[J_-,J_+]|\,\rangle &&= V(N-1). \end{aligned} \tag{9}$$

These equations are trivially solved, giving

$$\omega = (A^2 - B^2)^{1/2}, \tag{10}$$

$$Y = \left(\frac{A+\omega}{2\omega}\right)^{1/2}, \quad Z = -\left(\frac{A-\omega}{2\omega}\right)^{1/2}. \tag{11}$$

In Fig. 1, the excitation energies given by (10) are compared to the exact results for $N=8$ and 20 as a function of NV/ϵ. It is seen that ω vanishes at the critical value

$$V_{\text{crit}} = \epsilon/(N-1) \tag{12}$$

and for larger values of the interaction becomes imaginary. As is well known, V_{crit} is the value of the interaction at which the HF state becomes unstable and a new (deformed, i.e., parity-mixed) HF ground state emerges.

Transition matrix elements for the operator $(J_+ + J_-)$ are given in the RPA by

$$\begin{aligned} \langle 1|(J_+ + J_-)|0\rangle &\cong \langle\,|[O,(J_+ + J_-)]|\,\rangle \\ &= (Y+Z)\langle\,|[J_-,J_+]|\,\rangle^{1/2} \\ &= N^{1/2}(Y+Z). \end{aligned} \tag{13}$$

The values obtained from this expression, for different values of NV/ϵ, are shown on Fig. 1 in comparison with the exact values.

To obtain the correlated ground state, we need to solve the equation

$$O|0\rangle = 0. \tag{14}$$

For the model problem this equation has been solved exactly by Meshkov, Glick, and Lipkin[3] (MGL), with the result

$$|0\rangle = a_{-j}\sum_{n=0}^{j} b^n (c_n)^{1/2} |j, m=-j+2n\rangle, \tag{15}$$

where

$$\begin{aligned} (a_{-j})^{-2} &= \sum_{n=0}^{j} b^{2n} c_n, \\ b &= Z/Y, \\ c_n &= \binom{j}{n}^2 \binom{2j}{2n}^{-1}. \end{aligned} \tag{16}$$

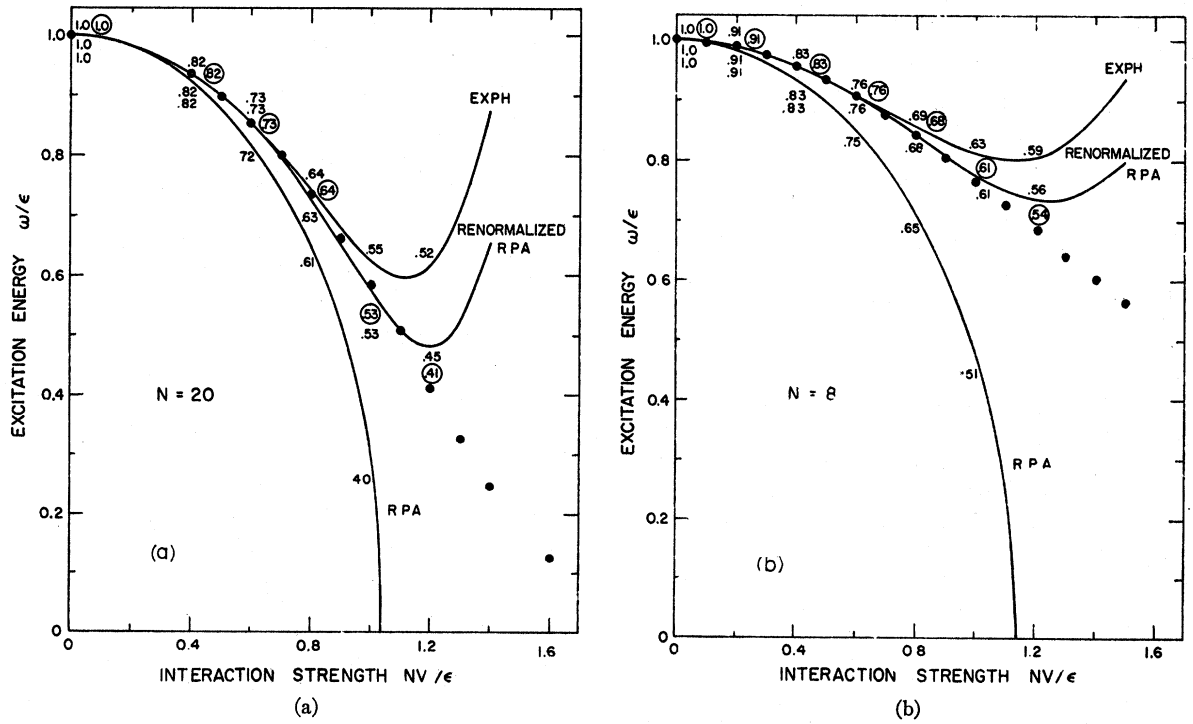

FIG. 1. The excitation energy $\omega/\epsilon = (E_1 - E_0)/\epsilon$ of the first excited state as a function of interaction strength for various approximate solutions of the equations of motion, (a) for 20 and (b) for 8 particles. Exact results are shown by filled circles. Transition matrix elements $\langle 1|(J_+ + J_-)|0\rangle$, normalized to unity at zero interaction, are shown as numbers on the curves for each approximation. The exact matrix elements are enclosed by circles.

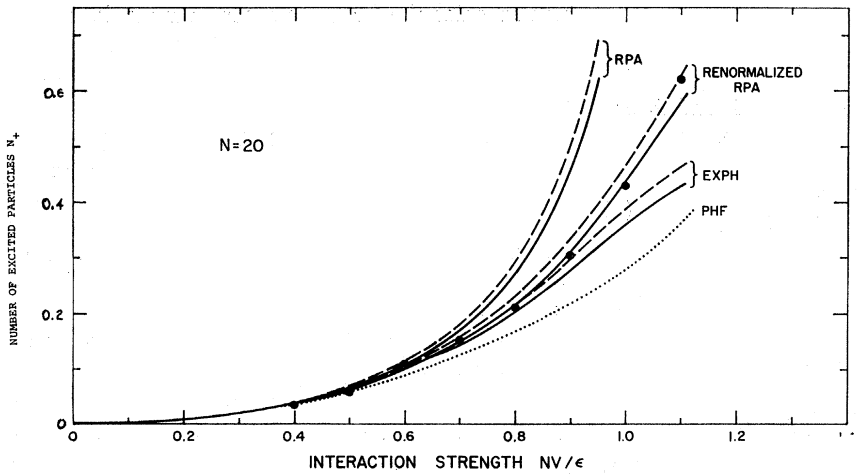

FIG. 2. The number of particles N_+ not occupying their HF orbitals as a function of interaction strength, calculated in various approximations. Dashed curves represent the MGL solutions and solid lines the quasiboson approximations. Exact results are shown by filled circles.

This gives the single-particle density N_+ [defined by Eq. (4)]

$$N_+=\sum_{n=0}^{j} 2nc_nb^{2n}\Big/\sum_{n=0}^{j} c_nb^{2n}. \tag{17}$$

This result, which we call the MGL result, is compared with the exact result in Fig. 2 for twenty particles. Qualitatively similar results were obtained for $N=8$.

Now the MGL method is peculiar to the model and cannot be used in general to solve Eq. (14). We therefore consider the approximate method based on the quasiboson approximation[4]

$$[J_-,J_+]\cong\langle\,|[J_-,J_+]|\,\rangle=-2\langle\,|J_z|\,\rangle=N. \tag{18}$$

The method has been described in I for the general problem. For the model it leads to the approximate ground state

$$|0\rangle\cong N_0\exp\left\{-\frac{1}{2N}\left(\frac{\epsilon-\omega}{\epsilon+\omega}\right)^{1/2}J_+J_+\right\}|\,\rangle \tag{19}$$

and to the single-particle density[5]

$$N_+=Z^2=(\epsilon-\omega)/2\omega. \tag{20}$$

Results using this expression are also included in Fig. 2. The interesting observation is that the quasiboson approximation gives a result which is extremely close to the MGL result, which is an exact solution of Eq. (14). Both methods give values for N_+ which are too large. This error can be attributed directly to the fact that the RPA underestimates ω.

Two expressions were given in I for the correlation energy: The *oscillator-projection method* gave

$$\Delta E=-\sum_{\lambda J}(2J+1)\omega_{\lambda J}\langle\,|O_{\lambda J}{}^\dagger O_{\lambda J}|\,\rangle \tag{21}$$

and the *method of generator coordinates* gave

$$\Delta E=\tfrac{1}{2}\sum_J(2J+1)\left\{\sum_\lambda\omega_{\lambda J}-\mathrm{Tr}A^{(J)}\right\}. \tag{22}$$

For the model problem in the RPA, these expressions are equivalent and give

$$\Delta E=\tfrac{1}{2}(\omega-\epsilon). \tag{23}$$

This prediction is compared to the exact results for 20 particles in Fig. 3, and is seen to be very good. Similar results were obtained for $N=8$.

4. EXACT 1-PARTICLE-HOLE (EXPH) EQUATIONS

In taking into account the effect of ground-state correlations in the equations of motion, it is convenient to express the excited-state creation operator

$$O^\dagger=(YJ_+-ZJ_-)/\langle 0|[J_-,J_+]|0\rangle^{1/2}, \tag{24}$$

where $|0\rangle$ is now the correlated ground state. With this denominator we then have the normalization[6]

$$\langle 0|[O,O^\dagger]|0\rangle=Y^2-Z^2=1. \tag{25}$$

Given the approximate expansion (24) for $O^\dagger$ and the exact ground state $|0\rangle$, it is possible to solve the equations of motion

$$\langle 0|[\delta O,H,O^\dagger]|0\rangle=\omega\langle 0|[\delta O,O^\dagger]|0\rangle \tag{26}$$

without any further approximation. One again obtains the matrix equation (8) of RPA form but with matrix

[4] E. A. Sanderson, Phys. Letters **19**, 141 (1965).

[5] Note that we here use the expression derived in I based on Sanderson's method but which differs from the expression he derives (also quoted in I) from the "factor pairing" approximation. For comparison we also calculated densities in the "factor pairing" approximation, but they were at all times inferior and are not shown in the figures.

[6] Note the distinction between these equations and the RPA equations (5) and (7) in which the correlated ground state is replaced by the HF particle-hole vacuum.

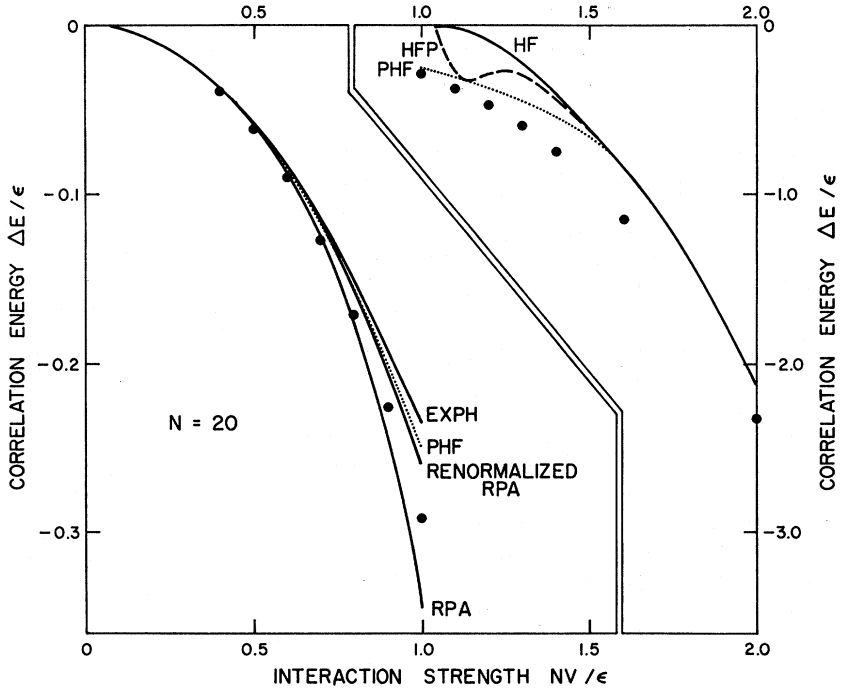

FIG. 3. The correlation energy $\Delta E/\epsilon$ as a function of interaction strength calculated in various approximations. Exact results are shown by filled circles.

elements

$$A=\frac{\langle 0|[J_-,[H,J_+]]|0\rangle}{\langle 0|[J_-,J_+]|0\rangle}=\epsilon+V\cdot\frac{\langle 0|J_-J_-|0\rangle}{\langle 0|J_z|0\rangle},$$

$$B=-\frac{\langle 0|[J_-,[H,J_-]]|0\rangle}{\langle 0|[J_-,J_+]|0\rangle}$$

$$=V\cdot\frac{-4\langle 0|J_z^2|0\rangle+\langle 0|J_+J_-+J_-J_+|0\rangle}{2\langle 0|J_z|0\rangle}. \quad (27)$$

These equations fully take into account ground-state correlations but are still approximate in as much as the true excitation operator should contain components in $(J_+)^3$, $(J_-)^3$, etc. They are therefore described as the exact 1-particle-hole (EXPH) equations.

The solution of these equations is again given by Eqs. (10) and (11), although, of course, with the EXPH values for A and B. The results for the excitation energy ω are plotted in Fig. 1. It is seen that good results are obtained for interaction strengths right up to V_{crit}.

Transition matrix elements for the operator (J_++J_-) are given in the EXPH model by

$$\langle 1|(J_++J_-)|0\rangle=\langle 0|[O,(J_++J_-)]|0\rangle$$
$$=(-2\langle 0|J_z|0\rangle)^{1/2}(Y+Z) \quad (28)$$

and are also shown in Fig. 1. Again the predictions are very much improved over the RPA.

To calculate the ground state we can again use the MGL method to solve Eq. (14). The expressions (15)–(17) remain unchanged except that $b=Z/Y$ is evaluated for the EXPH solutions. The predicted values for N_+ are plotted in Fig. 2 and are seen to be much improved, although now slightly underestimating the correlations for large values of the interaction.

Recognizing that the MGL method is not generally applicable, we also calculate the ground state in the renormalized quasiboson approximation:

$$[J_-,J_+]\cong\langle 0|[J_-,J_+]|0\rangle=-2\langle 0|J_z|0\rangle. \quad (29)$$

Following the methods described in I, we obtain

$$|0\rangle=N_0\exp\left[\frac{1}{4}\left(\frac{A-\omega}{A+\omega}\right)^{1/2}\frac{J_+J_+}{\langle 0|J_z|0\rangle}\right]|\ \rangle \quad (30)$$

and

$$N_+=Z^2=(A-\omega)/2\omega. \quad (31)$$

Results using this expression are shown in Fig. 2.

The expression (21) for the correlation energy is independent of the manner in which the excitation operators $O^\dagger$ are derived. In the EXPH approximation it gives, for the model,

$$\Delta E=N(A-\omega)/4\langle 0|J_z|0\rangle. \quad (32)$$

Values obtained with this expression are plotted in Fig. 3 and are accurate to 10% or better right up to $V=V_{\text{crit}}$. The agreement with the exact result is about as good as in the RPA but errs in the opposite direction. This in itself is a healthy trend, however, since any reliable method of estimating the ground-state energy should always give a value too large and never too small.

5. RENORMALIZED RPA

In any realistic problem we do not have sufficient knowledge of the correlated ground state to set up the EXPH equations. We therefore consider the renormalized RPA in which we use only information concerning the ground state which we believe we can estimate reliably in practice or calculate self-consistently. In particular, we believe that renormalized single-particle energies can be estimated experimentally and 1-particle densities can be calculated, but we do not anticipate being able to calculate 2-particle correlation functions reliably. However, since we wish to investigate the effect of ground-state correlations on the equations of motion and to test our ability to calculate ground-state correlations as two distinct problems, we have chosen not to proceed self-consistently in the present calculation. The information needed to set up the renormalized RPA equation was therefore extracted from the exact ground state of the model Hamiltonian.

The expansion (24) is again used for the excitation operator $O^\dagger$, so that the normalization (25) is retained. Y and Z remain solutions of the matrix equation (8), but with renormalized matrix elements. The general renormalized RPA expressions were derived by Rowe[2] and summarized in I. For the model problem the particle-hole energy ϵ, of the RPA, is replaced by $(\epsilon^{(+)}-\epsilon^{(-)})$, where $\epsilon^{(+)}$ and $\epsilon^{(-)}$ are defined by

$$\begin{aligned}\epsilon^{(+)}\langle 0|a_{p+}a_{p+}^\dagger|0\rangle&=\langle 0|a_{p+}[H,a_{p+}^\dagger]|0\rangle,\\ \epsilon^{(-)}\langle 0|a_{p-}^\dagger a_{p-}|0\rangle&=-\langle 0|a_{p-}^\dagger[H,a_{p-}]|0\rangle.\end{aligned}\tag{33}$$

Because of the symmetry, $\epsilon^{(+)}$ and $\epsilon^{(-)}$ are independent of p and are readily evaluated to give

$$A=\epsilon^{(+)}-\epsilon^{(-)}=\epsilon +2V[\langle 0|J_-J_-|0\rangle/(\langle 0|J_z|0\rangle-\tfrac{1}{2}N)].\tag{34}$$

Interaction matrix elements are obtained from the RPA by multiplying by the renormalization factor

$$\frac{2\langle 0|[J_-,J_+]|0\rangle-\langle\,|[J_-,J_+]|\,\rangle}{\langle 0|[J_-,J_+]|0\rangle}=\frac{4\langle 0|J_z|0\rangle+N}{2\langle 0|J_z|0\rangle}\tag{35}$$

giving

$$B=V(N-1)[2+N/2\langle 0|J_z|0\rangle].\tag{36}$$

It is seen that the renormalization factor involves evaluating the ground-state expectation of a 1-body operator but requires no specific knowledge of 2-body correlations. The renormalized single-particle energies do involve information concerning 2-body correlations, but in practice one would estimate $\epsilon^{(+)}$ and $\epsilon^{(-)}$ experimentally and not calculate them; $\epsilon^{(+)}$ is the centroid energy of the single-particle pickup strength while $\epsilon^{(-)}$ is the centroid of the stripping strength.

The solutions of the renormalized RPA equations are again given by Eqs. (10) and (11). Excitation energies are plotted in Fig. 1 and are seen to be extraordinarily good—better, in fact, than the EXPH results. Since the renormalized RPA makes more approximations than the EXPH model, the improved agreement is due to cancellation of errors. The important observation, however, is the close agreement between the renormalized RPA and the EXPH results, which indicates that specific two-body correlations (i.e., those which do not renormalize the single-particle energies) can be neglected in the equations of motion without introducing significant errors.

Transition matrix elements in the renormalized RPA are again given by (28) and are included in Fig. 1. Once more the renormalized RPA is in very good agreement with the EXPH and in even better agreement with the exact results.

The MGL expressions (15)–(17) for N_+ remain unchanged in the renormalized RPA as also do the renormalized quasiboson expressions (29)–(31). The predicted values are shown in Fig. 2. The quasiboson results, in particular, are seen to be virtually perfect.

Finally, the correlation energy given by Eq. (32) has been evaluated and is shown in Fig. 3. Once again the results are surprisingly good.

6. PROJECTION METHOD

It has been suggested in I that a good way to calculate the correlated ground state might be to project it from a determinant in which angular momentum is not a good quantum number. The analog in the present model is parity projection. If the interaction strength V exceeds the critical value V_{crit} [Eq. (12)], a HF ground state will emerge in which parity is not a good quantum number. To obtain an approximation for the true ground state, we might therefore project good parity out of the HF determinant. This is sometimes described as the HFP (Hartree-Fock variation followed by projection) method. Such calculations were carried out for the model problem by Agassi, Lipkin, and Meshkov[3] and lead to good results in the limit of large interaction strength. From a variational point of view, a much sounder approach would be to project first and perform the variation after.[7] This is sometimes described as the PHF (projection followed by Hartree-Fock variation) method. It was argued in I that this method should lead to a ground state with vibrational correlations, even when the interaction strength is well below the critical value at which a deformed (i.e., parity-mixed) HF solution first appears. One of the virtues of the PHF method is, therefore, that it is continuously applicable from the spherical to the strongly deformed limits.

The methods for performing the projection in the model problem were developed by Agassi *et al.*[3] and we shall merely summarize the pertinent results. An arbitrary determinant $|\alpha\rangle$ can be obtained from the HF determinant $|\,\rangle$ by a rotation through an angle α about

[7] H. Rouhaninejad and J. Yoccoz Nucl. Phys. 78, 353 (1966).

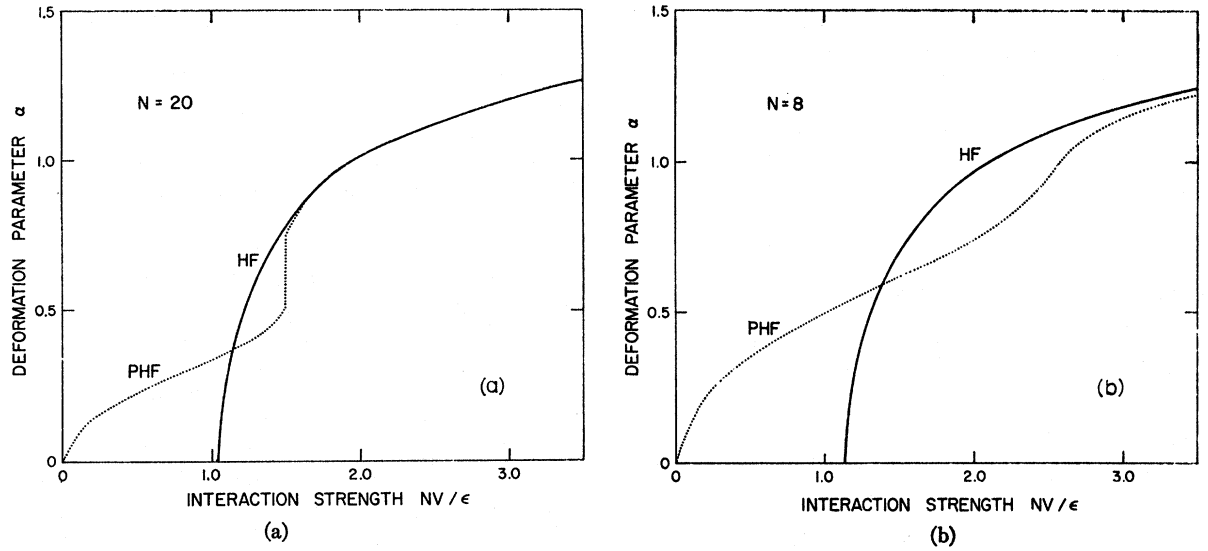

FIG. 4. The deformation parameter α of the intrinsic state as a function of interaction strength in the HF and PHF approximations, (a) for 20 and (b) for 8 particles.

the x axis in quasispin space[8]

$$|\alpha\rangle = e^{i\alpha J_x}|\ \rangle. \tag{37}$$

Instead of rotating the wave function, however, it is convenient to rotate the quasispin operators:

$$J_\mu{}^{(\alpha)} = e^{-i\alpha J_x} J_\mu e^{i\alpha J_x}. \tag{38}$$

The transformed Hamiltonian (2) then becomes

$$H^{(\alpha)} = e^{-i\alpha J_x} H e^{i\alpha J_x} = \epsilon(J_z\cos\alpha + J_y\sin\alpha) + V[J_x{}^2 - (J_y\cos\alpha - J_z\sin\alpha)^2]. \tag{39}$$

Thus we obtain the energy expectation of $|\alpha\rangle$

$$\langle\alpha|H|\alpha\rangle = \langle\ |H^{(\alpha)}|\ \rangle = -\epsilon j\{\cos\alpha + (V/\epsilon)(j-\tfrac{1}{2})\sin^2\alpha\}, \tag{40}$$

where $j = N/2$.

Now the positive parity component $|\alpha+\rangle$ of $|\alpha\rangle$ is given by

$$|\alpha+\rangle = |\alpha\rangle + |-\alpha\rangle \tag{41}$$

and its energy expectation by

$$\frac{\langle\alpha+|H|\alpha+\rangle}{\langle\alpha+|\alpha+\rangle} = \langle\alpha|H|\alpha\rangle\frac{1+(\cos\alpha)^{2j-1}}{1+(\cos\alpha)^{2j}}. \tag{42}$$

The PHF approximation to the ground state is the state $|\alpha+\rangle$ which minimizes this energy. This minimization we have performed numerically as a function of the interaction strength. Results for the ground-state energy are shown for $N=20$ in Fig. 3. Similar results were obtained for $N=8$. The agreement on the whole is satisfactory, although poorest in the transition region $V \approx V_{\text{crit}}$. One nevertheless is encouraged to use this method as a means of calculating ground-state wavefunctions for spherical and mildly deformed nuclei, as well as for strongly deformed nuclei, for which it was always a natural choice.

For comparison we have also shown in Fig. 3 the HF energy (i.e., the minimum energy $\langle\alpha|H|\alpha\rangle$) and the HFP energy (i.e., the energy of the positive-parity state projected from the HF state). For large values of the interaction it turns out to be immaterial whether one projects before or after variation—or, indeed, whether one projects at all.

To study the transition of the intrinsic state from the spherical to the strongly deformed limit, we have plotted, in Fig. 4, the values of α which minimize the PHF energy and which minimize the HF energy as a function of interaction strength. The HF deformation is zero for $V < V_{\text{crit}}$ and then suddenly increases very rapidly. For 20 particles it appears that the PHF deformation is finite for all nonvanishing interactions, but for a particular value of the interaction undergoes a sudden phase transition to a more deformed state. We surmise that this phase transition represents the dividing line between the vibrational and the rigid deformed states of the system, rather than the point at which a deformed HF solution first emerges. Thus we conjecture that before the PHF phase transition the deformation of the intrinsic state is associated with the mean deformation of the vibrational fluctuations. The negligible difference between the PHF and the HF deformations after the phase transition suggests that the vibrational correlations have suddenly become negligible. For $N=8$ the phase transition is largely smeared out. It will

[8] It is readily shown that, for V positive, the energy will always be minimized, whether one projects or not, by restricting the rotation in quasispin space to the yz plane. The argument is based on the observation that, for V positive, the relative phases of the $|j, m=-j\rangle$, $|j, m=-j+4\rangle$, $\cdots$, and the $|j, m=-j+2\rangle$, $|j, m=-j+6\rangle$, $\cdots$, components must be opposite.

be very interesting to see if such effects exist for nuclei.

The single-particle density operator $\hat{N}_+$, whose ground-state expectation is N_+, can be expressed

$$\hat{N}_+=\sum_p a_{p+1}^\dagger a_{p+1}=\tfrac{1}{2}N+J_z. \tag{43}$$

Transformed, it becomes

$$\hat{N}_+^{(\alpha)}=\tfrac{1}{2}N+J_z\cos\alpha+J_y\sin\alpha \tag{44}$$

and gives a ground-state expectation

$$N_+=\frac{\langle\alpha+|\hat{N}_+|\alpha+\rangle}{\langle\alpha+|\alpha+\rangle}=j(1-\cos\alpha)\frac{1-(\cos\alpha)^{2j-1}}{1+(\cos\alpha)^{2j}}. \tag{45}$$

Values predicted with this formula are shown in Fig. 2. They are not as good as those obtained with some of the other methods, but are nevertheless acceptable.

More detailed investigations of occupation probabilities were made by Agassi *et al.*[3] in the HF and HFP approximations, which naturally limited them to interaction strengths in excess of V_{crit}, for which there is a nontrivial HF solution. We, on the other hand, have concentrated on the PHF method and interaction strengths $V\approx V_{\text{crit}}$.

7. DISCUSSION

In this work we have investigated the importance of ground-state correlations on the solutions of the equations of motion and various approximate methods for calculating them in order to make the necessary corrections.

In the RPA two approximations are made.

(i) Neglect of 2nd RPA effects: By this we mean the restriction of the excitation operator $O^\dagger$ to be a 1-particle-hole operator. The true excitation operator should include 2-particle-hole, 3-particle-hole components, etc., which are included in a 2nd RPA calculation. (For the model problem the 2-particle-hole components are in fact suppressed by a parity-selection rule.)

(ii) Neglect of ground-state correlation effects: By this we mean the substitution of the uncorrelated HF state for the correlated ground state in the equations of motion.

Fig. 1 shows that these approximations lead to an excitation energy which is too low, while the transition matrix elements and single-particle densities of Figs. 1 and 2 show that it predicts correlations which are too large.

The EXPH equations still make approximations (i) but do not make approximation (ii). Thus the difference between the EXPH and the RPA is due entirely to ground-state correlation effects, while the difference between the EXPH and the exact results is due entirely to 2nd RPA effects. Inspection of Figs. 1 and 2 show that the EXPH model overestimates the excitation energy slightly and underestimates the correlations. This is a general result which can be understood on general grounds. It was shown in I that the excitation energy ω of the exact equations of motion for the operator $O^\dagger$ is equal to the centroid energy of the strength distribution of the state $O^\dagger|0\rangle$ among the exact eigenstates of the system. Thus, if the operator space of $O^\dagger$ is restricted, ω will always exceed the excitation energy of the lowest excited state. It is interesting that 2nd RPA errors are small for $V<V_{\text{crit}}$ but, for larger values of V, they suddenly become very large. It should be emphasized, however, that the model is not designed to investigate 2nd RPA corrections, which are almost certainly unrealistically small because of the suppression of the 2-particle-hole components in $O^\dagger$ by the parity-selection rule.

In the renormalized RPA, approximation (i) is again made but efforts are made to correct for (ii) in an approximate manner. From the small difference between the renormalized RPA and the EXPH results, we conclude that the renormalization procedure does indeed take into account by far the largest contribution from the ground-state correlations. The extraordinarily good agreement between the renormalized RPA and the exact results must to some extent be regarded as accidental since it is due to the fortuitous cancellation of errors. However, 2nd RPA and correlation corrections will in general tend to cancel, but not always so successfully.

An interesting and very encouraging observation from our results is that if one were given the excitation energy experimentally and chose an interaction to fit it in any of the above three approximations, one would simultaneously predict transition matrix elements and ground-state correlations very well. This argues, that, as far as the above properties are concerned, the various approximations can all be taken into account by the use of an effective interaction.