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Investigation of the One-Particle-Hole and Projected Hartree-Fock Approximations in C^{12} and O^{16}†

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Calculations are performed, in the one-particle-hole and projected Hartree-Fock (PHF) approximations, for the low-lying 2^+ and 3^- excitations in C^{12} and O^{16}, respectively. A new expression is derived for static moments of excited states in the random-phase approximation (RPA) and general one-particle-hole approximations. The purpose of this study was to investigate: the practical usefulness of the above approximations for nontrivial realistic problems; the validity of the one-particle-hole and PHF approximations for positive- as well as negative-parity excitations; the ability of the equations of motion and PHF methods to predict static moments of excited states; the magnitude of corrections to the RPA with explicit inclusion of ground-state correlations; and the validity of the inconsistent RPA procedure of including backward amplitudes at the expense of violating the Pauli principle. We conclude that the one-particle-hole approximation is particularly appropriate for negative-parity excitations and that the PHF approximation is appropriate for positive-parity excitations.

1. INTRODUCTION

Recent calculations[1-3] suggest that the equations-of-motion formalism[4] and the projected Hartree-Fock (PHF) approximation[5] may be complimentary in providing a powerful framework for the study of nuclear spectroscopy. In the equations-of-motion formalism it has been shown that, with a proper treatment of the Pauli principle, the particle-hole approximation is excellent for the description of negative-parity excitations of even nuclei – we restrict consideration here to even nuclei. On the other hand, the PHF approximation was found to be excellent, not only for the "rotational" excitations of highly deformed nuclei, but, with variation of the intrinsic wave function *after* projection, it is also surprisingly good for the vibrational and vibration-rotational excitations of spherical and transition nuclei.

Our objectives in the present investigation were to answer the following questions:

(i) Are the equations of motion and PHF methods useful for nontrivial realistic problems? In our early studies we considered a model problem and exploited its symmetry.[1] We also considered a nuclear problem[2] with a very restricted configuration space so that solutions could be obtained by brute-force methods. For the present investigation we have used more sophisticated techniques which are generally applicable.

(ii) Are the one-particle-hole equations of motion applicable to positive- as well as negative-parity excitations? Previously, we considered only negative-parity excitations which have the important distinction that two-particle-hole admixtures into predominantly one-particle-hole excitations tend to be suppressed by parity selection rules. Thus one suspected that the one-particle-hole approximation might be very much inferior for positive-parity excitations.

(iii) Are the equations of motion and PHF methods useful for calculating static moments of excited states? It has been shown, in a recent letter by Dreizler, Klein, and Do Dang,[6] that the random-phase approximation (RPA) predicts a static 2^J-pole moment of an excited state of angular momentum J which increases rapidly with increasing interaction strength and becomes unbounded as the RPA energy of that state approaches and becomes zero. Simple explicit expressions are derived in this paper for the 2^J-pole moments predicted by the RPA and general one-particle-hole approximations. We investigate, therefore, whether or not these expressions lead to meaningful results and how they compare with results obtained with the PHF and an exact shell-model diagonalization within the corresponding confuguration space.

(iv) Is the RPA an improvement over the Tamm-Dancoff approximation (TDA)? It has often been asked

whether the inclusion of particle-hole destruction operators in the RPA excitation operators represents a real improvement over the TDA or not. The question arises because the RPA extension to the TDA is achieved at the expense of violating the Pauli principle. We believe that our equations-of-motion formalism is particularly appropriate for answering this equation; since, for the first time, it enables one to extend the RPA to take the Pauli principle fully into account. We return to this question in Sec. 3.

To answer the above questions we have performed calculations on the $J^\pi = 3^-$, $T = 0$, 6.63-MeV state in O^{16} and on the $J^\pi = 2^+$, $T = 0$, 4.43-MeV state in C^{12}. For the O^{16} calculation we were not much concerned with testing the accuracy of the various approximations, since we had gathered this information from our earlier calculation.[2] Thus, we did the most realistic particle-hole and PHF calculations that we could within the $1p$ and $2s$-$1d$ active shells – unrestricted by the fact that an exact diagonalization in this space was out of the question. On the other hand, for the C^{12} calculation, where our main objective was to test the validity of the particle-hole approximation for a positive-parity excitation, it was important that an exact shell-model diagonalization should be possible. Thus, we restricted the space to the $1p$ shell. This is admittedly a small space in which to test the particle-hole approximations. Consequently, our results exagerate the effects of the Pauli principle and the limitations of the particle-hole models. However, nuclear excitations frequently are dominated by just a few particle-hole excitations; thus our stringent tests are not too unreasonable.

2. HAMILTONIAN

The Hamiltonian used in both calculations can be expressed

$$H = H_0 + :V:,$$

where H_0 is a single-particle Hamiltonian and $:V:$ is the two-body residual interaction. The dotted brackets indicate that it is arranged in normal order with respect to the O^{16} $(1s)^4(1p)^{12}$ closed-shell configuration. It is thus a residual interaction for O^{16} in the Hartree-Fock (HF) sense.

The single-particle energies of H_0, given in Table I, were taken from the experimental energies of the so-called "single-particle" states in O^{15} and O^{17} as quoted, for example, by Gillet and Vinh Mau.[7] The two-body interaction is a simple central Yukawa interaction with a Rosenfeld exchange mixture, of form identical to that used by Elliott and Flowers[8] but with a variable strength. It is given explicitly in Ref. 2.

In performing the calculations for C^{12} it was sometimes convenient to express this Hamiltonian in normal order with respect to the $(1s)^4$ particle-hole vacuum and sometimes with respect to the $(1s)^4(1p_{3/2})^8$ vacuum. We nevertheless maintained the same Hamiltonian so that, in whatever form or with whatever strength of residual interaction, it always generated the experimental O^{15}, O^{17} single-particle energies.

3. PARTICLE-HOLE APPROXIMATIONS

The particle-hole and equations-of-motion methods have been described many times previously[1-4]; therefore we restrict ourselves to just sufficient outline to introduce our notation and to give expressions for the static moment of an excited state.

The equations-of-motion approach is to seek excitation operators $O_\lambda^\dagger$ such that $O_\lambda^\dagger$ operates on the ground state $|0\rangle$ to generate an excited state $|\lambda\rangle$, while its Hermitian adjoint O_λ operates on the ground state to annihilate it; viz.

$$O_\lambda^\dagger|0\rangle = |\lambda\rangle, \qquad O_\lambda|0\rangle = 0. \tag{1}$$

These operators obey the equations of motion

$$\langle 0|[\delta O_\lambda, H, O_\lambda^\dagger]|0\rangle = \omega_\lambda \langle 0|[\delta O_\lambda, O_\lambda^\dagger]|0\rangle, \tag{2}$$

where ω_λ is the excitation energy $(E_\lambda - E_0)$ of the state $|\lambda\rangle$, δO_λ is an arbitrary variation on the operator O_λ, and the double commutator $[\delta O_\lambda, H, O_\lambda^\dagger]$ is defined

$$2[\delta O_\lambda, H, O_\lambda^\dagger] \equiv [\delta O_\lambda, [H, O_\lambda^\dagger]] + [[\delta O_\lambda, H], O_\lambda^\dagger]. \tag{3}$$

While the equations of motion, Eq. (2), are formally exact, two approximations must in general be introduced in order to solve them. Firstly, one

TABLE I. O^{16} single-particle energies ϵ_ν obtained from the ostensible single-particle states in O^{15} and O^{17}. The single-particle occupancy factors n_ν are those calculated for the O^{16} ground state with a 40-MeV residual interaction.

Single-particle state ν	$1d_{5/2}$	$1d_{3/2}$	$2s_{1/2}$	$1p_{3/2}$	$1p_{1/2}$	$1s_{1/2}$
ϵ_ν (MeV)	−4.15	0.93	−3.27	−21.80	−15.65	−50.00
n_ν	0.0247	0.0150	0.0046	0.9710	0.9501	0.9980

must assume a truncated space of basis operators. Secondly, one must replace the true ground state, $|0\rangle$, by some approximate model ground state $|\phi\rangle$.

In the particle-hole approximation, the excitation operators are expanded in terms of a finite set of particle-hole creation and destruction operators

$$O_{\lambda JT}^{\dagger} = \sum_{\mathrm{ph}} \frac{Y_{\mathrm{ph}}(\lambda JT) A_{\mathrm{ph}}^{\dagger}(JT) - Z_{\mathrm{ph}}(\lambda JT) A_{\mathrm{ph}}(\bar{J}\bar{T})}{\langle\phi|[A_{\mathrm{ph}}(JT), A_{\mathrm{ph}}^{\dagger}(JT)]|\phi\rangle^{1/2}}, \tag{4}$$

where

$$A_{\mathrm{ph}}^{\dagger}(JT) \equiv A_{\mathrm{ph}}^{\dagger}(JM, TM_T) = (a_{\mathrm{p}}^{\dagger} a_{\mathrm{h}})_{MM_T}^{JT},$$
$$A_{\mathrm{ph}}(\bar{J}\bar{T}) \equiv (-1)^{J+M+T+M_T} A_{\mathrm{ph}}(J-M, T-M_T). \tag{5}$$

In the TDA, the Z coefficients are put identically equal to zero and $|\phi\rangle$, in Eq. (4), is taken to be the HF particle-hole vacuum. The denominator in Eq. (4) then becomes equal to unity.

In the RPA, the particle-hole destruction operators – the so-called backward-going terms – are included, but $|\phi\rangle$ is still taken to be the HF particle-hole vacuum. From one point of view the RPA is therefore inconsistent; for, by admitting the backward-going terms, one recognizes the presence of correlations, i.e., excited particle-hole configurations, in the ground state; however, such correlations are not present in the model ground state $|\phi\rangle$. This inconsistency corresponds to violation of the Pauli principle in the quasiboson and Green's-function formalisms. In view of this inconsistency it is not obvious that the RPA is necessarily better than the TDA for a finite many-body system such as the nucleus.

To answer this question and to investigate the more general usefulness of the equations of motion we used the particle-hole expansion Eq. (4), but for $|\phi\rangle$ took the best shell-model ground state, within the active configuration space, that we could calculate. For O^{16} this meant that we diagonalized for the ground state in the space of zero plus all two-particle-hole configurations after elimination of the spurious center-of-mass excitations. The occupancies of single-particle states calculated for the O^{16} ground state are given in Table I. For C^{12} a complete diagonalization within the $1p$ shell was possible. Thus, for C^{12}, our equations-of-motion calculation corresponds to what we have previously described[1,2] as an "exact one-particle-hole" calculation.

The matrix elements that occur in the TDA and RPA secular matrix equations are very easy to evaluate and are well known. (The equations are given, for example, in Ref. 3.) This is because of the obviously special relationship that exists between particle-hole operators and the particle-hole vacuum. In the more general equations-of-motion calculation we used a mixed-configuration model ground state. It was therefore necessary to evaluate the double commutators that occur in the equations of motion [Eq. (2)] explicitly as a prelude to deriving their ground-state expectations. The methods used are described in detail in Ref. 3.

Transition matrix elements for a Hermitian one-body operator W are given in the one-particle-hole approximation by

$$\langle JT\|W^{JT}\|0\rangle = \sum_{\mathrm{ph}} \langle \mathrm{p}\|W^{JT}\|\mathrm{h}\rangle \times [Y_{\mathrm{ph}} + (-1)^{J+T} Z_{\mathrm{ph}}](n_{\mathrm{h}} - n_{\mathrm{p}})^{1/2}, \tag{6}$$

where n_ν is the fractional occupancy of the single-particle state ν and we take the Y, Z coefficients to be real.

The excitation energies for the 3^- state in O^{16} and the 2^+ state in C^{12}, calculated in the TDA, the RPA, and in the more exact equations-of-motion approximation (labeled E-of-M) are shown in Figs. 1 and 2. For C^{12}, Fig. 2, the results of the exact diagonalization are shown for comparison. Reduced transition probabilities, $B(EJ; J \to 0)$ for electric decay of the excited states are shown in oscillator units as numbers on the curves. The exact results, for C^{12} (Fig. 2), are encircled.

The Y and Z coefficients, together with the cofactor of $\langle \mathrm{p}\|W^{JT}\|\mathrm{h}\rangle$ in Eq. (6), are tabulated in Table II for the 40-MeV E-of-M calculation of the O^{16} 3^- excitation. Thus, to evaluate the transition matrix element of any one-body operator or, for example, calculate an electron scattering form factor, one has simply to multiply these cofactors by the appropriate single-particle reduced matrix elements and sum.

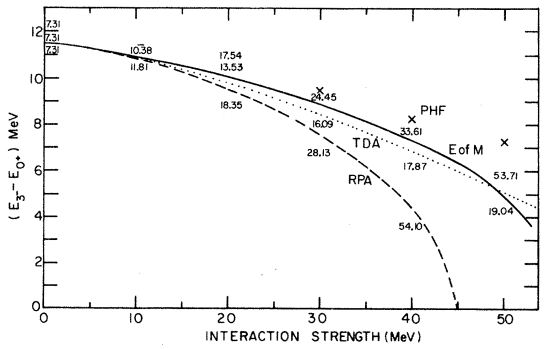

FIG. 1. Excitation energies for the first $J^\pi = 3^-$, $T = 0$ excited state in O^{16}, calculated in the PHF (X), TDA (. . .), RPA (--), and E-of-M (——) approximation, as a function of interaction strength. Reduced transition probabilities, $B(E3; 3 \to 0)$, are shown in oscillator units as numbers on the curves, for all but the PHF approximation.

TABLE II. E-of-M results for the $J^\pi = 3^-$, $T=0$ excitation in O^{16} with a 40-MeV residual interaction: $E_{3^-} - E_0 = 7.32$ MeV.

p h	$1d_{5/2}\,1p_{3/2}$	$1d_{5/2}\,1p_{1/2}$	$1d_{3/2}\,1p_{3/2}$
Y_{ph}	0.4312	0.8720	−0.3892
Z_{ph}	−0.1520	−0.2278	0.1510
$[Y_{ph} + (-1)^{J+T} Z_{ph}] \times (n_h - n_p)^{1/2}$	0.5673	1.0580	−0.5282

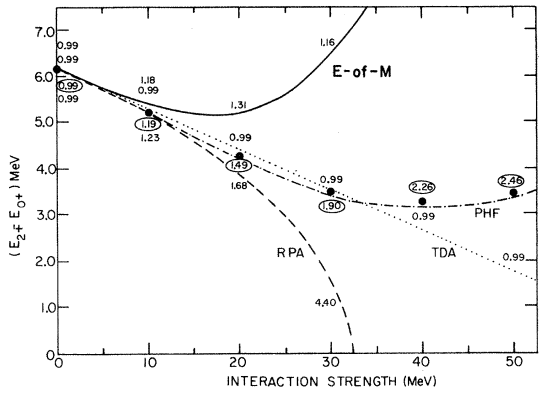

FIG. 2. Excitation energies for the first $J^\pi = 2^+$, $T=0$ excited state in C^{12}, calculated in the PHF (— • —), TDA (. . .), RPA (- -), and E-of-M (——) approximations, as a function of interaction strength. The results of exact diagonalization, within the $1p$ shell, are shown by filled circles. Reduced transition probabilities, $B(E2;\ 2 \rightarrow 0)$, are shown in oscillator units as numbers on the curves, for all but the PHF approximation. The circled numbers are the exact results.

For compactness we shall write $W^{\lambda\tau}$ as W^Λ, so that Λ stands for both angular momentum λ and isospin τ. The expectation of W^Λ in an excited state of angular momentum and isospin Γ is given, in the equations-of-motion formalism, by

$$\langle \Gamma | W^\Lambda | \Gamma \rangle = \langle 0 | [O_\Gamma, W^\Lambda, O_\Gamma{}^\dagger] | 0 \rangle . \tag{7}$$

This expression is readily evaluated. In the RPA, for example, one finds

$$\langle \Gamma \| W^\Lambda \| \Gamma \rangle = \sum_{\mathrm{ph}\,\mathrm{p'h'}} [Y_{\mathrm{ph}}{}^* Y_{\mathrm{p'h'}} + (-1)^\Lambda Z_{\mathrm{ph}} Z_{\mathrm{p'h'}}{}^*] \langle \mathrm{p(h)}^{-1}\Gamma \| W^\Lambda \| \mathrm{p'(h')}^{-1}\Gamma \rangle , \tag{8}$$

which is expanded to give

$$\begin{aligned}\langle \Gamma \| W^\Lambda \| \Gamma \rangle = \sum_{\mathrm{ph}\,\mathrm{p'h'}} & [Y_{\mathrm{ph}}{}^* Y_{\mathrm{p'h'}} + (-1)^\Lambda Z_{\mathrm{ph}} Z_{\mathrm{p'h'}}{}^*] \hat{\Gamma}^2 [\delta_{\mathrm{hh'}} W(\mathrm{hp}\Gamma\Lambda; \Gamma\mathrm{p'}) \langle \mathrm{p} \| W^\Lambda \| \mathrm{p'} \rangle \\ & - (-1)^\Lambda \delta_{\mathrm{pp'}} W(\mathrm{ph}\Gamma\Lambda; \Gamma\mathrm{h'}) \langle \mathrm{h'} \| W^\Lambda \| \mathrm{h} \rangle] ; \end{aligned} \tag{9}$$

we follow the notation of French[9] so that the Racah coefficients are really products of two Racah coefficients – one in angular momentum space and the other in isospin space. The same is true for the phase factor; i.e.,

$$(-1)^\Lambda \equiv (-1)^{\lambda+\tau} . \tag{10}$$

If Γ denotes angular momentum J and isospin T, the quantity $\hat{\Gamma}$ is defined

$$\hat{\Gamma} \equiv [(2J+1)(2T+1)]^{1/2} . \tag{11}$$

The general one-particle-hole equations-of-motion expression for static moments is

$$\begin{aligned}\langle \Gamma \| W^\Lambda \| \Gamma \rangle = \sum_{\mathrm{ph}\,\mathrm{p'h'}} & [Y_{\mathrm{ph}}{}^* Y_{\mathrm{p'h'}} + (-1)^\Lambda Z_{\mathrm{ph}} Z_{\mathrm{p'h'}}{}^*] \hat{\Gamma}^2 \\ & \times [\delta_{\mathrm{hh'}} W(\mathrm{hp}\Gamma\Lambda; \Gamma\mathrm{p'}) \langle \mathrm{p} \| W^\Lambda \| \mathrm{p'} \rangle - (-1)^\Lambda \delta_{\mathrm{pp'}} W(\mathrm{ph}\Gamma\Lambda; \Gamma\mathrm{h'}) \langle \mathrm{h'} \| W^\Lambda \| \mathrm{h} \rangle] \\ & \times \frac{1}{2} \left[\left(\frac{n_\mathrm{h} - n_\mathrm{p}}{n_\mathrm{h'} - n_\mathrm{p'}} \right)^{1/2} + \left(\frac{n_\mathrm{h'} - n_\mathrm{p'}}{n_\mathrm{h} - n_\mathrm{p}} \right)^{1/2} \right] . \end{aligned} \tag{12}$$

Results for the static quadrupole moment of the 2^+ state in C^{12} are shown for the three one-particle-hole approximations in Fig. 3.

4. PROJECTED HARTREE-FOCK APPROXIMATION

Ideally we should perform an unrestricted variation on an "intrinsic" determinantal wave function such that the energy expectation of the projected wave function, whose quantum numbers are those of the state desired, should be minimized. But, since the equations for such a variation are not self-consistent-field equations, such unrestricted variations are impractical. We therefore restrict the number of degrees of freedom that we vary after projection, according to the Lagrange-multiplier method that was proposed and used previous-

ly by some of us.[10]

Briefly, the method is to set up a new Hamiltonian $H(\lambda)$, related to the original H.

$$H(\lambda) = H - \lambda_1 Q_1 - \lambda_2 Q_2 - \ldots, \tag{13}$$

where λ corresponds to a set of Lagrange multipliers $(\lambda_1, \lambda_2, \ldots)$ which constrain the HF solution $\phi(\lambda)$ of $H(\lambda)$ to accept certain values for the static moments $\langle \phi(\lambda) | Q_i | \phi(\lambda) \rangle$. Thus the Q_i are a set of suitably chosen multipole operators. The method is to numerically project from $\phi(\lambda)$ the component having the quantum numbers of the state desired and to evaluate, for this projected state, the expectation of the Hamiltonian H. The appropriate set of multipliers are then the ones which minimize this energy expectation. To gain the advantages of variation after projection, the variation must, of course, be performed independently for different projected states.

Now it is clear that if one is interested, for example, in quadrupole excitations and quadrupole-quadrupole correlations in the ground state, then a quadrupole operator must be included in the set Q_i.

In the calculations reported here, we maintained axial symmetry, time-reversal invariance, and good isospin for the intrinsic wave function. We also restricted the number of Lagrange multipliers to one in each case. More general variations after projection can, however, be performed and lead to improved results.

For the 3^- calculation in O^{16}, we used an $r^3 Y_{30}$ operator to constrain the intrinsic wave function. For the 2^+ calculation in C^{12}, we used $r^2 Y_{20}$. The angular momentum projection was achieved numerically with a code supplied by Gunye.[11]

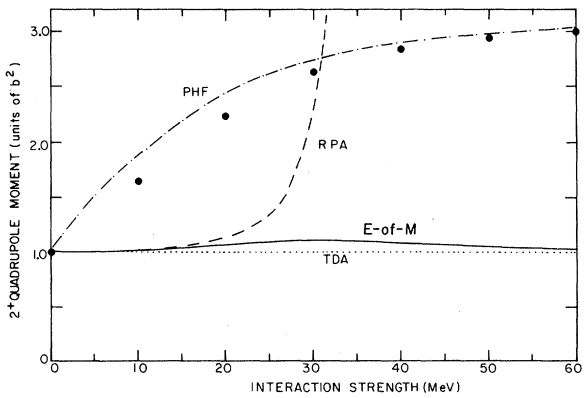

FIG. 3. The quadrupole moment of the first $J^\pi = 2^+$, $T = 0$ excited state in C^{12}, calculated in the PHF (—·—), TDA (. . .), RPA (--), and E-of-M (——) approximations as a function of interaction strength. The results of exact diagonalization within the $1p$ shell are shown by filled circles.

The result obtained for the excitation energies in O^{16} and C^{12} are shown, respectively, in Figs. 1 and 2. Since the ground and excited states were projected from different intrinsic determinants, transition matrix elements are more difficult to evaluate and are therefore not indicated, for this method, on the figure. However, the static quadrupole moment for the 2^+ state in C^{12} was calculated and is shown in Fig. 3.

5. DISCUSSION

As a result of our calculations we deduce that the general one-particle-hole equations-of-motion approximation provides a useful and practical procedure for the calculation of nuclear excitation energies and transitions. As found in our previous calculation,[2] the results for negative-parity excitations are excellent for small and intermediate interaction strengths, but deteriorate as the interaction strength increases beyond the value at which the HF phase transition occurs. In the present calculation the E-of-M excitation energy continues to fall, with increasing interaction strength, and eventually goes through zero and becomes imaginary. If the model ground state were exact this could not happen.[4] Our ground state, however, included only two-particle-hole excited configurations. Thus the fact that the E-of-M excitation energy goes imaginary indicates the buildup of many particle-hole configurations in the true ground state at large interaction strengths.

For positive-parity excitations the E-of-M results deteriorate much more rapidly with increasing strength. Since the ground state employed for the C^{12} calculation was exact within the configuration space considered, the deviation of the equations-of-motion results from the exact results can only be due to truncation of the 2^+ excitation operator to the one-particle-hole space. In this respect, positive-parity excitations differ in a fundamental way from negative-parity excitations for which two-particle-hole excitation processes tend to be suppressed by parity selection rules.

The PHF method is also useful, although for practical purposes its validity is restricted to the lowest excitations of a given spin and parity. Furthermore, in view of the fact that because of the repeated angular momentum projection PHF calculations are computationally much slower than corresponding HFP calculations (HF variation before projection), and because of the fact that negative-parity calculations in general involve a minimum of three major shells, the PHF approximation is much more appropriate for positive-parity states than for negative.

In view of the fact that one can only vary a very

restricted number of degrees of freedom, another limitation of the PHF method is that one must have some *a priori* physical insight into the nature of the correlations that are significant. For the so-called *collective* excitations, one gains this insight from the phenomenological models of volume-conserving vibrational shape fluctuations. Thus one naturally chooses constraining fields which resemble the self-consistent fields that would be generated by corresponding shape deformations of the nucleus. But this limitation is also an asset; for having generated correlated wave functions by such a PHF procedure, one has an immediate insight into their physical character. In particular, the PHF method is valuable for investigating the properties of the ground state and low-lying 2^+ state in the region of the HF phase transition.

Thus we find that the PHF and equations-of-motion methods are complementary; the PHF method can be used for the lowest positive-parity states, while the equations-of-motion method is ideally suited for negative-parity excitations. For open-shell nuclei, this suggests the possibility of using the PHF procedure to generate an uncorrelated ground state for a subsequent equations-of-motion calculation of negative-parity excitations built upon it.[12]

We find (Fig. 3) that the PHF method gives satisfactory results for static moments, particularly in the strong-interaction limit, but none of the one-particle-hole approximations is acceptable in this respect. In particular, the divergence of the RPA result at the point of the HF phase transition is completely spurious. This divergence can be attributed directly to the uncontrolled buildup of the backward-going amplitudes in the RPA which are constrained by the Pauli principle in the more exact equations-of-motion treatment. The inadequacy of the one-particle-hole approximations is due to the neglect of two-particle-hole components in the excitation operators. These components are less important for the calculation of transition matrix elements. Since transition operators are one-body operators, the two-particle-hole components only participate indirectly through the normalization. For static moments, however, they contribute directly in a big way. In the small interaction limit, one can readily show that the amplitude of the two-particle-hole components enter quadratically in the expression for the excitation energy and transition matrix elements, but linearly for static moments. This is confirmed by inspection of Figs. 2 and 3.

Finally, we find (Fig. 2), as in previous calculations,[1,2] that the inclusion of backward-going amplitudes, as in the RPA, lowers the excitation energy; but the inclusion of explicit ground-state correlations, as in the exact one-particle-hole equations, raises the excitation energy. Thus the RPA excitation energies are too low, whereas the TDA, which ignores both effects, is much closer to the results of an exact diagonalization. On the other hand, the reduced transition probability for decay of the excited state is given much better in the RPA and better still in the exact one-particle-hole approximation. If the practical procedure is adopted in an RPA calculation of taking single-particle energies from experiment and adjusting the strength of the residual interaction to fit the excitation energy, then good results can be obtained for transition matrix elements by including occupancy renormalization factors according to Eq. (6). Methods for calculating single-particle occupancies have been discussed in many papers.[1,2,13]

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