

# Scalar ground-state observables in the random phase approximation

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We calculate the ground-state expectation value of scalar observables in the matrix formulation of the random phase approximation (RPA). Our expression, derived using the quasiboson approximation, is a straightforward generalization of the RPA correlation energy. We test the reliability of our expression by comparing against full diagonalization in  $0\hbar\omega$  shell-model spaces. In general the RPA values are an improvement over mean-field (Hartree-Fock) results, but are not always consistent with shell-model results. We also consider exact symmetries broken in the mean-field state and whether or not they are restored in RPA.

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## I. INTRODUCTION

Mean-field theory is the starting point for most microscopic models of many-body systems such as nuclei. In fact, for *global* studies of nuclear properties, such as nuclear binding energies, mean-field theory in the form of Hartree-Fock (HF) and related approximations is still the only viable microscopic approach [1]; otherwise one turns to semiclassical methods such as the liquid drop [2] and Thomas-Fermi methods [3].

Unfortunately, mean-field theory ignores particle-hole correlations and can break fundamental symmetries such as rotational and translational invariance. The next logical step beyond the static mean field is known as the random phase approximation (RPA) which can be derived in the small amplitude limit of time-dependent mean-field theory, and which implicitly allows for small correlations in the ground state [4–6].

The main applications of RPA have been to transition strengths and excitation spectra. One can also calculate the correction to the ground state energy due to RPA correlations, which was the basis of a recent proposal to use mean-field + RPA to compute global binding energy systematics [7].

There are other potential quantities of interest, namely, the ground state expectation value of observables other than the Hamiltonian. An important application is the root-mean-square radius. Any global fit of nuclear systematics involves both binding energies and nuclear radii. Indeed, most global fits to binding energies and radii with nonrelativistic phenomenological interactions such as Skyrme require density-dependent forces, although we will not deal specifically with that issue in this paper. Further challenges to mean-field calculations are isotopic shifts in the charge radius [8], and parity-violating electron scattering, which is sensitive to the difference between the neutron and proton rms radii [9].

In Sec. II of this paper we present an expression for the

ground-state expectation value of a general observable in RPA. This expression is derived using the quasiboson approximation, in exact analogy with the RPA correlation energy, and is a generalization of the RPA one-particle density derived by Rowe [4,10]. Because the RPA ground state is approximated by a quasiboson vacuum, one can read off directly the expectation value without having to construct an explicit wave function. Other, more recent work [11] discusses briefly the computation of RPA observables using the response-function formalism, but does not make any systematic study.

Having an expression is not sufficient. Does it produce useful and reliable results? After all, RPA is an approximation, and because it violates the Pauli exclusion principle RPA is not even variational. Despite this, rigorous tests of the accuracy of RPA calculations have been spotty. For example, although the RPA correlation energy has been in the literature for decades, the only tests were in toy models [12]. Recently we compared the RPA correlation energy against exact shell-model results [13]. We found that generally RPA gave very good agreement—albeit with some significant failures which reduce the reliability of RPA binding energies.

We continue this program by computing the ground-state expectation value of observables both in exact shell-model calculations and in RPA. As discussed below, in this paper we limit ourselves to scalar operators. Unfortunately in  $0\hbar\omega$  harmonic oscillator model spaces  $\langle R^2 \rangle$  is trivial, so we instead compute and compare the expectation values of a one-body operator: the number of particles outside the  $0d_{5/2}$  orbit; and several two-body operators:  $S^2$ ,  $L^2$ ,  $Q^2$ , and the pairing Hamiltonian  $H_{\text{pair}} = P^\dagger P$ .

The results are found in Sec. III. In general, RPA offers an improvement over the mean-field (HF) expectation values. This is not always the case, however, and even when HF + RPA is closer to the exact shell-model results than HF values, the improved agreement is sometimes still unsatisfactory. (The situation is reminiscent of variational calculations, where one typically gets much better agreement in energy than in the wave function. But again, RPA is not a variational theory.)

In Sec. IV we turn to another issue of relevance to RPA:

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the restoration of symmetries, such as rotational invariance, broken by the mean field. We compute the expectation value of  $J^2$  and compare the exact shell-model result against the Hartree-Fock and RPA values. If RPA “restores” the broken symmetry then one expects that either one regains the correct ground state value of  $J^2$  or gets a much better value than the Hartree-Fock value. We find that, although often  $\langle J^2 \rangle$  is improved by RPA corrections, one does not always regain a very good estimate of the ground state angular momentum. We interpret this to mean that RPA only approximately restores broken symmetries.

Nonetheless, we consider our results relevant. The RPA is not new, but we remind the reader that for global approaches to nuclear structure the state of the art is still mean-field theory; *ab initio* methods can only be applied to very light nuclei, and shell model diagonalization can only be applied piecewise. Consistent calculations using HF+RPA throughout the nuclides is conceivable, however, and this paper is part of a larger program to rigorously test the reliability of RPA as an approximation to much larger microscopic calculations.

## II. CORRECTIONS TO A GENERAL OPERATOR IN RPA

Before we derive the expectation value of an operator in RPA, we first begin with a brief pedagogical review of the derivation of the RPA correlation energy, including proper treatment of zero modes that correspond to broken symmetries. The RPA expectation value of a general operator then follows naturally.

There are many ways to derive RPA [5,6]. One approach is to expand the energy about the Hartree-Fock minimum. Let  $|\text{HF}\rangle$  be the Hartree-Fock Slater determinant, and let  $|\Psi(\vec{Z})\rangle = \exp(\sum_m Z_m^* \hat{c}_m^\dagger \hat{c}_i) |\text{HF}\rangle$  be small perturbations from the Hartree-Fock state. We follow the usual convention where  $m, n$  denote single-particle states above the Fermi surface in the Hartree-Fock state, or “particle” states, while  $i, j$  denote “hole” states below the Fermi surface. Then one can expand the energy surface  $E(\vec{Z})$  in the vicinity of the Hartree-Fock minimum in terms of the particle-hole amplitudes  $\{Z_{mi}\}$  up to second order:

$$E(\vec{Z}) = E_{\text{HF}} + \vec{z}^\dagger \mathbf{A} \vec{z} + \frac{1}{2} \vec{z}^\dagger \mathbf{B} \vec{z}^* + \frac{1}{2} \vec{z}^T \mathbf{B} \vec{z}, \quad (1)$$

where

$$A_{nj,mi} \equiv \langle \text{HF} | [\hat{c}_j^\dagger \hat{c}_n, [\hat{H}, \hat{c}_m^\dagger \hat{c}_i]] | \text{HF} \rangle, \quad (2)$$

$$B_{nj,mi} \equiv \langle \text{HF} | [[\hat{H}, \hat{c}_n^\dagger \hat{c}_j], \hat{c}_m^\dagger \hat{c}_i] | \text{HF} \rangle. \quad (3)$$

We restrict ourselves to real wave functions, so that  $\mathbf{A}$ ,  $\mathbf{B}$  are also real. There is no linear term in Eq. (1) because  $\langle \text{HF} | [\hat{H}, \hat{c}_m^\dagger \hat{c}_i] | \text{HF} \rangle = 0$  by the definition of the Hartree-Fock state. This quadratic surface can be mapped to a harmonic oscillator, replacing the  $Z_{mi}$  by boson operators  $b_{mi}^\dagger$

$$\hat{H}_B = E_{\text{HF}} + \vec{b}^\dagger \mathbf{A} \vec{b} + \frac{1}{2} \vec{b}^\dagger \mathbf{B} \vec{b}^\dagger + \frac{1}{2} \vec{b} \mathbf{B} \vec{b}, \quad (4)$$

which has analogous commutation relations, e.g.,  $A_{nj,mi} = \langle 0 | [\hat{b}_{nj}, [\hat{H}_B, \hat{b}_{mi}^\dagger]] | 0 \rangle$ , etc. The boson Hamiltonian can be written in matrix form, which induces an additional constant term

$$H_B = E_{\text{HF}} - \frac{1}{2} \text{Tr} \mathbf{A} + \frac{1}{2} (\vec{b}^\dagger \vec{b}) \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix} \begin{pmatrix} \vec{b} \\ \vec{b}^\dagger \end{pmatrix}. \quad (5)$$

We want to put Eq. (5) into diagonal form, the first step of which is to solve the well-known RPA matrix equation

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix} \begin{pmatrix} \vec{X} \\ \vec{Y} \end{pmatrix} = \Omega \begin{pmatrix} \vec{X} \\ \vec{Y} \end{pmatrix}. \quad (6)$$

The solutions have normalization  $\vec{X}^2 - \vec{Y}^2 = 1$ .

Before going on one must treat carefully the case of zero modes  $\Omega_\nu = 0$ . Zero modes arise in RPA when an exact symmetry is broken. Suppose the HF state is deformed. The HF energy will not change as the orientation is rotated; this invariance is reflected in  $E(\vec{Z})$  and resurfaces as RPA zero modes. (This is also a good check of one’s RPA codes. One expects three zero-frequency modes for triaxially deformed states, and two zero modes for an axisymmetric deformed state: rotation about an axis of symmetry takes one to the same, indistinguishable state. If one’s model space admits spurious center-of-mass motion, then one would expect three additional zero modes as well.) One cannot define properly normalized  $\vec{X}, \vec{Y}$  for zero modes. Instead one introduces collective coordinates  $\vec{Q}_\nu$  and conjugate momenta  $\vec{P}_\nu$  [4,5,14], which satisfy

$$\begin{aligned} \mathbf{A} \vec{P}_\nu - \mathbf{B} \vec{P}_\nu^* &= i M_\nu \Omega_\nu^2 \vec{Q}_\nu, \\ \mathbf{A} \vec{Q}_\nu - \mathbf{B} \vec{Q}_\nu^* &= -\frac{i}{M_\nu} \vec{P}_\nu. \end{aligned} \quad (7)$$

Here  $M_\nu$  is a constant, interpretable as mass or moment of inertia but whose value depends on the normalization of  $P, Q$ , which are only constrained by

$$\vec{Q}_\lambda^* \cdot \vec{P}_\nu - \vec{Q}_\lambda \cdot \vec{P}_\nu^* = i \delta_{\lambda\nu}. \quad (8)$$

Now one obtains a generalized Bogoliubov transformation of the boson operators  $\hat{b}, \hat{b}^\dagger$ , not only to quasibosons  $\hat{\beta}, \hat{\beta}^\dagger$ , but also to the zero-mode collective coordinate operator  $\hat{Q}_\nu$  and conjugate momentum operator  $\hat{P}_\nu$ :

$$\begin{aligned} \hat{b}_{mi} &= \sum_{\lambda, \Omega_\lambda > 0} (X_{mi,\lambda} \hat{\beta}_\lambda + Y_{mi,\lambda} \hat{\beta}_\lambda^\dagger) \\ &\quad - i \sum_{\nu, \Omega_\nu = 0} (P_{mi,\nu} \hat{Q}_\nu - Q_{mi,\nu} \hat{P}_\nu). \end{aligned} \quad (9)$$

Application of Eq. (9) and its Hermitian conjugate to Eq. (5) puts it in diagonal form:

$$H_B = E_{\text{RPA}} + \sum_{\lambda} \Omega_{\lambda} \beta_{\lambda}^{\dagger} \beta_{\lambda} + \sum_{\nu, \Omega_{\nu}=0} \frac{\hat{P}_{\nu}^2}{2M_{\nu}}. \quad (10)$$

The ground state is the quasiboson vacuum, and one can easily read off the RPA ground state energy, which is just the zero-point energy

$$E_{\text{RPA}} = E_{\text{HF}} - \frac{1}{2} \text{Tr}(A) + \frac{1}{2} \text{Tr}(\Omega). \quad (11)$$

One can expand

$$\mathbf{A} = \mathbf{X}\Omega\mathbf{X}^{\dagger} + \mathbf{P}\mathbf{M}^{-1}\mathbf{P}^{\dagger}, \quad (12)$$

where the second term is restricted to zero modes, and then obtain an expression equivalent to Eq. (11),

$$E_{\text{RPA}} = - \sum_{\lambda} \Omega_{\lambda} |\vec{Y}_{\lambda}|^2 - \frac{1}{2} \sum_{\nu, \Omega_{\nu}=0} \frac{1}{M_{\nu}} |\vec{P}_{\nu}|^2, \quad (13)$$

an expression which explicitly segregates out the contribution from zero modes.

The above derivation of the RPA correlation energy  $-\frac{1}{2} \text{Tr}(A) + \frac{1}{2} \text{Tr}(\Omega)$  is well known. We derive the RPA expectation value of any generator operator  $\hat{\mathcal{O}}$  in exactly analogous fashion. Define  $\tilde{A}$ ,  $\tilde{B}$  as in Eqs. (2) and (3), respectively, by replacing the Hamiltonian by the observable  $\mathcal{O}$ , that is,

$$\tilde{A}_{nj,mi}(\mathcal{O}) \equiv \langle \text{HF} | \hat{c}_j^{\dagger} \hat{c}_n \cdot [\hat{\mathcal{O}}, \hat{c}_m^{\dagger} \hat{c}_i] | \text{HF} \rangle, \quad (14)$$

$$\tilde{B}_{nj,mi}(\mathcal{O}) \equiv \langle \text{HF} | [[\hat{\mathcal{O}}, \hat{c}_n^{\dagger} \hat{c}_j], \hat{c}_m^{\dagger} \hat{c}_i] | \text{HF} \rangle, \quad (15)$$

and define  $o_{mi} = \langle \text{HF} | [c_m^{\dagger} c_i, \mathcal{O}] | \text{HF} \rangle$ , which does not in general vanish. (Because we restrict the Hartree-Fock state to real Slater determinants  $\tilde{A}$ ,  $\tilde{B}$ , and  $o$  are real.) Please note that in computing  $\tilde{A}$ ,  $\tilde{B}$ , and  $o$  one still uses the Hartree-Fock state from minimizing the Hamiltonian  $\hat{H}$ , *not* from minimizing  $\hat{\mathcal{O}}$ ; we are finding the expectation value  $\langle \hat{\mathcal{O}} \rangle$  in the vicinity of the minimum of  $\langle \hat{H} \rangle$ .

The form of the operator in the harmonic oscillator bosons is

$$\begin{aligned} \hat{\mathcal{O}}_B = & \mathcal{O}_{\text{HF}} - \frac{1}{2} \text{Tr} \tilde{\mathbf{A}} + \begin{pmatrix} \vec{o} & \vec{o} \end{pmatrix} \cdot \begin{pmatrix} \vec{b} \\ \vec{b}^{\dagger} \end{pmatrix} \\ & + \frac{1}{2} \begin{pmatrix} \vec{b}^{\dagger} & \vec{b} \end{pmatrix} \cdot \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathbf{B}} \\ \tilde{\mathbf{B}} & \tilde{\mathbf{A}} \end{pmatrix} \cdot \begin{pmatrix} \vec{b} \\ \vec{b}^{\dagger} \end{pmatrix}. \end{aligned} \quad (16)$$

By transforming to the collective quasibosons (9), we again can trivially read off the quasiboson vacuum expectation value, which is the RPA ground-state expectation value, without explicit construction of a wave function:

$$\mathcal{O}_{\text{RPA}} = \mathcal{O}_{\text{HF}} - \frac{1}{2} \text{Tr} \tilde{\mathbf{A}} + \frac{1}{2} \text{Tr} \Theta, \quad (17)$$

where

$$\Theta = \mathbf{X}^T \cdot \tilde{\mathbf{A}} \cdot \mathbf{X} + \mathbf{Y}^T \cdot \tilde{\mathbf{A}} \cdot \mathbf{Y} + \mathbf{X}^T \cdot \tilde{\mathbf{B}} \cdot \mathbf{Y} + \mathbf{Y}^T \cdot \tilde{\mathbf{B}} \cdot \mathbf{X}. \quad (18)$$

Substitution of Eq. (6) with  $A, B$  derived from the Hamiltonian immediately regains the RPA binding energy (11). It is important to emphasize again that the  $X, Y$  used here are those calculated from Eq. (6) using the *original*  $A, B$  matrices (from the Hamiltonian); one does *not* compute  $X, Y$  using  $\tilde{A}, \tilde{B}$ .

As before we can rewrite Eq. (17) into an expression with explicit segregation of the zero modes

$$\begin{aligned} \mathcal{O}_{\text{RPA}} = & \mathcal{O}_{\text{HF}} + \sum_{\lambda(\Omega_{\lambda}>0)} \sum_{mi,nj} (\tilde{A}_{mi,nj} Y_{mi,\lambda} Y_{nj,\lambda} \\ & + \tilde{B}_{mi,nj} Y_{mi,\lambda} X_{nj,\lambda}) \\ & - \frac{1}{2} i \sum_{\mu(\Omega_{\mu}=0)} \sum_{mi,nj} \tilde{A}_{mi,nj} (P_{mi,\mu}^* Q_{nj,\mu} - Q_{mi,\mu}^* P_{nj,\mu}). \end{aligned} \quad (19)$$

We have confirmed numerically that Eq. (19) yields the same values as Eq. (17).

As we will see in the next section, Eq. (17) reduces to that derived by Rowe for one-particle densities in spherical nuclei [4,10]. If  $\hat{\mathcal{O}}$  is a scalar, so that it is invariant under rotation, translation, etc., then the above is sufficient. Nonscalar observables require a little more thought. In particular, consider observables that are angular momentum tensors  $\hat{\mathcal{O}}_{\kappa,\mu}$ , with a nonzero rank  $\kappa$ . Here  $\mu$  is the magnetic quantum number. If one applies the generalized Bogoliubov transformation (9) then the linear terms in  $o_{mi}$  do not vanish. The linear terms proportional to the quasiboson operators  $\hat{\beta}, \hat{\beta}^{\dagger}$  are transitions to excited states; but, for nonscalars, there will be terms also proportional to  $\hat{Q}_{\nu}$  and to  $\hat{P}_{\nu}$ . Furthermore, there will be quadratic terms, such as  $\hat{\beta}^{\dagger} \hat{\beta}, \hat{\beta} \hat{\beta}$ , etc., which manifestly do not contribute to the ground state, but also terms quadratic in  $\hat{Q}, \hat{P}$ . These terms arise from rotations (and in the more general case, translations, etc.): because they correspond to zero-frequency modes, they connect only to the ground state, but in a different orientation. If  $\hat{\mathcal{O}}_{\kappa,\mu}$  is a spherical tensor, we know how it transforms under a rotation, and the linear and quadratic terms in  $\hat{Q}$ , etc., are simply the linear and quadratic terms for small rotation angles. Nonetheless, the issue of nonscalar observables is not trivial, and we leave it to future work.

To summarize a first result of the present work, we have extended the usual expansion of the Hamiltonian operator in the neighborhood of the HF solution to any operator, with the purpose to incorporate RPA correlations in computation of expectation values of relevant observables. In the next section we test the reliability of this formula in a nontrivial model, that is, the shell-model restricted space using realistic Hamiltonians.

### III. RPA vs SHELL MODEL FOR SCALAR OBSERVABLES

In this section we test the RPA expectation value found in Eqs. (17), (19), against an exact numerical solution computed by diagonalizing a Hamiltonian in a shell-model basis. We work in complete  $0\hbar\omega$  spaces where the valence particles are restricted to the single-particle states of a single major harmonic oscillator shell, e.g.,  $1s_{1/2}-0d_{3/2}-0d_{5/2}$  for  $sd$  or  $1p_{1/2}-1p_{3/2}-0f_{5/2}-0f_{7/2}$  for  $pf$  shell. The cores are inert,  $^{16}\text{O}$  for the  $sd$  and  $^{40}\text{Ca}$  for the  $pf$  shell. In the the valence space we use realistic interactions: Wildenthal ‘‘USD’’ in the  $sd$  shell [15] and the monopole-modified Kuo-Brown ‘‘KB3’’ in the  $pf$  shell [16]. Note that a  $0\hbar\omega$  model space does not admit any spurious center-of-mass motion, because the generators of center-of-mass motion are  $1\hbar\omega$  in character [17].

As mentioned in the Introduction, an operator one would like to measure is  $R^2$ . Unfortunately in a  $0\hbar\omega$  shell-model space  $\langle R^2 \rangle$  is trivial. The operator  $R^2$  has two pieces, a one-body piece  $r^2$ , which has a constant expectation value in a single major harmonic oscillator shell, and a two-body piece  $r(1) \cdot r(2)$ ; but because  $r$  is an odd-parity operator, the two-body piece is nonzero only across major shells. Therefore in this paper we consider other one- and two-body operators.

#### A. One-body operators

Using the quasiboson approximation, Rowe derived the RPA one-particle densities for spherical nuclei [4,10]; related formulas have been used to compute the isotope shift in calcium [8], ignoring the two-body contribution. Let  $\rho_M = \langle c_M^\dagger c_M \rangle$  be the number of particles excited above the Fermi surface into the particle state  $M$ . ( $M$  is not a magnetic quantum number.) Here  $\tilde{A}_{mi,nj} = \delta_{ij} \delta_{mM} \delta_{nM}$  and from Eq. (19)

$$\rho_M = \sum_{\lambda} \sum_i |Y_{Mi,\lambda}|^2, \quad (20)$$

which is Rowe’s result for *spherical* Hartree-Fock states. If the HF state is deformed, however, one has to take into account zero modes. The second term in Eq. (19) can be simplified if one sums over all particle states  $M$ , that is, the total number of particles excited above the Fermi surface; in that case one can use Eq. (8) and find

$$\sum_M \rho_M = \sum_{\lambda} \sum_{Mi} |Y_{Mi,\lambda}|^2 - \frac{1}{2} N_{\text{zero}}, \quad (21)$$

where  $N_{\text{zero}}$  is the number of zero modes,  $N_{\text{zero}}=2$  for an axisymmetric Hartree-Fock state, such as for  $^{20}\text{Ne}$ , and  $=3$  for a triaxial state, found for  $^{24}\text{Mg}$ . We find Eq. (21) often leads to negative occupation numbers. Note, however, that  $\sum \rho_M$  is not an angular momentum scalar, nor even a spherical tensor of fixed rank, for deformed states.

Instead we considered the only scalar one-body operators in our system, the occupation numbers of a  $j$  shell. Table I tabulates the Hartree-Fock, RPA, and exact shell-model (SM) values of  $n(d_{3/2}) + n(s_{1/2})$ . The results are rather poor, ex-

TABLE I. The number of particles in the  $d_{3/2}+s_{1/2}$  orbits ( $\dagger=f_{7/2}$  orbit for  $^{48}\text{Ca}$ ). An asterisk denotes nuclides with spherical Hartree-Fock states.

Nucleus	HF	RPA	SM
$^{20}\text{Ne}$	1.60	1.75	1.60
$^{22}\text{Ne}$	1.49	1.64	1.47
$^{24}\text{Mg}$	2.13	1.85	2.31
$^{28}\text{Si}$	3.87	3.77	3.15
$^{20}\text{O}$	0.24	0.46	0.54
$^{21}\text{O}$	0.06	0.53	0.38
$^{22}\text{O}^*$	0.00	0.67	0.54
$^{24}\text{O}^*$	2.00	2.50	2.25
$^{48}\text{Ca}^{\dagger}$	8.00	7.73	7.78
$^{22}\text{Na}$	1.51	1.69	1.52
$^{26}\text{Al}$	2.29	2.51	2.18
$^{19}\text{F}$	1.02	1.10	1.52
$^{21}\text{F}$	0.84	0.56	0.87
$^{25}\text{Mg}$	2.21	3.09	1.96

cept for three cases with spherical Hartree-Fock states,  $^{22}\text{O}$ ,  $^{24}\text{O}$ , and  $^{48}\text{Ca}$  [for which we instead tabulate  $n(f_{7/2})$ ].  $^{21}\text{O}$  is weakly deformed and also shows a reasonable, albeit imperfect, improvement as one goes from the Hartree-Fock value to the RPA value.

To explore this issue further, we took  $^{28}\text{Si}$  and lowered the  $d_{5/2}$  single-particle energy; eventually the Hartree-Fock state changes from deformed to spherical. The results are plotted in Fig. 1. Again we see reasonable agreement for the spherical region, but poor agreement in the deformed regime.

To summarize our results for one-body operators: we regain, for spherical Hartree-Fock states, Rowe’s one-particle occupation numbers, and get improved values over the Hartree-Fock occupation numbers. For deformed nuclides, however, the RPA value is generally worse than the HF value. The fault does not appear to lie in the corrections due to zero modes; in the next section, we will find that the RPA expectation value of  $J^2$  is more accurate in the deformed regime than in the spherical regime.

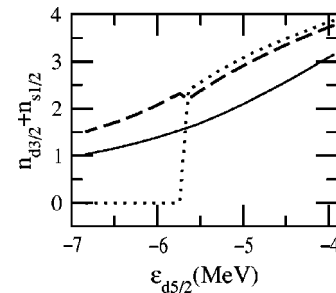


FIG. 1.  $n(d_{3/2}) + n(s_{1/2})$  in  $^{28}\text{Si}$  as the  $d_{5/2}$  single-particle energy is lowered relative to the other single-particle energies. The solid line is the (exact) shell-model value, the dotted line the HF value, and the dashed line the RPA value.

TABLE II. Ground-state expectation values of  $S^2$  and  $L^2$  for several nuclei in  $sd$  and  $pf$  shells. For each observable we show the SM, HF, and RPA estimates. The nuclides have been grouped into even-even, single-species, odd-odd, and odd- $A$ .

Nucleus	$S^2$			$L^2$		
	HF	RPA	SM	HF	RPA	SM
$^{20}\text{Ne}$	0.35	0.33	0.26	15.90	-0.25	0.26
$^{22}\text{Ne}$	1.48	0.48	0.88	16.76	0.31	0.88
$^{24}\text{Mg}$	1.39	1.38	1.03	20.65	-1.17	1.03
$^{26}\text{Mg}$	2.04	1.14	1.45	18.94	-0.34	1.45
$^{28}\text{Si}$	1.62	1.28	1.45	21.50	-0.75	1.45
$^{44}\text{Ti}$	1.03	0.75	0.64	30.34	-2.48	0.64
$^{46}\text{Ti}$	2.24	1.20	1.36	29.72	-2.94	1.36
$^{48}\text{Cr}$	3.12	0.99	1.70	29.77	5.38	1.70
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$^{20}\text{O}$	1.50	0.45	0.75	6.80	0.92	0.75
$^{22}\text{O}$	2.40	-0.15	1.26	2.40	6.36	1.26
$^{24}\text{O}$	2.40	-0.27	1.29	2.39	6.06	1.29
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$^{20}\text{F}$	2.00	1.44	1.74	14.21	8.09	3.55
$^{22}\text{Na}$	2.20	1.90	2.14	21.32	9.08	8.07
$^{26}\text{Al}$	3.14	1.96	1.45	29.56	20.14	1.45
$^{46}\text{V}$	2.51	1.50	1.36	35.39	16.33	1.36
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$^{19}\text{F}$	1.09	0.80	0.87	12.61	4.39	0.22
$^{21}\text{F}$	2.11	0.76	1.52	13.31	5.60	6.41
$^{21}\text{Ne}$	1.11	0.44	1.00	17.55	10.11	3.22
$^{23}\text{Na}$	2.02	0.88	1.15	18.81	7.46	3.93
$^{25}\text{Mg}$	2.04	0.38	1.73	22.56	11.77	7.68

### B. Two-body operators

We now turn to two-body operators, or more properly operators with both one- and two-body pieces. (We investigated the pure two-body pieces but found no qualitative differences; the pure two-body pieces performed neither better nor worse on the whole than the one-body pieces, which here are linear combinations of number operators.)

In Table II we show results for  $S^2$  (total spin) and  $L^2$  (total orbital angular momentum). The RPA expectation value is generally a significant improvement over the Hartree-Fock value, relative to the exact result. On the other hand, the RPA values, while closer to the mark, are not in very good agreement with the exact shell-model values, and sometimes overcorrect to negative, nonphysical expectation values (this can happen because RPA does not respect the Pauli exclusion principle).

In Table III we consider the expectation value of the pairing interaction,  $P^\dagger P$  where  $P^\dagger = \sum_{j,m>0} a_{j,m}^\dagger a_{j,-m}^\dagger$ , and of  $Q^2$ . We also show the ratio of correlation energies [13] which is a measure of how well the RPA binding energy tracks the exact binding energy. There appears to be no correspondence: a good RPA value for the binding energy does not correspond to a good RPA expectation value. In particular, note the single-species (oxygen) results, where the RPA binding energy is particularly bad; yet for these nuclides  $\langle P^\dagger P \rangle$  and  $\langle Q^2 \rangle$  are very good.

TABLE III. Ground-state expectation values of  $P^\dagger P$  (pairing) and  $Q^2$ . The final column is the ratio of the RPA correlation energy to the shell-model correlation energy, and =1 when the RPA binding energy is equal to the exact binding energy.

Nucleus	Pairing			$Q^2$			$\frac{E_{\text{HF}} - E_{\text{RPA}}}{E_{\text{HF}} - E_{\text{SM}}}$
	HF	RPA	SM	HF	RPA	SM	
$^{20}\text{Ne}$	2.99	5.47	6.81	715	825	793	0.75
$^{22}\text{Ne}$	3.99	7.25	9.31	876	1007	944	0.97
$^{24}\text{Mg}$	5.99	10.14	11.72	1167	1263	1268	0.92
$^{26}\text{Mg}$	6.99	11.51	14.56	1001	1104	1048	0.94
$^{28}\text{Si}$	8.99	12.73	15.16	1304	1389	1214	0.90
$^{20}\text{O}$	2.00	5.18	7.25	257	353	339	1.09
$^{22}\text{O}$	3.00	5.83	6.20	163	277	270	1.67
$^{24}\text{O}$	4.00	6.52	6.58	122	194	191	1.83

Again we look at the transition from deformed to spherical in  $^{28}\text{Si}$  for  $\langle Q^2 \rangle$  and  $\langle P^\dagger P \rangle$ , in Fig. 2, which clearly shows the RPA values are in better agreement in the spherical regime than in the deformed regime. (As it happens, of the nuclides we investigated  $^{28}\text{Si}$ , while convenient for comparing spherical vs deformed regimes, is the only nuclide for which the RPA value of  $Q^2$  is worse than the HF value, using the original Wildenthal single-particle energies.) This is not universal behavior; as seen in Table II and will be seen in the next section for  $J^2$ , the RPA expectation value for some operators is better in the deformed regime.

An obvious step will be to try quasiparticle-RPA (QRPA), which may improve performance in the deformed regime. On the other hand, we reran our calculations with all the explicit pairing matrix elements set to zero, and found no qualitative change in our results, much as was found for the RPA correlation energy [13].

### IV. RESTORATION OF BROKEN SYMMETRIES?

The random phase approximation respects broken symmetries by separating out exactly, as zero modes, spurious

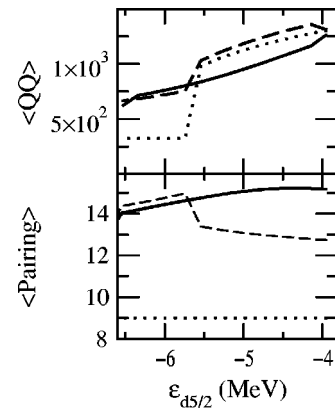


FIG. 2.  $\langle Q^2 \rangle$ ,  $\langle P^\dagger P \rangle$  in  $^{28}\text{Si}$  as the  $d_{5/2}$  single-particle energy is lowered relative to the other single-particle energies. The solid line is the (exact) shell-model value, the dotted line the HF value, and the dashed line the RPA value.

TABLE IV. Ground-state expectation value  $\langle J^2 \rangle$  for selected nuclides, grouped into even-even, single-species, odd-odd, and odd-A.

Nucleus	HF	RPA	SM
<sup>20</sup> Ne	16.06	-0.45	0
<sup>22</sup> Ne	17.17	-1.16	0
<sup>24</sup> Mg	20.13	-2.52	0
<sup>26</sup> Mg	18.61	-1.72	0
<sup>28</sup> Si	20.89	-1.99	0
<sup>44</sup> Ti	31.65	-3.10	0
<sup>46</sup> Ti	31.53	-5.00	0
<sup>48</sup> Cr	29.37	4.72	0
<sup>20</sup> O	6.07	1.76	0
<sup>22</sup> O	0.00	7.99	0
<sup>24</sup> O	0.00	7.38	0
<sup>20</sup> F	18.46	12.41	6
<sup>22</sup> Na	25.57	14.57	12
<sup>26</sup> Al	35.98	27.92	0
<sup>46</sup> V	39.56	20.00	0
<sup>19</sup> F	15.12	5.52	0.75
<sup>21</sup> F	15.51	9.47	8.75
<sup>21</sup> Ne	19.05	12.68	3.75
<sup>23</sup> Na	19.42	11.87	3.75
<sup>25</sup> Mg	23.87	14.51	8.75

motion. This is sometimes interpreted as an “approximate restoration of the symmetry” [5]. The restoration cannot be exact, because the RPA wave function is valid only in the vicinity of the Hartree-Fock state [14] and cannot be extrapolated to, for example, large rotation angles.

Still, we now have a tool to further explore symmetry restoration, by computing Casimir operators of symmetry groups. Specifically, we consider  $\langle J^2 \rangle$ . Ideally, if the RPA restores a broken symmetry, one might imagine that one either regains the exact ground state value of  $\langle J^2 \rangle$  or gets very close to it.

We present our results in Table IV. The pattern is the same as with other operators:  $\langle J^2 \rangle$  is generally better in RPA than in Hartree-Fock but not always very close to the exact shell-model value. Even worse are the cases with a closed shell in HF, such as <sup>22,24</sup>O: the HF value is correct, while the RPA value is terrible.

To examine this issue more closely, in Fig. 3 we again plot, for <sup>28</sup>Si,  $\langle J^2 \rangle$  versus the  $d_{5/2}$  single-particle energy through the transition from deformed to spherical HF state. The results are better for the deformed HF state, although we obtain slightly negative, and thus nonphysical, values of  $\langle J^2 \rangle$ .

Calculation of  $\langle J^2 \rangle$  is not necessarily the only test of restoration of symmetry. One would also expect, for nuclides with  $J=0$  ground states, that  $\langle J_i \rangle = 0, i=x, y, z$ . This will be an important test of the restoration of symmetry, but as  $J_i$  is a nonscalar observable it is beyond the scope of the present paper. Note, however, that for even-even nuclides,  $\langle J_i \rangle = 0$

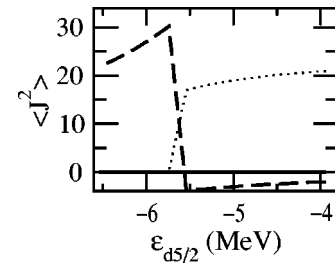


FIG. 3.  $\langle J^2 \rangle$  in <sup>28</sup>Si as the  $d_{5/2}$  single-particle energy is lowered relative to the other single-particle energies. The solid line is the (exact) shell-model value, the dotted line the HF value, and the dashed line the RPA value.

for the Hartree-Fock state due to time-reversal invariance. The question then becomes whether or not for deformed states the RPA corrections to  $\langle J_i \rangle$  are also zero. In the near future we will perform these calculations as evidence for or against the restoration of rotational symmetry in the RPA.

An additional test of symmetry restoration would be computation of the expectation value of other nonscalar observables, such as the magnetic dipole moment or electric quadrupole moment, for a deformed nucleus with a  $J=0$  shell-model ground state. We have preliminary, unpublished calculations which suggest that indeed the RPA ground state of even-even nuclides retains a significant quadrupole moment, another piece of evidence that symmetry is incompletely restored.

There are other observables one would like to compute relevant to broken symmetries. Aside from the Casimir itself, the dispersion of a Casimir would be a useful measure. For example, consider quasiparticle RPA (QRPA), where particle number is broken in the Hartree-Fock-Bogoliubov state. One would like to see the QRPA value of the dispersion  $\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$  move close to zero. Another example would be proton-neutron RPA (pnRPA) or pnQRPA, allowing protons and neutrons to mix, so that  $T_z = Z - N$  is no longer a good quantum number; this is applicable to beta decay. Here one might consider  $\langle \hat{T}_z^2 \rangle - \langle \hat{T}_z \rangle^2$ . Unfortunately, we suspect that the dispersion would also signal incomplete symmetry restoration.

## V. SUMMARY AND CONCLUSION

We derived an expression for the ground-state expectation value of observables in the matrix formulation of RPA, using the quasiboson approximation, and tested it against exact shell-model calculations for selected scalar operators. The RPA value was in general an improvement over the Hartree-Fock value, but failed to be a consistent and reliable estimate of the exact expectation value.

There are a number of generalizations and modifications to the RPA: the number-operator method, renormalized RPA, self-consistent RPA, modified RPA, etc. [10,18–22]. Rowe [10] and others [23] compared the quasiboson approximation for occupation numbers with the number-operator method, and found the quasiboson overestimated the occupation number by a factor of 2. This factor of 2 is often attributed to

double counting (but see footnote 15 of Ref. [10], which suggests it may be due to the failure of the quasiboson approximation to fully satisfy the Pauli principle). On the other hand, Dukelsky, Hirsch, and Schuck [24] recently compared the occupation number for the Lipkin model in the RPA, the number-operator method, and the self-consistent RPA, and found the latter gave consistently better results.

In this paper we have restricted ourselves to the simplest RPA approach, but considered a more general operator in a more realistic model. Clearly the next step would be to de-

rive expressions for a general scalar observable in the number-operator method, self-consistent RPA, and so on, and compare against nontrivial shell-model calculations. This we leave to future work.

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