Ground-state Correlation Effects in Extended RPA Calculations

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Abstract

We study normalization problems associated with use of perturbatively correlated ground-states in extended RPA schemes in the context of a specific but typical example. The sensitivity of the results to the amount of $2p2h$ admixtures to the correlated ground state is also investigated in terms of a modification of the standard perturbative approach.

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Some time ago Van Neck et al.[1] pointed out that some annoying numerical inconsistencies result from the evaluation of consistently derived perturbative expressions in the context of the nuclear many-body problem. Specifically, they pointed out that an often used procedure of evaluating the number of nucleons perturbatively excited above the Fermi level (including normalization factors expanded to the appropriate perturbative order) leads to grossly overestimated results. This happens due to the fact that, as the perturbation adds a very large number of relatively small excited $2p2h$ components to the $0p0h$ wave function, the relative weight of the former in the perturbed wavefunction is typically large enough numerically so that the perturbatively expanded normalization becomes inadequate. This type of difficulty affects also linear response calculations done in the context of the so called extended second random phase approximation (ESRPA) [2], which uses a perturbatively generated ground state wavefunction with $2p2h$ admixtures, in addition to including two-body operators in the structure of the phonons. In this note we work out an example that shows that this numerical normalization error tends in fact to inflate significantly ESRPA strength distributions, as was also pointed out in Ref. [1]. Moreover, considerable excess strength still remains over the results obtained by using just the unperturbed ground state (second random phase approximation (SRPA)) when one attends to the numerical normalization problem. This excess strength appears to be related to the relative importance of the $2p2h$ admixtures to the unperturbed ground state.

In order to explore this point we give also results obtained for a modified ESRPA in which $2p2h$ ground state correlations are introduced by means of the Brillouin-Wigner (BW) perturbation theory, which has the effect of reducing appreciably their importance. This happens through the lowering of the ground state energy produced by solving the appropriate dispersion equation. The resulting strength distribution, for reduced but still non negligible $2p2h$ admixtures to the unperturbed ground state, comes out close to the simple SRPA result. We take these facts as an indication of enough sensitivity of the calculated strengths to the correlation structure of the ground-state so as to warrant the development and implementation in realistic situations of better controlled extensions of the standard quasi-boson random-phase approximation.

We base our argument on the linear response $R(E)$ to an external field $\hat{F}$, which admits the spectral representation

$$R(E) = \sum_\nu \left[\frac{\langle 0|\hat{F}|\nu\rangle\langle\nu|\hat{F}^\dagger|0\rangle}{E - E_\nu + i\eta} - \frac{\langle 0|\hat{F}^\dagger|\nu\rangle\langle\nu|\hat{F}|0\rangle}{E + E_\nu - i\eta} \right]. \tag{1}$$

Here $|0\rangle$ and $|\nu\rangle$ are the exact ground state and excited eigenstates of the full hamiltonian $\hat{H}$. The excited states $|\nu\rangle$ can be written as

$$|\nu\rangle = \Omega_\nu^\dagger|0\rangle; \;\; \Omega_\nu^\dagger = \sum_i X_i^\nu C_i^\dagger - \sum_j Y_j^\nu C_j, \tag{2}$$

where the set $\{C_i, C_i^\dagger\}$ constitutes a complete operator basis. In the SRPA this set is restricted to one and two particle-hole annihilation and creation operators out of the Hartee-Fock (HF) ground state $|HF\rangle$ and the coefficients X_i^ν and Y_i^ν are determined from the equations of motion [4]

$$\langle HF| \left[\Omega_\mu, \left[\hat{H}, \Omega_\nu^\dagger\right]\right] |HF\rangle = E_\nu \langle HF| \left[\Omega_\mu, \Omega_\nu^\dagger\right] |HF\rangle = E_\nu \delta_{\mu\nu}. \tag{3}$$

The ESRPA hinges on the idea that the inclusion of $2p2h$ operators among the C_i requires a modification of the quasi-boson approximation in which the HF ground state is allowed to include perturbative $2p2h$ correlations. Hence, in evaluating Eq. (3) one uses in this case a ground state of the form

$$|\tilde{0}\rangle = c_0 \left[|HF\rangle + \sum_{2_0} c_{2_0} |2_0\rangle \right], \tag{4}$$

where the amplitudes c_{2_0} are evaluated in the first order Rayleigh-Schrödinger (RS) perturbation theory, i.e.,

$$c_{2_0} = \frac{\langle 2_0|\hat{V}|HF\rangle}{-E_{2_0}}. \tag{5}$$

Here $2_0 \equiv (p_1 p_2 h_1 h_2)_0$ indicates $2p2h$ excitations with independent-particle energy E_{2_0}, $\hat{V}$ is the residual interaction, and c_0 is a normalization factor. Since Eq. (4) is thought of as a perturbatively generated expression, c_0 is generally set equal to 1.

In general Eq. (3) leads to a secular problem of the form

$$\mathcal{A}\mathcal{X}^\nu = E_\nu \mathcal{N}\mathcal{X}^\nu, \tag{6}$$

with

$$\mathcal{A} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}, \quad \mathcal{X}^\nu = \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}, \quad \mathcal{N} = \begin{pmatrix} N & 0 \\ 0 & -N^* \end{pmatrix}. \tag{7}$$

where the submatrices A, B and N given by

$$A_{i,j} = \langle\tilde{0}| \left[C_i, \left[\hat{H}, C_j^\dagger\right]\right] |\tilde{0}\rangle, \;\; B_{i,j} = \langle\tilde{0}| \left[C_i, \left[\hat{H}, C_j\right]\right] |\tilde{0}\rangle, \;\; N_{i,j} = \langle\tilde{0}| \left[C_i, C_j^\dagger\right] |\tilde{0}\rangle. \tag{8}$$

Furthermore, one can write Eq. (1) in a representation independent form as

$$R(E) = \mathcal{F}^\dagger (E\mathcal{N} + i\eta\mathcal{I} - \mathcal{A})^{-1}\mathcal{F}, \tag{9}$$

where the matrix $\mathcal{F}$ represents the operator $\hat{F}$ and is defined as

$$\mathcal{F} \equiv \begin{pmatrix} F^A \\ F^B \end{pmatrix}, \quad \text{with} \begin{cases} F_i^A = \langle\tilde{0}| \left[C_i, \hat{F}\right] |\tilde{0}\rangle, \\ F_i^B = F_i^{A*}(\hat{F} \to \hat{F}^\dagger). \end{cases} \tag{10}$$

Eq. (9) can be reduced with the help of projection operators P and Q onto subspaces involving $1p1h$ and $2p2h$ excitations respectively. One gets

$$R(E) = \tilde{\mathcal{F}}_P^\dagger(E)\mathcal{G}_P(E)\tilde{\mathcal{F}}_P(E) + \mathcal{F}_Q^\dagger \mathcal{G}_Q(E)\mathcal{F}_Q, \tag{11}$$

where

$$\mathcal{G}_P(E) = \left[E\mathcal{N}_P + i\eta\mathcal{I}_P - \mathcal{A}_P - \left(\mathcal{A}_{PQ} - \mathcal{N}_{PQ}E\right)\mathcal{G}_Q(E)\left(\mathcal{A}_{QP} - \mathcal{N}_{QP}E\right)\right]^{-1}, \tag{12}$$

with

$$\mathcal{G}_Q(E) = \left[E\mathcal{N}_Q + i\eta\mathcal{I}_Q - \mathcal{A}_Q\right]^{-1}, \tag{13}$$

and

$$\tilde{\mathcal{F}}_P(E) = \mathcal{F}_P - \mathcal{N}_{PQ}\mathcal{F}_Q + \mathcal{A}_{PQ}\mathcal{G}_Q(E)\mathcal{F}_Q. \tag{14}$$

When using the ESRPA some more complicated two-body effects are trimmed by keeping terms up to second order in $\hat{V}$ for the forward sector within the P space, terms linear in $\hat{V}$ for the backward sector within the P space and for the coupling between the P and Q spaces, and only terms of zeroth order within the Q space. The usual argument (see e.g. Ref. [2]) for this procedure involves again the limitations stemming from the perturbative dressing of the ground state, Eq. (4).

Finally, we set up a modified extended second RPA (MESRPA) in which Eq. (4) is replaced by the corresponding expression obtained from the BW perturbation theory. This in fact coincides with the ESRPA result but the coefficients c_{2_0} are now given as

$$c_{2_0} = \frac{\langle 2_0|\hat{V}|HF\rangle}{E_0 - E_{2_0}}, \tag{15}$$

where the ground state energy E_0 is the lowest solution of the secular equation

$$E_0 = \sum_{2_0} \frac{|\langle 2_0|\hat{V}|HF\rangle|^2}{E_0 - E_{2_0}}. \tag{16}$$

This leads to increased energy denominators in Eq. (15) and hence to reduced $2p2h$ admixtures to the HF ground state. One obtains in this way

$$N_{ij} = \delta_{ij} + \Delta N_{ij} \tag{17}$$

where $i \equiv ipih$ and the nonzero ΔN_{ij} are just

$$\Delta N_{11'} = |c_0|^2 \sum_{2_0, 2'_0} c^*_{2_0} c_{2'_0} \langle 2_0|\hat{D}_{11'}|2'_0\rangle, \tag{18}$$

where $\hat{D}_{11'} = \left[\hat{C}_1, \hat{C}^\dagger_{1'}\right] - \delta_{11'}$. (Note that within the quasi-boson approximation $\hat{D}_{11'} \equiv 0$). The explicit result for the matrix element $\langle 2_0|\hat{D}_{11'}|2'_0\rangle$ is

$$\begin{aligned} \langle (p_1 p h_1 h_2)_0|\hat{D}_{ph,p'h'}|(p'_1 p'_2 h'_1 h'_2)_0\rangle &= -\left[1 + P(h_1, h_2)P(h_{1'}, h_{2'})\right] \\ \times \quad & \left[\delta_{p,p'}\delta_{h_1,h'}P^-(h, h_2)P^-(p_1, p_2)\delta_{h_{1'},h}\delta_{h_2,h_{2'}}\delta_{p_2,p_{2'}}\delta_{p_1,p_{1'}}\right] + p \leftrightarrow h, \end{aligned} \tag{19}$$

where $P^{-}(i,j) \equiv [1 - P(i,j)]$, while the operator $P(i,j)$ exchanges the arguments i and j. The matrix elements of $\mathcal{A}$ are

$$A_{ij} = \delta_{ij} E_j + V_{ij} + \Delta A_{ij}, \tag{20}$$

where $V_{ij} \equiv \langle i\hat{V}|j\rangle$ and the nonzero matrix elements ΔA_{ij} are:

$$\Delta A_{11'} = |c_0|^2 \sum_{2_0,2'_0} (E_1 - E_{2_0} + E_0) c^*_{2_0} c_{2'_0} \langle 2_0|\hat{D}_{11'}|2'_0\rangle. \tag{21}$$

Finally the matrix elements of $\mathcal{F}$ are:

$$F_i^A = \begin{cases} f_1 + \sum_{1'} \Delta N_{11'} f_{1'} & \text{for } i = 1 \\ c_0 \sum_{2_0} c_{2_0} f_{22_0} & \text{for } i = 2, \end{cases} \tag{22}$$

where

$$f_1 \equiv \langle 1|\hat{F}|HF\rangle, \text{ and } f_{22_0} \equiv \langle 2|\hat{F}|2_0\rangle. \tag{23}$$

Note that the corresponding ESRPA quantities are obtained by setting $c_0 = 1$ and $E_0 = 0$ in the MESRPA expressions.

We next give numerical results for the GT resonance ($\hat{F}_{\pm} \equiv \vec{\sigma} t_{\pm}$) in ^{48}Ca using the MY3 force [7] in the $0\hbar\omega - 3\hbar\omega$ oscillator space. Four different ways of handling the nuclear ground state will be compared. The first one is just the plain SRPA in which the equations of motion (3) are evaluated with the HF ground state. We give also results for the ESRPA (for which the normalization coefficient c_0 is set equal to 1), for a normalized version of this approximation (NESRPA) in which c_0 is determined so that $\langle\tilde{0}|\tilde{0}\rangle = 1$ with the c_{2_0} coefficients given by Eq. (5), and finally for the MESRPA, which uses a normalized ground state with amplitudes c_{2_0} evaluated using Eq. (15). In order to obtain smooth strength functions $S(E) \equiv -\frac{1}{\pi} Im\ R(E)$ with $R(E)$ given by Eq. (11), the energy variable is taken to be complex: $E \to E + i\Delta$, with $\Delta = 1$ MeV for the $1p1h$ and $\Delta = 3$ MeV for the $2p2h$ subspace respectively. Solving the dispersion equation Eq. (16) gives $E_0 = -29$ Mev, which amounts to about 8% of the experimental ground state binding energy. The results are shown in Fig. 1 and in Table 1 below. The positive branch of the GT sum rule $\mathcal{S}_+ - \mathcal{S}_- = 3(N - Z)$ with $\mathcal{S}_{\pm} \equiv \int S_{\pm}(E) dE$ is divided into a low energy part $\mathcal{S}_+^<$ ($E < 20$ Mev) and a high energy part $\mathcal{S}_+^>$ ($E > 20$ Mev).

These quantities are the relevant ones for the problem of the quenching of GT strength. In the usual RPA the low energy part $\mathcal{S}_+^<$ essentially exhausts the sum rule. When $1p1h-2p2h$ coupling is introduced via the SRPA, 30% of this strength is shifted to the high energy region. This amount is somewhat reduced when ground state correlations are introduced via the ESRPA. This results from the combined effect of the Q-space part of Eq. (11) and of the interference effects generated by the last term of Eq. (14) [3]. Furthermore one gets now also a contribution in the negative branch $\mathcal{S}_-$ so that $\mathcal{S}_+^<$ increases to 82% (third line in Table 1). As shown in the first two columns of Table 1, the ground state wavefunction involved in the derivation of the ESRPA expressions has a serious normalization problem. In the NESRPA this is fixed by suitably reducing the value of c_0. This has only a relatively small effect on $\mathcal{S}_+^<$ and reduces both $\mathcal{S}_+^>$ and the negative branch contribution $\mathcal{S}_-$ (fourth line of Table 1). When ground state correlations are introduced via the MESRPA, on the other hand, the percentage of $2p2h$ admixtures to the ground state is reduced from 62% to 31% while the strength distribution becomes quite similar to the simple SRPA result. This last feature indicates important sensitivity to the amount of ground state correlations which therefore, as stated above, deserves a more controlled treatment. It is worth noticing that, when the interaction among the $2p2h$ configurations is neglected, the BW approximation for the ground state wavefunction coincides with the diagonalization procedure [6]. This means that the $0p0h-2p2h$ coupling in the initial nucleus is treated at the same footing as the $1p1h-2p2h$ coupling in the final nucleus. Thus we feel that, in the context of the present calculations, it is more consistent to use the BW perturbation theory than the RS one.

Even though the present discussion has been limited to one specific case involving the Gamow-Teller response within the extended RPA, the observed trends should apply also to other schemes which include ground state correlation effects perturbatively, both for this [7] and for other types of response functions, notably the longitudinal and transverse inclusive responses in quasi-free electron scattering [8, 9, 10]. In all cases ground-state normalization is numerically important and sensitivity to the amount of $2p2h$ correlations should be high, so that a moderate reduction of the $2p2h$ ground state component will lead to results which are not far from those obtained in the simple SRPA.

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References

[1] D. Van Neck, M. Waroquier, V. Van der Sluys and J. Ryckebusch, Phys. Lett. **274B**, 143 (1992).

[2] K. Takayanagi, K. Shimizu and A. Arima, Nuc. Phys. **A477**, 205 (1988).

[3] S. Drożdż, S. Nishizaki, J. Speth and J. Wambach, Phys. Rep. **197**, 1 (1990).

[4] D.J. Rowe, Nuclear Collective Motion (Methuen, London 1970).

[5] S. Drożdż, V. Klemt, J. Speth and J. Wambach, Phys. Lett. **166B**, 253 (1986).

[6] A. Bohr and B. Mottelson, *Nuclear Structure* Vol. I, p. 302 (Benjamin, New York).

[7] G.F. Bertsch and I. Hamamoto, Phys. Rev. **C26**, 1323 (1982).

[8] W.M. Alberico, M. Ericson and A. Molinari, Ann. Phys. (NY) **154**, 356 (1984).

[9] K. Takayanagi, Phys. Lett. **233B**, 271 (1989).

[10] A. Mariano, E. Bauer, F. Krmpotić, and A.F.R de Toledo Piza, Phys. Lett. **268B**, 332 (1991).

TABLES

Table 1: Ground state normalization factor, summed weights of $2p2h$ components (see Eq. (4)), GT integrated strength $\mathcal{S}_+$ in the resonance region (<), above it (>), and total GT strengths $\mathcal{S}_+$ and $\mathcal{S}_-$. The first column identifies the approximation scheme. Strengths are given in percent of $3(N-Z)$.

	$\lvert c_0\rvert^2$	$\sum_{2_0} \lvert c_{2_0}\rvert^2$	$\mathcal{S}_+^<$	$\mathcal{S}_+^>$	$\mathcal{S}_+$	$\mathcal{S}_-$
RPA	1	0	100	0	100	0
$SRPA$	1	0	70	30	100	0
$ESRPA$	1	1.60	82	27	109	9
$NESRPA$	0.38	1.60	80	23.5	103.5	3.5
$MESRPA$	0.69	0.45	72.8	28	100.8	0.8

FIGURES

Figure 1: Folded Gamow-Teller strength distributions in ^{48}Ca for different approximation schemes.