Zero-temperature second random phase approximation and its formal properties

Constantine Yannouleas
The Niels Bohr Institute, DK-2100 Copenhagen Ø, Denmark
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We derive the zero-temperature second random phase approximation using Rowe's double-commutator equation. Subsequently, we show that the zero-temperature second random phase approximation exhibits formal properties in analogy with the usual 1p-1h random phase approximation. In particular, the second random phase approximation preserves the energy-weighted sum rule.

Recently, an extension of the simple random phase approximation (RPA), referred to as the second RPA, was formulated in Ref. 1 following Rowe's equations-of-motion method.[2] This extension accounts for residual couplings to (and inside) the 2p-2h subspace in addition to the couplings inside the 1p-1h subspace.

This second RPA has been employed[3] to describe a variety of aspects of nuclear dissipation. In particular, the second RPA is very efficient in describing properties of giant vibrations like the spreading widths.[4,5] The second RPA can also provide an answer to the question of the missing strength in the case of the Gamow-Teller excitations[6] as well as to the question of the screening of the tensor force in finite nuclei.[7]

The aim of this Brief Report is to supplement the presentation in Ref. 1 by showing that the zero-temperature second RPA exhibits formal properties in complete analogy with the simple RPA.[8] At the same time, it can also serve as a brief, but self-contained, introduction to the theory of the second RPA as a whole.[9–12]

As is the case with the simple RPA,[2] the search for formal properties of the second RPA is greatly simplified by the fact that the second RPA excitation operator $O_\nu^\dagger$—which creates a one-phonon state—satisfies the following double-commutator equation:

$$\langle \mathrm{HF}\,|\,[R,[H,O_\nu^\dagger]]\,|\,\mathrm{HF}\rangle = \hbar\omega_\nu \langle \mathrm{HF}\,|\,[R,O_\nu^\dagger]\,|\,\mathrm{HF}\rangle \ , \quad \text{for all } R \ , \tag{1}$$

where $\hbar\omega_\nu$ is the excitation energy, $|\,\mathrm{HF}\rangle$ is the Hartree-Fock ground state of the nucleus, and R is any operator in the same space as $O_\nu^\dagger$. H is the exact many-body Hamiltonian.

The double-commutator equation (1) was introduced in Ref. 2, where its equivalence to the simple RPA was also shown. As we will subsequently outline, not only the simple RPA, but also the second RPA equations can result from an equation-of-motion like Eq. (1). Notice, however, that even though the generic structure of Eq. (1) remains unaltered when the extension of the first to the second RPA is implemented, the pivotal new element is the difference in the approximation for the excitation operator $O_\nu^\dagger$. Specifically, the second RPA $O_\nu^\dagger$ comprises 2p-2h components in addition to the familiar case of 1p-1h components, namely

$$O_\nu^\dagger = \sum_{mi} [\,Y_{mi}(\omega_\nu)a_m^\dagger a_i - Z_{mi}(\omega_\nu)a_i^\dagger a_m\,] + \sum_{m<n,i<j} [\,Y_{mnij}(\omega_\nu)a_m^\dagger a_n^\dagger a_j a_i - Z_{mnij}(\omega_\nu)a_i^\dagger a_j^\dagger a_n a_m\,] \ . \tag{2}$$

In Eq. (2), the a's are fermion-creation and fermion-annihilation operators, while the Y's and Z's are forward and backward going amplitudes. Indices m,n,p,q denote particle states, while indices i,j,k,l denote hole states.

Equipped with Eqs. (1) and (2), one can repeat the steps in Sec. III of Ref. 2 and show that all the formal properties familiar from the simple RPA hold for the zero-temperature second RPA as well. In particular, these formal properties are the following:

(1) The solutions of the second RPA appear in pairs having symmetric positive and negative eigenvalues.

(2) The second RPA solutions have real energies when Thouless's stability condition is fulfilled.

(3) Spurious solutions reflecting the center-of-mass motion separate out and have exactly zero energy.

(4) The second RPA solutions are orthonormal.

(5) The nonspurious second RPA solutions form a complete set.

(6) The matrix elements of any operator W calculated in the second RPA preserve the energy-weighted sum rule.

Since the steps associating the formal properties listed above with the second RPA are similar to the steps in the case of the simple RPA, henceforth for illustration purposes, we will focus only on the energy-weighted sum rule. This selection has also been motivated by the prominent role that the energy-weighted sum rule plays in the discussion of the properties of giant vibrations.[13–15] Moreover, we will discuss this sum rule in connection with a non-Hermitian operator.

However, before proceeding further with the discussion of the energy-weighted sum rule, we first outline for completeness how the second RPA equations result from the double-commutator equation (1).

Indeed, it is a matter of algebra to show that insertion of expansion (2) in Eq. (1) yields the following linear set of second RPA equations:

$$\begin{bmatrix} \mathscr{A} & \mathscr{B} \\ -\mathscr{B}^* & -\mathscr{A}^* \end{bmatrix} \begin{bmatrix} \mathscr{Y}(\omega_\nu) \\ \mathscr{Z}(\omega_\nu) \end{bmatrix} = \hbar\omega_\nu \begin{bmatrix} \mathscr{Y}(\omega_\nu) \\ \mathscr{Z}(\omega_\nu) \end{bmatrix} , \tag{3}$$

where $\mathcal{A}$ and $\mathcal{B}$ are 2×2 matrices,

$$\mathcal{A}=\begin{bmatrix} A_{mi,pk} & A_{mi,pqkl} \\ A_{mnij,pk} & A_{mnij,pqkl} \end{bmatrix}, \tag{4a}$$

$$\mathcal{B}=\begin{bmatrix} B_{mi,pk} & B_{mi,pqkl} \\ B_{mnij,pk} & B_{mnij,pqkl} \end{bmatrix}, \tag{4b}$$

and

$$\mathcal{Y}(\omega_\nu)=\begin{bmatrix} Y_{mi}(\omega_\nu) \\ Y_{mnij}(\omega_\nu) \end{bmatrix}, \quad \mathcal{Z}(\omega_\nu)=\begin{bmatrix} Z_{mi}(\omega_\nu) \\ Z_{mnij}(\omega_\nu) \end{bmatrix}. \tag{5}$$

The form (3) for the second RPA equations is quite analogous to the simple RPA form as introduced by Thouless.[8] The difference lies in the larger dimensions of the matrices $\mathcal{A}$ and $\mathcal{B}$.[16]

The elements of the matrix $\mathcal{A}$ are defined as

$$A_{mi,pk}=\langle \mathrm{HF}\,|\,[a_i^\dagger a_m,[H,a_p^\dagger a_k]]\,|\,\mathrm{HF}\rangle\ , \tag{6a}$$

$$A_{mi,pqkl}=\langle \mathrm{HF}\,|\,[a_i^\dagger a_m,[H,a_p^\dagger a_q^\dagger a_l a_k]]\,|\,\mathrm{HF}\rangle\ , \tag{6b}$$

$$A_{mnij,pk}=\langle \mathrm{HF}\,|\,[a_i^\dagger a_j^\dagger a_n a_m,[H,a_p^\dagger a_k]]\,|\,\mathrm{HF}\rangle\ , \tag{6c}$$

$$A_{mnij,pqkl}=\langle \mathrm{HF}\,|\,[a_i^\dagger a_j^\dagger a_n a_m,[H,a_p^\dagger a_q^\dagger a_l a_k]]\,|\,\mathrm{HF}\rangle\ . \tag{6d}$$

The elements of the matrix $\mathcal{B}$ have the same form as the elements of the matrix $\mathcal{A}$ apart from the following two differences:

(i) In the second product of fermion operators, the particle indices p and q are interchanged with the hole indices k and l, respectively.

(ii) A minus sign appears in front of the whole expression.

For example, the matrix element $B_{mi,pqkl}$ is

$$B_{mi,pqkl}=-\langle \mathrm{HF}\,|\,[a_i^\dagger a_m,[H,a_k^\dagger a_l^\dagger a_q a_p]]\,|\,\mathrm{HF}\rangle\ . \tag{7}$$

A lengthy, but straightforward, calculation shows that the matrix elements of $\mathcal{A}$ can be expressed as

$$A_{mi,pk}=\mathcal{N}_{m,i}(\epsilon_m-\epsilon_i)\delta_{mp}\delta_{ik}+\mathcal{N}_{m,i}\mathcal{N}_{p,k}V_{mkip}\ , \tag{8a}$$

$$A_{mi,pqkl}=\mathcal{N}_{m,i}[\mathcal{U}(pq)\mathcal{N}_{kl,p}V_{klip}\delta_{mq}-\mathcal{U}(kl)\mathcal{N}_{pq,k}V_{mkpq}\delta_{il}]\ , \tag{8b}$$

$$A_{mnij,pk}=\mathcal{N}_{mn,ij}[\mathcal{U}(mn)V^*_{ijkm}\delta_{pn}-\mathcal{U}(ij)V^*_{pimn}\delta_{kj}]\ , \tag{8c}$$

$$\begin{aligned} A_{mnij,pqkl}=\mathcal{N}_{mn,ij}[&(\epsilon_m+\epsilon_n-\epsilon_i-\epsilon_j)\mathcal{U}(pq)\mathcal{U}(kl)\delta_{mp}\delta_{nq}\delta_{jl}\delta_{ik}-\mathcal{U}(mn)\mathcal{U}(ij)\mathcal{U}(pq)\mathcal{U}(kl)\mathcal{N}_{p,l}V_{mlpj}\delta_{nq}\delta_{ik} \\ &+(\bar{n}_q-n_p)\mathcal{U}(kl)V_{mnpq}\delta_{ik}\delta_{jl}+(n_l-\bar{n}_k)\mathcal{U}(pq)V_{klij}\delta_{mp}\delta_{nq}]\ . \end{aligned} \tag{8d}$$

Here, the matrix elements of the two-body force V are antisymmetrized. The single-particle energies ϵ are the stationary Hartree-Fock energies, namely

$$\epsilon_\alpha=t_{\alpha\alpha}+\sum_j V_{j\alpha j\alpha}\ , \tag{9}$$

where t refers to the kinetic energy contribution and $\alpha,\beta,\gamma,\delta$ are free indices. $\mathcal{U}(rs)$ is the antisymmetrizer for the indices r,s. The definition of the symbols $\mathcal{N}$ is

$$\mathcal{N}_{\alpha,\beta}=\bar{n}_\alpha n_\beta-n_\alpha\bar{n}_\beta=n_\beta-n_\alpha\ , \tag{10a}$$

$$\mathcal{N}_{\alpha\beta,\gamma}=\bar{n}_\alpha\bar{n}_\beta n_\gamma+n_\alpha n_\beta\bar{n}_\gamma\ , \tag{10b}$$

and

$$\mathcal{N}_{\alpha\beta,\gamma\delta}=\bar{n}_\alpha\bar{n}_\beta n_\gamma n_\delta-n_\alpha n_\beta\bar{n}_\gamma\bar{n}_\delta\ . \tag{10c}$$

The symbols n_α, $\bar{n}_\alpha=1-n_\alpha$ denote the occupation probability of a hole and a particle state, respectively, at zero temperature. They result from corresponding fermion-creation—fermion-annihilation (or *vice versa*) contractions over the Hartree-Fock ground state and assume either the value 1 or 0.

For the B matrices, one finds

$$B_{mi,pk}=\mathcal{N}_{m,i}\mathcal{N}_{p,k}V_{mpik} \tag{11a}$$

and

$$B_{mi,pqkl}=B_{mnij,pk}=B_{mnij,pqkl}=0\ . \tag{11b}$$

Since the factors $\mathcal{N}$ in Eqs. (8) and (11) contribute only with the value 1, the 2×2 matrices $\mathcal{A}$ and $\mathcal{B}$ exhibit symmetries in complete analogy with the simple RPA,[17] i.e.,

$$\mathcal{A}^\dagger=\mathcal{A}\ \text{(Hermitian)}\ , \tag{12a}$$

$$\tilde{\mathcal{B}}=\mathcal{B}\ \text{(symmetric)}\ . \tag{12b}$$

Additionally, in analogy with the simple RPA, the second RPA amplitudes can be expressed as

$$Y_{mnij}(\omega_\nu)=\langle \mathrm{RPAII}\,|\,a_i^\dagger a_j^\dagger a_n a_m O_\nu^\dagger\,|\,\mathrm{RPAII}\rangle\ , \tag{13a}$$

$$Z_{mnij}(\omega_\nu)=\langle \mathrm{RPAII}\,|\,a_m^\dagger a_n^\dagger a_j a_i O_\nu^\dagger\,|\,\mathrm{RPAII}\rangle\ , \tag{13b}$$

$$Y_{mi}(\omega_\nu)=\langle \mathrm{RPAII}\,|\,a_i^\dagger a_m O_\nu^\dagger\,|\,\mathrm{RPAII}\rangle\ , \tag{13c}$$

$$Z_{mi}(\omega_\nu)=\langle \mathrm{RPAII}\,|\,a_m^\dagger a_i O_\nu^\dagger\,|\,\mathrm{RPAII}\rangle\ . \tag{13d}$$

In Eq. (13), $|\,\mathrm{RPAII}\rangle$ is the correlated second RPA ground state defined by

$$O_\nu\,|\,\mathrm{RPAII}\rangle=0,\ \text{for all}\ \nu\ . \tag{14}$$

To show the validity of Eq. (13), one uses Eq. (14) to introduce an intermediate commutator and then calculates this commutator by replacing the correlated ground state by the Hartree-Fock determinant. This procedure is similar to the treatment of the simple RPA amplitudes.

From the structure of Eq. (3), there results the following orthonormality relation for the second RPA solutions:

$$(\mathscr{Y}^*(\omega_\mu),\mathscr{Z}^*(\omega_\mu))\begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}\begin{bmatrix} \mathscr{Y}(\omega_\nu) \\ \mathscr{Z}(\omega_\nu) \end{bmatrix}=\delta_{\mu\nu}\frac{\omega_\nu}{|\omega_\nu|} \quad (15a)$$

or

$$\langle \mathrm{HF}|[O_\mu,O_\nu^\dagger]|\mathrm{HF}\rangle=\delta_{\mu\nu}\,, \quad (15b)$$

where I is the unit 2×2 matrix.

Finally, as is the case with the simple RPA, the 1p-1h and 2p-2h base vectors obey boson commutation relations, i.e.,

$$\langle \mathrm{HF}|[a_i^\dagger a_m,a_\alpha^\dagger a_\beta]|\mathrm{HF}\rangle=\mathscr{N}_{m,i}\delta_{m\alpha}\delta_{i\beta}\,, \quad (16a)$$

$$\langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m,a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta]|\mathrm{HF}\rangle =\mathscr{N}_{mn,ij}\mathscr{U}(mn)\mathscr{U}(ij)\delta_{m\alpha}\delta_{n\beta}\delta_{j\gamma}\delta_{i\delta}\,, \quad (16b)$$

$$\langle \mathrm{HF}|[a_i^\dagger a_m,a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta]|\mathrm{HF}\rangle=0\,. \quad (16c)$$

We return now to the discussion of the energy-weighted sum rule for an operator W, not necessarily Hermitian. Such a non-Hermitian operator, for example, arises in the case of the Gamow-Teller excitations.

The energy-weighted sum rule for any operator W is specified by the relation[15]

$$S_W^E+S_{W^+}^E=\sum_\nu (E_\nu-E_0)|\langle\nu|W|0\rangle|^2 +\sum_\nu (E_\nu-E_0)|\langle\nu|W^\dagger|0\rangle|^2 =\langle 0|[W,[H,W^\dagger]]|0\rangle\,, \quad (17)$$

where E_ν and $|\nu\rangle$ refer to the excitation energies and corresponding states of the system, while the index 0 refers to the ground state of the system. Observe that the right-hand side (rhs) of Eq. (17) does not depend on the excitation energies and states.

Relation (17) is an identity when the corresponding exact quantities are used. Thus the preservation of this sum rule is a crucial test for the accuracy of any given approximation. In particular, for the second RPA the following statement applies: When one evaluates the left-hand side (lhs) of Eq. (17) by using the second RPA eigenenergies $(E_\nu-E_0)_{\mathrm{RPAII}}=\hbar\omega_\nu$ and the second RPA expressions $\langle\nu|W|0\rangle_{\mathrm{RPAII}}$ for the transition matrix elements, one finds the same result as when calculating the rhs of Eq. (17) by replacing the exact ground state $|0\rangle$ by the Hartree-Fock determinant, $|\mathrm{HF}\rangle$.

To proceed with the proof of this statement, one needs the second RPA expression for the transition matrix elements. This expression is given by

$$\langle\nu|W|0\rangle_{\mathrm{RPAII}}=\langle \mathrm{RPAII}|[O_\nu,W]|\mathrm{RPAII}\rangle \cong\langle \mathrm{HF}|[O_\nu,W]|\mathrm{HF}\rangle\,. \quad (18)$$

Since the second RPA eigenvectors form a complete base, any operator W devoid of spurious components can be expanded as

$$W=\sum_{\lambda>0}\{\langle \mathrm{HF}|[O_\lambda,W]|\mathrm{HF}\rangle O_\lambda^\dagger -\langle \mathrm{HF}|[O_\lambda^\dagger,W]|\mathrm{HF}\rangle O_\lambda\}\,, \quad (19)$$

where $O_\lambda^\dagger$ and O_λ are the second RPA eigenvectors. Substituting expansion (19) into the expression

$$\langle HF|[W,[H,W^\dagger]]|\mathrm{HF}\rangle\,, \quad (20)$$

and using the equation-of-motion (1), the orthonormality relation (15), and expression (18), one can see immediately that the zero-temperature second RPA preserves the energy-weighted sum rule.

In summary, we have derived the zero-temperature second RPA through an application of the double-commutator equation introduced in Ref. 2 and have shown that it exhibits formal properties in analogy with the simple RPA.

[1] C. Yannouleas, M. Dworzecka, and J. J. Griffin, Nucl. Phys. **A397**, 239 (1983), in particular Appendix A.

[2] D. J. Rowe, Rev. Mod. Phys. **40**, 153 (1968).

[3] C. Yannouleas and S. Jang, Nucl. Phys. **A455**, 40 (1986).

[4] S. Drożdż, V. Klemt, J. Speth, and J. Wambach, Nucl. Phys. **A451**, 11 (1986).

[5] S. Adachi and N. Van Giai, Phys. Lett. **149B**, 447 (1984).

[6] S. Drożdż, V. Klemt, J. Speth, and J. Wambach, Phys. Lett. **166B**, 18 (1986).

[7] S. Drożdż, J. L. Tain, and J. Wambach, Phys. Rev. C **34**, 345 (1986).

[8] D. J. Thouless, Nucl. Phys. **22**, 78 (1961).

[9] For the first time in nuclear physics, the second RPA was introduced through a different approach by Sawicki (Ref. 10). However, Ref. 10 introduced the second RPA with the aim of explaining the 6.06 MeV 0^+ state in ^{16}O. Later, Refs. 11 and 12 introduced a quasiparticle Bardeen-Cooper-Schrieffer (BCS) second RPA with the aim of explaining the anharmonic splitting of the two-phonon low-lying collective states. On the contrary, Refs. 1 and 3 introduced the second RPA as a tool to account for the spreading widths of giant resonances, as well as for various other aspects of nuclear dissipation (see, in particular, the introduction in Ref. 3).

[10] J. Sawicki, Phys. Rev. **126**, 2231 (1962).

[11] T. Tamura and T. Udagawa, Nucl. Phys. **53**, 33 (1964).

[12] M. Savoia, J. Sawicki, and T. Tomasini, Nuovo Cimento **32**, 991 (1964).

[13] O. Bohigas, A. M. Lane, and J. Martorell, Phys. Rep. **51**, 267 (1979).

[14] M. Barranco, A. Polls, and J. Martorell, Nucl. Phys. **A444**, 445 (1985).

[15] A. Abbas, Nucl. Phys. **A452**, 61 (1986).

[16] Elimination of the 2p-2h components, however, leads to an RPA-type problem whose matrices have the same dimensions as in the usual RPA, but with frequency dependent elements (Ref. 3).

[17] At finite temperatures, however, this symmetry does not result automatically, and an appropriate symmetrization must be implemented (Ref. 3).