

Bulk and spectroscopic nuclear properties within an *ab initio* renormalized random-phase approximation framework

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A modern chiral potential incorporating the three-body force is adopted to investigate bulk properties, spectra, and nuclear responses of closed-(sub)shell nuclei throughout the nuclear chart within a particle-hole (p-h) renormalized random-phase approximation (RRPA) scheme using a Hartree-Fock (HF) single-particle basis. Our analysis shows that all instabilities induced by the quasiboson approximation (QBA) underlying RPA are removed and an overall better consistency with the experiments is achieved for all observables of the investigated nuclei. The residual discrepancies point out the need of going beyond the p-h space.

Introduction. RPA is one of the most widely adopted methods devoted to the study of nuclear spectroscopy. It can be derived from the equation of motion method [1] or from the linear response theory [2].

It was implemented within many different frameworks, some using non-relativistic (e.g. Refs. [3, 4]) or relativistic (e.g. Refs. [5, 6]) density functionals, other exploiting the Green's function formalism (e.g. Refs. [7, 8]). The latter approach allows one to go beyond the harmonic approximation by coupling the RPA modes to complex configurations. Other extensions using Skyrme forces were proposed [9]. The investigations based on modern realistic potentials are few and rather recent [10–15].

RPA is known to be an extension of Tamm-Dancoff approximation (TDA). In both approaches, the eigenvalue problem is formulated within a p-h or two quasiparticle (2qp) spaces. In TDA, the ground state is the HF vacuum. In RPA, it is assumed to be correlated in the formal derivation of the equations of motion, but is replaced by an uncorrelated HF wavefunction in the actual calculation of the RPA matrix elements. This simplification, known as quasi-boson approximation (QBA), induces instabilities at low excitation energies.

Most of the recipes for obviating this shortcoming were enumerated and developed long ago by Rowe [16, 17]. They consist in reintroducing the correlations into the ground state without spoiling the simple structure of the RPA eigenvalue equations. Few investigations were conducted along this line since then [18–20]. An important extension was achieved and applied to metal clusters in Refs. [21, 22].

It is worth mentioning a more recent approach using the realistic Argonne v18 potential [23], as well as a dressed (D) RPA study performed within a self-consistent Green's function scheme [14]. A variety of works aiming to go beyond RPA is presented and discussed in a recent review [24].

Other approaches for computing ground-state correla-

tions are available. We mention an extension of TDA [25], a time-dependent density matrix (TDDM) formalism [26], a many-body perturbative approach [27], in-medium similarity renormalization group (IMSRG) [28] and an equation of motion multiphonon method (EMPM) [29].

The need for restoring the ground-state correlations is also dictated by the fact that HF accounts only for a fraction of the binding energy of all closed-(sub)shell nuclei throughout the periodic table if modern realistic potentials are adopted. This emerges blatantly from the results presented in Ref. [29].

In the present work, we perform a systematic study of bulk properties, nuclear responses, and spectra of a large number of nuclei ranging from ⁴He to ²⁰⁸Pb. We use the chiral potential $\Delta\text{N}^2\text{LO}_{\text{GO}}(394)$ [30], incorporating the three-body force, to generate a self-consistent HF basis and then solve the eigenvalue equations within TDA, RPA, and RRPA.

To our knowledge, this is the first *ab initio* extension of RPA which removes the instabilities induced by the QBA. It accounts for the nuclear bulk properties and provides a unified scheme where energy levels and responses are referred to the true correlated (rather than unperturbed) ground state.

The RRPA formalism. Following the procedure of Refs. [17, 21, 22] we consider states of the form

$$|\nu\rangle = Q_\nu^\dagger |0\rangle = \sum_{ph} [X_{ph}^\nu B_{ph}^\dagger - Y_{ph}^\nu B_{ph}] |0\rangle. \quad (1)$$

Here $B_{ph}^\dagger = D_{ph}^{-1/2} a_p^\dagger a_h$ denotes a renormalized p-h creation operator with respect to the HF vacuum, and

$$D_{ph} = n_h - n_p, \quad (2)$$

where $n_r = \langle 0 | a_r^\dagger a_r | 0 \rangle$ are the particle ($r = p$) and hole ($r = h$) ground-state occupation numbers. The ground

state is obtained by imposing the condition

$$Q_\nu |0\rangle = 0. \quad (3)$$

In the QBA underlying RPA, $|0\rangle$ is replaced by the unperturbed HF wavefunction so that $n_p = 0$, $n_h = 1$ and $D_{ph} = 1$.

Using the equation of motion method [17], one obtains

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar\omega_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}, \quad (4)$$

where $\hbar\omega_\nu = E_\nu - E_0$ and

$$\begin{aligned} \mathcal{A}_{ph,p'h'} &= \langle 0 | [B_{ph}, H, B_{p'h'}^\dagger] | 0 \rangle, \\ \mathcal{B}_{ph,p'h'} &= -\langle 0 | [B_{ph}^\dagger, H, B_{p'h'}^\dagger] | 0 \rangle, \end{aligned} \quad (5)$$

having introduced the symmetrized double commutator

$$[A, B, C] = \frac{1}{2}([A, [B, C]] + [[A, B], C]). \quad (6)$$

The calculation of the block matrices yields

$$\begin{aligned} \mathcal{A}_{ph,p'h'} &= D_{php'h'} (\epsilon_{pp'} \delta_{hh'} - \epsilon_{hh'} \delta_{pp'}) \\ &\quad + D_{ph}^{1/2} D_{p'h'}^{1/2} \langle hp' | V | ph' \rangle, \\ \mathcal{B}_{ph,p'h'} &= D_{ph}^{1/2} D_{p'h'}^{1/2} \langle hh' | V | pp' \rangle, \end{aligned} \quad (7)$$

where ($r = p, h$ and $s = p, h$)

$$D_{php'h'} = \frac{1}{2}(D_{ph}^{1/2} D_{p'h'}^{-1/2} + D_{ph}^{-1/2} D_{p'h'}^{1/2}), \quad (8)$$

$$\begin{aligned} \epsilon_{pp'} &= \langle p' | t | p \rangle + \sum_r n_r \langle p' r | V | pr \rangle \\ &\quad + \frac{1}{2} \sum_{r,s} n_r n_s \langle p' r s | V | prs \rangle, \end{aligned} \quad (9)$$

$$\begin{aligned} \epsilon_{hh'} &= \langle h | t | h' \rangle + \sum_r n_r \langle hr | V | h' r \rangle \\ &\quad + \frac{1}{2} \sum_{r,s} n_r n_s \langle h r s | V | h' r s \rangle. \end{aligned} \quad (10)$$

The occupation numbers n_r are to be obtained from the one-body density matrix (OBDM)

$$\begin{aligned} \langle 0 | a_p^\dagger a_{p'} | 0 \rangle &= \sum_{\nu, \mu, h} \left[\delta_{\nu\mu} - \frac{1}{2} \sum_{q,g} D_{qg} X_{qg}^\mu X_{qg}^{\nu*} \right] \\ &\quad \cdot D_{ph}^{1/2} D_{p'h}^{1/2} Y_{ph}^\nu Y_{p'h}^{\mu*} + \mathcal{O}(|Y|^6), \\ \langle 0 | a_h^\dagger a_{h'} | 0 \rangle &= \delta_{hh'} - \sum_{\nu, \mu, p} \left[\delta_{\nu\mu} - \frac{1}{2} \sum_{q,g} D_{qg} X_{qg}^\mu \right. \\ &\quad \cdot X_{qg}^{\nu*} \left. \right] D_{ph}^{1/2} D_{p'h'}^{1/2} Y_{ph}^\nu Y_{p'h'}^{\mu*} + \mathcal{O}(|Y|^6). \end{aligned} \quad (11)$$

The above system of nonlinear coupled equations is solved iteratively. Each iteration gives a new OBDM whose diagonalization yields a new set of occupation numbers n_r ($r = p, h$) and defines a new natural orbital

single-particle basis. The iteration ends when the convergence is reached.

The whole process implies a double iteration. One starts with solving the standard RPA eigenvalue problem, obtaining thereby the initial amplitudes X and Y . These amplitudes together with the HF occupation numbers are used to determine the density matrices in Eqs. (11). The diagonalization of these latter quantities yields the new occupations numbers and a natural orbital basis to be used for solving again the RPA eigenvalue problem (Eq. (4)). A new set of RPA amplitudes is obtained thereby. The above procedure is iterated until the OBDM converges to a fixed point.

Final RPA amplitudes define excited states built on top of the correlated ground state and can be used to evaluate the ground-state transition amplitudes of any one-body operator F

$$\langle \nu | F | 0 \rangle = \sum_{p,h} D_{ph}^{1/2} (X_{ph}^{\nu*} \langle p | F | h \rangle + Y_{ph}^{\nu*} \langle h | F | p \rangle). \quad (12)$$

Note that in the limit $D_{ph} \rightarrow 1$ the standard RPA expressions are recovered.

Numerical implementation and results. The Hamiltonian is composed of the intrinsic kinetic energy T_{int} and the chiral potential $\Delta\text{N}^2\text{LOGO}(394)$ [30].

A HF basis was generated within an harmonic oscillator (HO) space covering all major shells up to $N_{\text{max}} = 14$. Such a basis was adopted to determine the matrix elements of the interaction. The NuHamil numerical code was used for this purpose [31].

All matrix elements of the three-body potential up to $N_{\text{max}}^{(3)} \equiv \min(3N_{\text{max}}, 28)$ are included at the normal ordered two-body (NO2B) level [32]. These are the only ones entering in calculations performed within a p-h configuration space as in our case. Such a p-h basis, with the exception of the HF vacuum, is also free of spurious center of mass admixtures. These are removed by an orthogonalization procedure [33].

The ground-state energy is given by

$$E_0 = E_{\text{HF}} + E_{\text{corr}}, \quad (13)$$

where E_{HF} is the HF term and

$$E_{\text{corr}} = - \sum_\nu \hbar\omega_\nu \sum_{p,h} |Y_{ph}|^2 \quad (14)$$

comes from the correlations. The neutron ($\tau = \nu$) and proton ($\tau = \pi$) square radii

$$\langle r_\tau^2 \rangle = \frac{1}{N_\tau} \langle 0 | \sum_{i=1}^{N_\tau} (\vec{r}_\tau(i) - \vec{R}_{\text{c.m.}})^2 | 0 \rangle \quad (15)$$

are referred to the center of mass (c.m.) in order to minimize the spurious admixtures present in the HF vacuum. The empirical charge radii are deduced from $\langle r_\pi^2 \rangle$ through the formula given, for instance, in Refs. [27, 34].

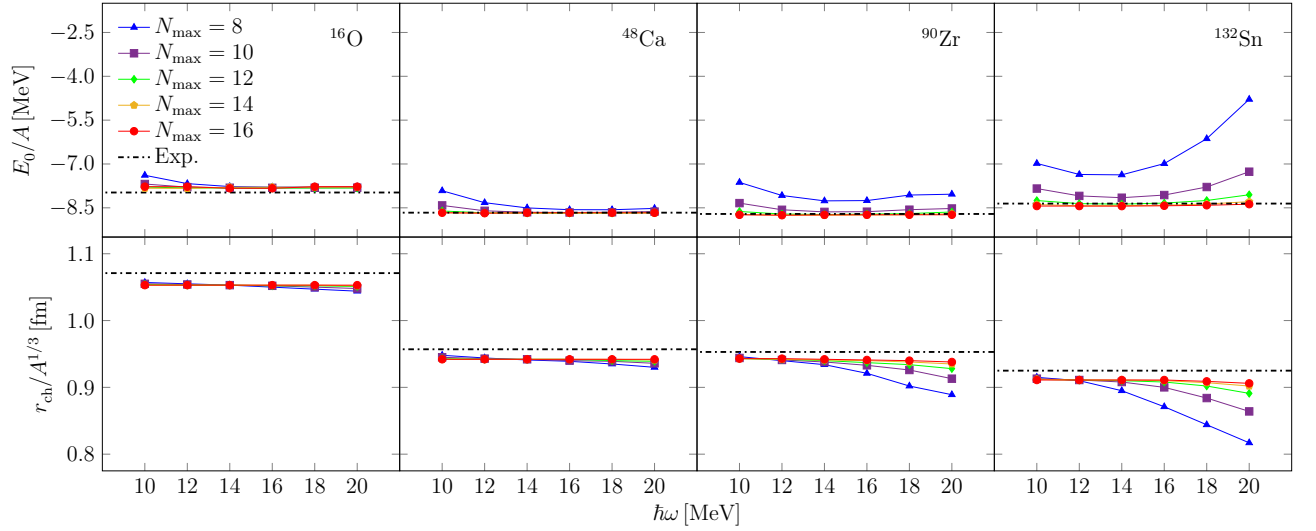


FIG. 1. (Color online) Convergence of the RRPA binding energy per nucleon, and charge radii versus the HO frequency $\hbar\omega$ for different numbers $N_{\max}$ of HO major shells. The dash-dotted lines indicate experimental values [35, 36].

As shown in Fig. 1, the ground-state energies as well as the charge radii become insensitive to the HO frequency only in a space encompassing an increasing number of major shells as we move from light to heavy nuclei. An overall fair agreement between computed and empirical

values is attained. For nuclei up to ^{90}Zr the employed model space is large enough to yield stable results, being their dependence on the HO frequency $\hbar\omega$ very weak. Thus, the numerical results are presented for a single choice $\hbar\omega = 12$ MeV.

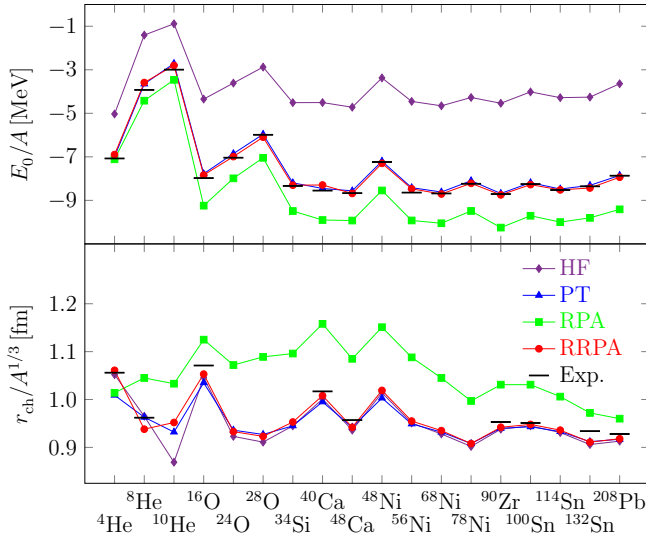


FIG. 2. (Color online) Systematic of the HF, PT, RPA, and RRPA binding energies per nucleon, and charge radii versus the empirical values taken from [35, 36].

The systematics presented in Fig. 2 prove that HF underestimates severely the binding energy of all studied nuclei. On the other hand, a strong over-binding is obtained once we add the contribution from the RPA ground-state correlations. The quenching action of the RRPA restores the consistency with the empirical val-

ues. The close agreement of the RRPA energies with the corresponding quantities obtained in HF + second-order perturbation theory (PT) is noteworthy.

RPA tends to overestimate also the nuclear radii (Fig. 2). RPA restores the agreement between theoretical and empirical quantities.

Next, we discuss the effect of renormalisation on selected excited states. In RPA, few levels of the ^{16}O and ^{90}Zr spectra are strongly pushed down toward the ground state (Fig. 3). This is a general feature occurring in all nuclei investigated. In some of them, like ^{40}Ca , the lowest level collapses and the energy becomes imaginary. These instabilities are removed within the RRPA and the consistency with the experiments is restored.

Further insight can be obtained from the transition probabilities. The ground-state correlations, accounted for in RRPA, do not produce any significant further fragmentation of the strength with respect to RPA. On the other hand, because of the energy downshift and damping of the main E1 peak they cause, the energy-weighted sum rule, preserved in RPA, is sensibly underestimated (Fig. 4). This impact is to be attributed to the depletion of few single particle (hole) states since the majority of the states involved in the transitions, being far from the Fermi surface, are empty (full) (Fig.5).

The depletion of single-particle levels around such a surface affects strongly the low-lying octupole transitions (Table I). In fact, the E3 ground-state reduced strength of the transition to the 3_1^- , practically negligible in TDA, increases dramatically as we move to RPA which system-

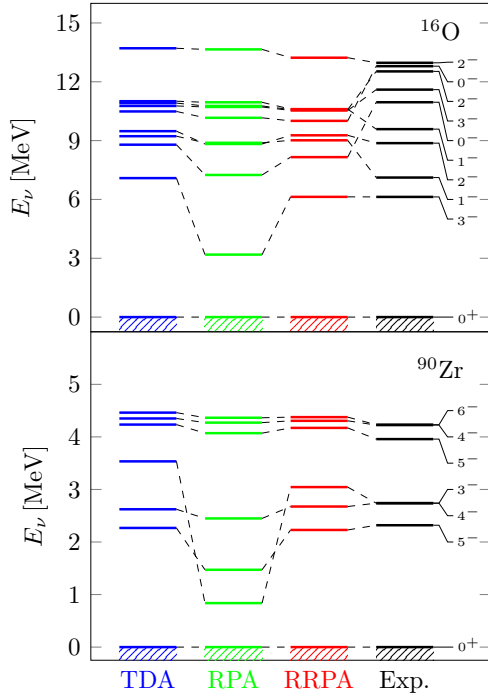


FIG. 3. (Color online) Selected low-lying levels of ^{16}O (top) and ^{90}Zr (bottom) calculated within TDA, RPA, and RRPA.

atically overestimates the measured values. These are sensibly underestimated in RRPA as a consequence of the drastic quenching of the Y amplitudes (Fig. 5).

It is not difficult to find the reason of these dramatic changes in going from one approach to the other. Small variations in the X and Y amplitudes are strongly amplified by their mutual interference produced once the transition amplitudes get squared.

	TDA	RPA	RRPA	Exp.
^{16}O	0.7	2.9	1.2	1.5 ± 0.1
^{40}Ca	5.4	14.8	12.6	20.4 ± 1.7
^{48}Ca	5.7	17.2	9.6	8.3 ± 0.2
^{68}Ni	2.2	21.7	8.0	38.0 ± 9.0
^{90}Zr	27.1	396.6	58.7	108.0 ± 9.0
^{114}Sn	7.0	87.6	34.8	100.0 ± 12.0
^{208}Pb	123.6	773.8	277.7	611.0 ± 9.0

TABLE I. Reduced E3 transition strengths $B(\text{E}3, 0_1^+ \rightarrow 3_1^-)$ [$10^3 \cdot \text{e}^2 \cdot \text{fm}^6$] for transitions from the ground to the first octupole state in selected nuclei within TDA, RPA, and RRPA. The experimental values are taken from [38].

Concluding remarks. The limits of RPA emerge definitely from the present systematic based on the use of modern realistic potentials: The overestimation of binding energies and charge radii, the softness of some excited levels toward the ground state.

The origin of these deficiencies is suggested by the plot

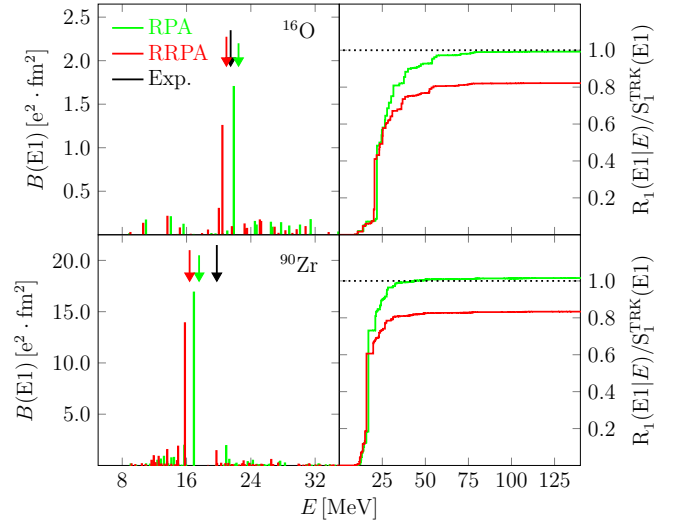


FIG. 4. (Color online) RPA versus RRPA reduced E1 strength distributions (left) and the energy-weighted running sums normalized to Thomas-Reiche-Kuhn (TRK) sum rule (right). Arrows indicate the energy centroids calculated as ratio between energy-weighted and non-weighted sums m_1/m_0 . Experimental values were adopted from [37] (Ahrens et al. 1972 & Askin et al. 1972 data sets).

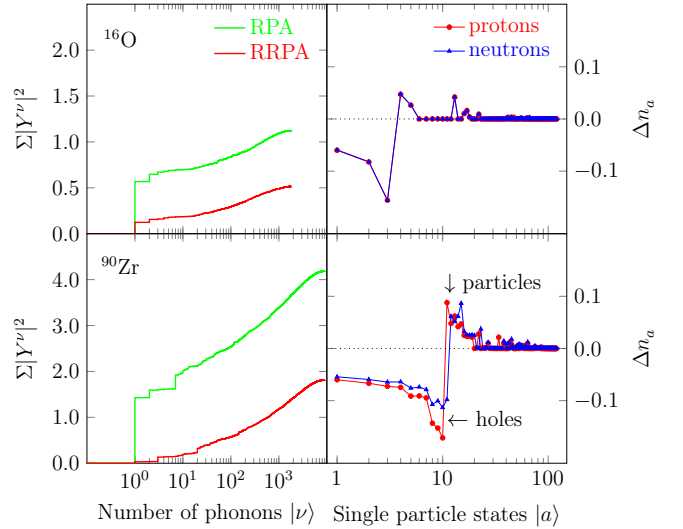


FIG. 5. (Color online) Running sum of RPA and RRPA backward amplitudes (left), and deviations of the RRPA from the HF occupation numbers $\Delta n_a = n_a^{\text{RRPA}} - n_a^{\text{HF}}$ (right) in ^{16}O and ^{90}Zr . Phonons and single-particle states are ordered according to energy.

in Fig. 5. We infer from the too large values of the backward Y amplitudes that the strong ground-state correlations induced by modern realistic potentials invalidate the QBA underlying RPA. Once this approximation is removed, the amplitudes are damped and the inconsistencies removed.

The present approach achieves such a remarkable re-

sult without spoiling the simple structure of the RPA eigenvalue equations. One needs to account for the deviations of the single particle occupation numbers from 0 or 1. These deviations are quite pronounced in proximity of the Fermi surface and vanish rapidly as we move away from (Fig. 5). Moreover, it is necessary to include the contribution coming from the non-diagonal particle-particle (pp') and hole-hole (hh') (Eqs. 11) terms entering the OBDMs, as proposed in Ref. [22], in order to reproduce the charge radii, strongly overestimated in RPA.

As pointed out already, the RRPA levels and responses are referred to the true correlated ground state. A significant link with no-core shell model [39] and coupled-cluster [40] is established thereby. Such a link will be reinforced once the method will be recast in terms of Bogoliubov quasiparticles (qp), a feasible task, so as to cover a large fraction of open shell nuclei.

Even so reformulated, however, RRPA cannot be considered a complete alternative to no-core shell model. Being confined within a p-h or 2qp configuration space, RRPA can account only for a fraction of the energy levels forming the nuclear spectra and is unable to fully satisfy the energy-weighted sum rule. One needs to enlarge the

space so as to include $np - nh$ ($n > 1$) or nqp ($n > 2$) configurations in order to cover the full energy spectrum and, hopefully, to reduce the persisting discrepancies between theoretical and experimental responses.

This upgrade is not at all trivial if we stick on RPA and its extensions. It is more natural to resort to a closely related and reliable alternative represented by the EMPM in its qp version [41].

We can therefore conclude that, within the limits of its validity, the present self-consistent RRPA approach offers, from first principles, a simple reliable unified systematic of bulk and spectroscopic properties of finite closed (sub-)shell nuclei, and is especially useful in the regions of medium and heavy nuclei, not easily accessible to more complete *ab initio* approaches.

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