Correlation energies in the random phase approximation using realistic interactions

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The random phase approximation (RPA) based on a correlated realistic nucleon-nucleon interaction is used to evaluate correlation energies in closed-shell nuclei beyond the Hartree-Fock level. The relevance of contributions associated with charge exchange excitations as well as the necessity to correct for the double counting of the second order contribution to the RPA ring summation are emphasized. Once these effects are properly included, the RPA ring summation provides an efficient tool to assess the impact of long-range correlations on binding energies throughout the whole nuclear chart, which is of particular importance when starting from realistic interactions.

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The picture of a collection of independent particles moving in a common mean field is a common starting point for the description of several microscopic many-body systems, ranging from solid state physics to chemistry and nuclear structure. However, this notion, which leads directly to the Hartree-Fock (HF) theory, is just a first approximation and significant effort is required to adequately describe the correlations beyond mean field. For simple atoms and molecules, as an example, many-body perturbation theory (MBPT) allows to predict correlation energies already at the level of a per cent [1], while more accurate approaches such as Green's function [2, 3] and coupled-cluster [4] methods are also available. The situation is less favorable in the case of nuclear physics, where one has to face both, the difficulties in solving the nuclear many-body problem and the ambiguities in the models of the nuclear interaction. Due to the strong short-range and tensor components of the interaction, exact ab-initio calculations have so far been restricted to the lightest systems [5, 6]. For larger nuclei the most accurate scheme to obtain nuclear masses are still phenomenological energy density functionals, e.g. Skyrme functionals, which lead to rms-deviations from the experimental biding energies of the order of 1 MeV [7–9]. This remains somewhat larger than the accuracies of a few hundred keV required for applications in nuclear astrophysics.

Recently, realistic nucleon-nucleon (NN) interactions have been regulated for the use with standard nuclear structure methods using two novel approaches: (i) low-momentum interactions $V_{\mathrm{low}k}$ derived from renormalization group theory [10] and (ii) correlated interactions V_{UCOM} constructed in the framework of unitary correlation operator method [11]. In connection with these interactions, the HF approximation leads to bound nuclei but underestimates the binding energy due to its inability to describe long-range correlations. In recent HF studies based on $V_{\mathrm{low}k}$ and V_{UCOM}, these have been accounted for via many-body perturbation theory (MBPT) up to third order [12, 13]. In general, correlations beyond HF are more relevant in studies based on realistic NN interactions than in models based on energy density functionals, because the latter already mimic part of the many-body correlations through the phenomenological fit.

Going beyond low-order MBPT, correlation energies can be obtained using the random phase approximation (RPA) as a tool to evaluate a partial summation over particle-hole ring diagrams. In the language of RPA, ground state correlations emerge from a coupling to giant resonances and surface vibrations [14–17]. By applying the RPA method, these excitations are approximated as harmonic vibrations. The total binding energy can then be evaluated as the sum of the zero-point energies of all the possible modes. The RPA framework has been employed in several studies of the ground-state correlation energies mainly associated with quadrupole and octupole modes, and pairing vibrations [18–22]. It should be noted that for systems made of more than one fermion species, other modes, e.g. Gamow-Teller transitions in nuclei, become possible. However, no discussion is usually found in the literature regarding the relevance of these charge exchange excitations.

In this work we study RPA correlation energies in conjunction with correlated realistic NN interactions derived from the Argonne V18 potential [23] in the framework of the unitary correlation operator method (UCOM). The short-range central and tensor correlations induced by the realistic potential are described by a unitary state-independent transformation [11, 24]. Only the short-range, system-independent correlations are described explicitly by the unitary transformation, long-range correlations have to be accounted for by the many-body method employed. The unitary transformation of the Hamiltonian defines a correlated interaction V_{UCOM} which is phase-shift equivalent to, but much softer than the original potential. The application of V_{UCOM} in no-core shell model calculations for ^{3}H and ^{4}He shows a dramatic improvement of the convergence behavior [24]. At the same time, the tensor correlator can be tuned in order to minimize the contribution to the binding energy of the net three-body force, which is the sum of the genuine three-body potential supplementing the bare NN potential and the three-body terms induced

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by the unitary transformation of the Hamiltonian. As no-core shell model calculations show, the two-body $V_{\rm UCOM}$ provides a good quantitative description of ground and low-lying excited states throughout the p-shell. Using the same correlated interaction $V_{\rm UCOM}$ we have performed HF+MBPT and HF+RPA calculations for closed shell nuclei throughout the nuclear chart [13, 25]. In the following we show that correlations beyond HF estimated in these ways lead to good agreement with experimental binding energies [13].

In the present work we investigate the effect of long-range correlations in the framework of RPA [25]. Using the single-particle basis resulting from HF, the RPA configuration space is built and the generalized eigenvalue problem posed by the RPA equations is solved,

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} , \qquad (1)$$

where the eigenvalues ω_ν correspond to RPA excitation energies. The forward and backward-going particle-hole amplitudes, X^ν_{ph} and Y^ν_{ph}, respectively, are related to the transition amplitudes to the excited states $|\Psi_\nu\rangle$ by

$$\langle\Psi_\nu| c^\dagger_\alpha c_\beta |\Psi_0\rangle \;=\; \sum_{p\,h} \left[\delta_{\alpha,p}\delta_{\beta,h}\, X^\nu_{ph} \;+\; \delta_{\alpha,h}\delta_{\beta,p}\, Y^\nu_{ph}\right] . \qquad (2)$$

Here and in the following, the indices p (h) always label particle (hole) states while Greek letters refer to any orbits. $c^\dagger$ (c) are the usual creation (annihilation) operators. The HF+RPA scheme is applied in a fully consistent way, i.e. the same translational invariant Hamiltonian $H_{\rm int} = T - T_{\rm cm} + V_{\rm UCOM}$, is used in the HF equations that determine the single-particle basis and in the RPA matrices **A** and **B**. This ensures that the RPA amplitudes do not contain spurious components associated with the center-of-mass translational motion [25].

In the quasi-boson approximation the ground state energy is described as the zero point energy of a collection of harmonic vibrations. Using the oscillator-projection method by Rowe [15], one is led to express the intrinsic energy of the system as

$$E = E_{\rm HF} + E_{\rm RPA}, \qquad (3)$$

where in addition to the HF binding energy a contribution of the RPA correlation energy,

$$E_{\rm RPA} = -\sum_{\nu>0} \hbar\omega_\nu \sum_{p\,h} |Y^\nu_{ph}|^2 \;, \qquad (4)$$

appears. Eq. (4) involves the RPA eigenvalues ω_ν and backward-going amplitudes Y^ν_{ph}. We note that the kinetic energy of the center of mass, $T_{\rm cm}$, has been fully subtracted in the intrinsic Hamiltonian and no correction associated with the zero energy mode ($\nu = 0$) is needed. Although it has been shown that this contribution to the correlation energy amounts to subtracting the kinetic energy of the center of mass [26, 27], this does not apply to the intrinsic Hamiltonian. To see what happens in this case, we have considered an Hamiltonian of the form $H(\alpha) = H_{\rm int} + \alpha T_{\rm cm}$ and repeated the derivation of Ref. [34]. We found that the RPA energy is given by

$$E_{\rm RPA} = -\sum_{\nu\neq 0} \hbar\omega_\nu \sum_{p\,h} |Y^\nu_{ph}|^2 \;-\; \frac{\alpha}{2M_T} < HF|\mathcal{P}_0^2|HF > , \quad (5)$$

where the operator $\mathcal{P}_\nu \equiv \sum_{p,h}[P^\nu_{ph} c^\dagger_p c_h + (P^\nu_{ph})^* c^\dagger_h c_p]$ is defined in terms of the amplitudes of the collective momentum [27] and M_T is the total mass of the system. $< HF|\,\mathcal{P}_0^2\,|HF >$ gives the square of the momentum of the center of mass. Thus one finds a contribution proportional to the fraction of $T_{\rm cm}$ actually included in the Hamiltonian. We have verified numerically that the contribution from the zero energy mode vanishes with α.

In comparison to an order-by-order summation of particle-hole ring diagrams in MBPT, Eq. (4) implicitly double counts the second-order contribution, as pointed out by Fukuda et al. [14] and Ellis [28]. To show this, we expand the RPA eigenvalues ω_ν and the amplitudes X^ν_{ph} and Y^ν_{ph} in a perturbation series of the interaction $H_{\rm int}$, as done in Ref. [14]. Inserting these into Eq. (4) one obtains,

$$E_{\rm RPA} = 2E^{(2)} + E^{(3)}_{\rm ring} + O(H^4) , \qquad (6)$$

where $E^{(2)}$ corresponds to the second order contribution in MBPT

$$E^{(2)} = -\frac{1}{4} \sum_{p_1 p_2 h_1 h_2} \frac{H_{p_1 p_2, h_1 h_2}\; H_{h_1 h_2, p_1 p_2}}{\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2}} , \qquad (7)$$

and $E^{(3)}_{\rm ring}$ to the contribution of the ring diagram at third order

$$E^{(3)}_{\rm ring} \;=\; \sum_{p_1 p_2 p_3} \sum_{h_1 h_2 h_3} \frac{H_{p_1 p_2, h_1 h_2}\; H_{p_3 h_2, h_3 p_2}\; H_{h_1 h_3, p_1 p_3}}{(\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2})(\epsilon_{p_1} + \epsilon_{p_3} - \epsilon_{h_1} - \epsilon_{h_3})} . \qquad (8)$$

These relations reveal two important points. First, the double counting of the second order contribution $E^{(2)}$ is evident and has to be corrected for explicitly. Second, the sum over all possible combinations of proton and neutron orbits in Eq. (7) is not achieved without including the charge exchange modes in Eq. (4).

The double counting of $E^{(2)}$ is intrinsic to the quasi-boson approximation and can be avoided only in a formalism that (beyond the RPA approach) explicitly recouples particle and hole states between different phonons. This can be achieved at the level of the many-body self-energy [29, 30]. Beyond the second order, the expansion (6) of $E_{\rm RPA}$ does not introduce any further overcountings [14]. However, one has to keep in mind that the particle-hole ring summation does not include all possible diagrams, e.g., the third order ring term $E^{(3)}_{\rm ring}$ is only one of three third-order contributions and two-particle two-hole diagrams are neglected by Eq. (4). The latter are known to be approximately compensated by Pauli exchange effects between different phonons at high order [31].

The inclusion of charge-exchange modes arises naturally, for example, in the presence of isospin symmetry: the coupling of isospins trivially leads to a factor of $(2T + 1)$ in front

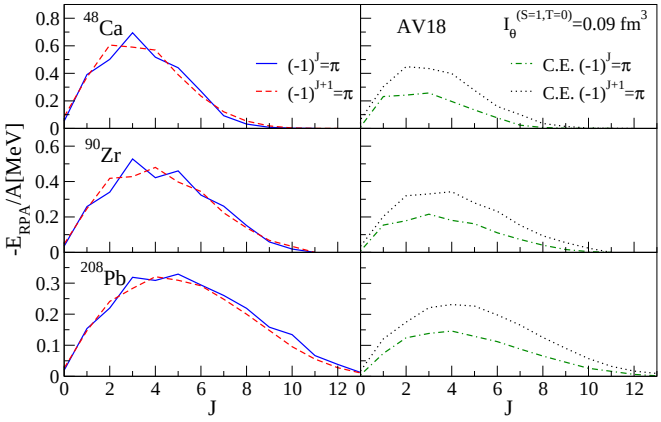

FIG. 1: (Color online) Partial contributions to the RPA correlation energies in ^{40}Ca, ^{90}Zr, and ^{208}Pb as a function of multipolarity J. Solid and dashed lines correspond to contributions from natural and unnatural parity excitations, respectively (left panel). The contributions from charge exchange excitations (C.E.) are shown in the right panel.

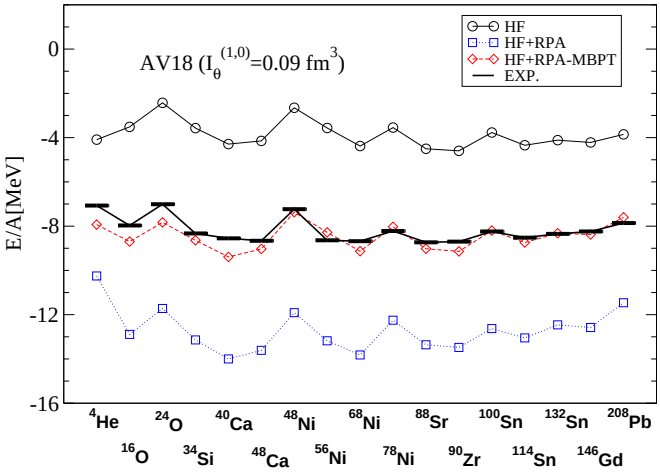

FIG. 2: (Color online) Binding energies per nucleon for a series of closed-shell nuclei in comparison with experiment. Shown are the HF energy, the energy including RPA correlations according to Eq. (4) , and those including RPA correlations corrected for the double counting of the second order (denoted HF+RPA-MBPT). All calculations are based on the correlated Argonne V18 interaction.

of Eq. (4) [28]. Also in the Green's function formalism, the Lehman representation of the polarization propagator includes the completeness of all states of A particles, regardless of the total charge [3]. In this case, both the standard RPA and the charge-exchange RPA arise naturally as different channels of the same Bethe-Salpeter equation. Simply, the eigenstates of the nuclei with (A,$Z \pm 1$) should be regarded as possible excitations of the system. And the zero-point energy of these modes contributes to Eq. (4).

For a microscopic theory based on realistic nucleon-nucleon interactions, the correlation energy beyond the simple HF approximation is sizable. This remains true even after regularizing the interaction to take into account short-range correlations. The residual long-range correlations manifest themselves in a sizable second-order contribution, $E^{(2)}$ [13]. Therefore, the naive application of Eq. (4) would lead to a strong overestimation of the correlation energy. In the context of phenomenological models, Eq. (4) is often applied without corrections for double countings [18–22]. This might be partially compensated by also neglecting the contribution from charge exchange terms. However, this constitutes a completely uncontrolled approximation.

We apply the above scheme to evaluate correlation energies for closed-shell nuclei throughout the nuclear chart based on a realistic NN interaction. We employ the $V_{\rm UCOM}$ derived from the Argonne V18 interaction using the optimal correlation operators determined in Ref. [24]. The range of the tensor correlator in the triplet-even channel was fixed to reproduce the binding energies of $A \leq 4$ nuclei in no-core shell model calculations ($I_\vartheta = 0.09\,\mathrm{fm}^3$). The same correlator was used successfully in HF and MBPT calculations reported in Ref. [13]. For a systematic calculation of the RPA correlations, Eq. (1) was projected onto good angular momentum J and parity π and all available multipolarities were taken into account. All calculations were performed using 13 major harmonic oscillator shells. For both MBPT and RPA this is sufficient to obtain convergence for light nuclei; heavier isotopes still show changes of ~ 0.5MeV per nucleon when going to 15 shells.

In Fig. 1 we display the individual contributions to the correlation energies evaluated with Eq. (4) for ^{48}Ca, ^{90}Zr, and ^{208}Pb. Shown are the contributions to $E_{\rm RPA}$ as function of the multipolarity $J^\pi = 0^\pm - 13^\pm$ separated into natural parity, $\pi = (-1)^J$, and unnatural parity, $\pi = (-1)^{J+1}$, excitations as well as charge exchange excitations. In general, the RPA correlation energy increases with J, reaches the maximum for $J = 3 - 4$, and slowly decreases towards higher multipolarities. Both, natural and unnatural parity states are equally important and charge exchange excitations also have significant contributions to the correlation energy. Although in all nuclei the largest contributions come from the $J = 3 - 4$ excited states, one obviously needs to include all other multipolarities as well. This is especially important for heavier nuclei, where the correlation energies are widely distributed over various multipolarities up to $J = 13$.

The overall sum of correlation energies displayed in Fig. 1 provides the correction to the binding energies in finite nuclei. In Fig. 2 we show binding energies per nucleon for several closed-shell nuclei obtained in HF with and without the inclusion of the RPA correlation energies, in comparison to the experimental binding energies [32]. The plain HF calculations underestimate the binding energies due to the inadequate description of long-range correlations. Inclusion of the correlation energies resulting from Eq. (4) without correction for the double-counting of the second order contribution leads to a strong overbinding. As discussed by da Providencia [33], only after explicit correction for the double counting by subtracting the second order contribution, i.e. by using $E_{\rm HF} + E_{\rm RPA} - E^{(2)}$, we obtain a proper estimate for the binding energy including correlation effects which is in good agreement with experiment.

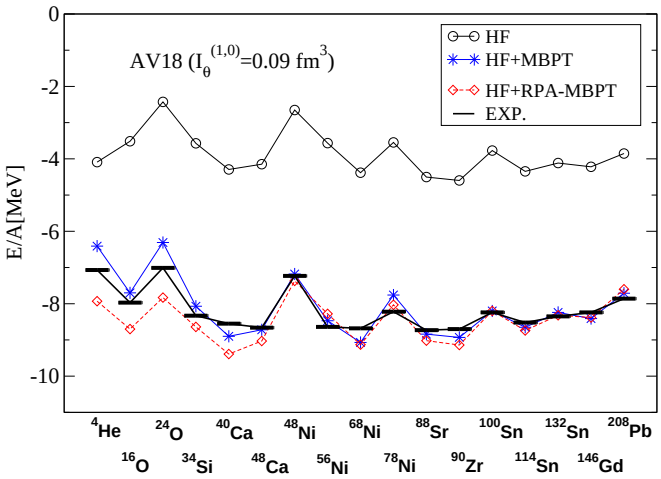

FIG. 3: (Color online) Binding energies per nucleon including RPA correlations and second-order correction (HF+RPA-MBPT) compared to energies resulting from second-order perturbation theory only (labeled HF+MBPT). Compare to Fig. 2.

For a more detailed discussion, in Fig. 3 we show the corrected RPA energies, $E_{\rm HF} + E_{\rm RPA} - E^{(2)}$, in comparison to the direct second-order perturbative estimate, $E_{\rm HF} + E^{(2)}$. The binding energies per nucleon obtained by employing the second-order perturbation theory agree rather well with the results of the RPA ring summation. Although the second-order correction to the HF energy is large, the higher order contributions included in the ring summation seem to have a relatively small net effect. Beyond ^{48}Ca the binding energies per nucleon including $E_{\rm RPA}$ are in excellent agreement with the perturbative second-order results and also with experimental values. The ring summation provides systematically larger correlation energies than the plain second-order.

For a more quantitative comparison of our calculated binding energies with the experimental data, we evaluate the rms-deviation $\sigma_{\rm rms}$ [7]. Using the set of 17 nuclei considered in the present study, we obtain $\sigma_{\rm rms}$=24.1 MeV for HF+RPA-MBPT binding energies. In comparison, phenomenological models based on energy density functionals result in rms-deviations of typically 0.7 to 4.4 MeV [7, 9, 34], i.e. one order of magnitude smaller. Given that the present approach does not contain any parameters adjusted to nuclei beyond $A = 4$ this result is remarkable. Refinements, such as the inclusion of a weak residual three-body interaction, are presently under investigation.

In conclusion, we have employed a consistent RPA approach to evaluate correlation energies based on a correlated realistic NN-potential beyond the HF level. We point out the need to sum over all possible excitation modes, including charge exchange excitations, and to correct for the double counting of the second-order contribution, when using standard expressions like Eq. (4) to evaluate the correlation energy. Then the RPA ring summation provides an efficient tool to evaluate correlation energies throughout the nuclear chart. In connection with $V_{\rm UCOM}$, the RPA correlation energies generally confirm the results of second order MBPT, indicating that the net contribution of higher-order ring-diagrams are moderate although the second order itself is large. Both, RPA ring summation and low-order MBPT, provide efficient tools for nuclear structure calculations with correlated realistic NN-interactions.

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