Integral representation of the RPA correlation energy

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Using the spectral function $F'(z)/F(z)$ the RPA correlation energy and other properties of a finite system can be written as a contour integral in a compact way. This yields a transparent expression and reduces drastically the numerical efforts for obtaining reliable values. The method applied to pairing vibrations in rotating nuclei as an illustrative example.

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Various problems considered in many-body physics of finite quantum systems can be treated in terms of a Hamiltonian which is quadratic in the creation and annihilation operators (see for example [1]). The mean field approximation (MF) and the random phase approximation (RPA) are the well known examples where the dynamics of complicated system is reducing to dynamics described by a quadratic Hamiltonian. These approximations have been proven to be quite successful in many applications to mesoscopic systems like nuclei [2-4] and metallic clusters [5].

One of the long standing problems in the RPA is how to calculate practically the correlation energy of the Hamiltonian $H = H_0 + V$, where $H_0$ is a mean field Hamiltonian and $V$ is a two-body residual interaction. The solution of this problem could allow also to calculate properly other physical quantities which depend on the whole set of the RPA eigen frequencies. The MF description is only a first approximation and the RPA correlations can essentially improve the description of experimental observables.

The Hamiltonian, written in terms of the RPA phonon operators $O_n^+(O_n)$, takes the simple form [6].
\[ H = E_{MF} + \sum_{n>0} \omega_n O_n^+ O_n + \frac{P^2}{2\mu} - \sum_{n>0} \omega_n Y^n + Y^n \]  

Here the first term is the MF energy and the second term is the Hamiltonian of the RPA (normal) modes. The third term is associated with the contribution of a spurious mode arisen due to a broken continuous symmetry (for example translation or rotation). The fourth term, where \( Y_n \) is the vector of the backward-going amplitudes of the RPA solution, is a correlation energy \( \varepsilon_{corr} \) caused by the normal modes. The eigen frequencies \( \omega_\nu \) of the RPA are derived from the singularities of the RPA response function \[ R(\omega) = (1 - R^0(\omega)\chi)^{-1}R^0(\omega) , \]  

where \( R^0 \) is the known unperturbed response function and \( \chi \) is a coupling constant. Accordingly, these frequencies are obtained as the zeros of the determinant \[ F(\omega) = det (1 - R^0(\omega)\chi) . \]  

The total correlation energy \( E_{corr} \), which is essentially the energy gain of the RPA ground state relative to the MF ground state, can be expressed as \[ E_{corr} = -\frac{<P^2>_{MF}}{2\mu} - \varepsilon_{corr} \equiv \frac{1}{2}(\sum \omega_\nu - \sum E_\mu) - E_{ex} , \]  

where \( E_{ex} \) is the known exchange energy of the interaction \( V \) and \( E_\mu \) are the poles of the \( R^0 \). The eigen frequencies \( \omega_\nu \) appear in actual situations as rather closely spaced zeros of the determinant \( F(\omega) \), Eq.(3). Since the number of roots of \( F(\omega) \) is practically of the order \( 10^4 \), for example, for heavy nuclei \( (A \approx 150) \) and none of these roots can be neglected, the calculation of the correlation energy \( E_{corr} \) is known to be rather difficult even in the case of the separable interactions. In addition, in many physical applications it is necessary to study the dependence of the correlation energy on the variation of the MF parameters. The method, proposed in [8] for the calculation of the rotational dependence of the correlation energy, does not allow treat the contribution of the spurious modes. Furthermore, it should be used with a dense grid to approach the necessary convergence in the integration procedure.
to obtain reliable results regarding the contribution of the normal modes. The contour integral representation presented in our paper remedies these deficiencies and in addition is a transparent method which has further advantages discussed below.

Let us consider a general eigenvalue equation

$$F(z) = 0 \quad (5)$$

where $F(z)$ is a supposed to be an analytical function in some region of the complex variable $z$. The complex continuation of the determinant Eq.(3) is an example for an appropriate function $F(z)$ studied below in detail. Another example is any finite matrix eigenvalue problem $F(z) = \det (H - z) = 0$ written in terms of a finite matrix $H$, for instance, the Hamiltonian of the shell model [9]. We define for our purpose the spectral function $S(z)$ as

$$S(z) = \frac{F'(z)}{F(z)} = \frac{d}{dz} \log F(z) \quad (6)$$

using the derivative $F'(z)$ in the $z$-region where $F(z)$ is analytical. The meaning of $S(z)$ becomes obvious for the example $F(z) = \det (H - z)$. Assuming $H$ is diagonalizable we may express $F$ in terms of the eigenvalues $\omega_\nu$ as the product $F(z) = \Pi_\nu (\omega_\nu - z)$ and obtain

$$S(z) = \frac{F'(z)}{F(z)} = \sum_\nu \frac{1}{\omega_\nu - z} \quad (7)$$

which yields the spectral decomposition of the matrix $H$. Returning to the general case, it is suggestive to apply Cauchy’s theorem to the above spectral function $S(z)$. In particular, we obtain straightforwardly by forming the following closed contour integral

$$I [g(z)] = \frac{1}{2\pi i} \oint dz g(z) S(z) = \frac{1}{2\pi i} \oint dz g(z) \frac{F'(z)}{F(z)}$$

$$= \sum_\nu n_\nu g(\omega_\nu) - \sum_\mu m_\mu g(p_\mu) \quad (8)$$

where $g(z)$ is an arbitrary complex function which is analytical in the enclosed region. Further, the sum $\nu$ includes all roots $\omega_\nu$ of $F(z)$ and the sum $\mu$ accounts for all poles $p_\mu$ of the derivative $F'(z)$ enclosed by the chosen contour. The integers $n_\nu$ and $m_\mu$ mean the multiplicity of the root $\omega_\nu$ and the order of the pole $p_\nu$, respectively.
The integration formula Eq.(8) is now applied to the RPA case. For the sake of the discussion let us consider a two-body residual interaction which is a sum of separable multipole-multipole interactions, i.e.

$$V = \sum_{\rho} \chi_{\rho} \hat{Q}_{\rho}^+ \hat{Q}_{\rho}$$

$$\hat{Q}_{\rho} = \sum_{\alpha<\beta} q_{\rho}(\alpha,\beta) a_{\alpha,\beta}^+ + h.c. = \hat{Q}_{\rho}^+$$

where $a^+$ is a quasiparticle creation operator. This interaction is widely used in nuclear physics [2–4] and nowadays it is successfully employed for the description of the plasmon frequencies in metallic clusters [10]. The unperturbed matrix response function $R^0$ associated with the interaction Eq.(9) is defined as the matrix

$$R^0_{\rho\sigma}(\omega) = \sum_{\mu} \frac{q_{\rho}^*(\mu) q_{\sigma}(\mu)}{E_\mu - \omega} + \frac{q_{\rho}(\mu) q_{\sigma}^*(\mu)}{E_\mu + \omega}$$

where the double index $\mu = (i, j)$ is running over all independent quasiparticle pairs $i > j = 1, n$ and $E_\mu \equiv e_i + e_j$ denotes the two-quasiparticle energy. The function $F(z)$ is specified as the determinant Eq.(3) with matrix elements Eq.(10). The location of its roots $\omega_\nu$ is not needed but these RPA roots are known to lie on the real axis symmetrically around the origin and in addition appear at $z = 0$, if there are spurious RPA solutions. One can easily obtain the derivative $F'(z)$ to form $S(z)$. Apparently, the poles of $F'(z)$ coincide with the known two-quasiparticle energies $E_\mu$. For our goal the appropriate contour of the integration Eq.(8) goes around all positive roots of $F(z)$ and likewise all two-quasiparticle poles as shown in Fig.1. Hence the desired contribution to the RPA correlation energy Eq.(4) is obtained as the contour integral

$$\frac{1}{2} \left( \sum \omega_\nu - \sum E_\mu \right) \equiv \frac{1}{4\pi i} \oint dz \frac{F'(z)}{F(z)}$$

Usually, the integration will be done numerically. The crucial practical advantage of the formula Eq.(11) is that we are free to choose the rectangular contour (Fig.1) sufficiently

$^1$the case of complex RPA solutions is normally excluded but could be similarly treated
distant from the poles such that the spectral function \( S(z) = F'(z)/F(z) \) becomes smooth while integrating on this path.

Then, the necessary grid needs not to be dense any more. In practical cases considered so far the number of integration points were reduced by a factor \( 10^2 \) without loss of a precision which reduces the CPU time drastically. The contribution of the possible spurious RPA solutions with \( \omega_0 = 0 \) is correctly accounted for, since the equivalent sum expression Eq.\((4)\) implies such contributions. Notice that, when integrating in Eq.\((11)\) separately around such a spurious pole at \( z = 0 \), there arises no a finite energy contribution due to the \( z^{-1} \) factor in the integrand. The precision of the numerical integration of the correlation energy \( E_{corr} \) can be conveniently checked by evaluating the analogous contour integral for \( g(z) = 1 \) which gives according Eq.\((8)\) an integer number. For the RPA spectral function \( S(z) \) the difference between the number of RPA roots and the number of quasiparticle states is counted, i.e. one expects a zero if there are no spurious \( \omega_0 = 0 \) solutions.

We specify discussion to the RPA spectral function \( S(z) \) derived from the determinant Eqs.\((3),(10)\). However, a similar treatment may hold for more general cases. Even, if the characteristic function \( F(z) \), Eq.\((3)\), can be defined only numerically in the vicinity of an appropriate integration path one may calculate the spectral function \( S(z) \) and apply the integration method. Now, we are going to employ the free choice of any physically relevant weight function \( g(z) \) in the integral formula Eq.\((8)\). In addition, also the integration contour can be adapted to the physical problem under study. For \( g(z) \equiv 1 \) information on the number and distribution of levels can be obtained. First, we define the two-quasiparticle

FIG. 1. A schematic picture of the integration contour (dashed line) in the complex plane. The roots \( \omega_\nu \) and the poles \( E_\mu \) of the function \( F(z) \) are marked with crosses.
spectral function by

\[ S^o(z) = \sum_\mu \frac{1}{E_\mu - z}. \tag{12} \]

Let us assume for simplicity, that the derivative \( F'(z) \) of the RPA determinant Eqs.(3), (10), has simple poles, i.e. \( m_\nu = 1 \). Then, in the spectral function

\[ \tilde{S}(z) = S(z) - S^o(z) \tag{13} \]

the two-quasiparticle poles are removed. Hence the integral \( \mathcal{I}[g = 1] \) using the spectral function \( \tilde{S} \) is counting the number of all RPA states \( \omega_\nu \) enclosed in the contour. The presence of a spurious solution at \( z = 0 \) can be checked when calculating \( \mathcal{I}[g = 1] \) with a narrow rectangular contour around zero which cannot be seen directly from the correlation energy Eq.(11). The simplest form of a level density distribution can be calculated analogously by slices like \( \mathcal{I}[g = 1]/\Delta \omega \) by integrating repeatedly along rectangular stripe contours around a given \( \omega \)--value with an appropriate width \( \Delta \omega \). A more refined representation of the level distribution follows from Eq.(8) when inserting the Lorentzian weight function

\[ g(z) \equiv L(z) = \frac{\Delta^2}{(\omega - z)^2 + \Delta^2} \tag{14} \]

which has poles at \( z = \omega \pm i\Delta \). The RPA spectral function \( \tilde{S}(z) \) yields the relation

\[ D(\omega, \Delta) \equiv \sum_\nu \frac{\Delta^2}{(\omega - \omega_\nu)^2 + \Delta^2} = \Delta \text{Im} \tilde{S}(\omega - i\Delta) + \mathcal{I}[L(z)] \tag{15} \]

where the sum includes all eigenvalues \( \omega_\nu \) within the chosen contour. Actually it is the r.h. side of this relation which can be evaluated numerically and thus it provides us the RPA level distribution \( D(\omega, \Delta) \) averaged by the width parameter \( \Delta \). Taking the contour at infinity outside all poles (assuming a finite number of roots) the integral becomes zero due to the Lorentzian fall off. Hence the integral term in Eq.(15) is the Lorentzian "background" contribution from the roots not included in the contour. Again, the contour integral involved can be calculated conveniently with a smooth integrand as mentioned above.

To demonstrate the viability and utility of the method, we have applied it to analyze the influence of the correlation energy on the description of the g-band of \(^{178}W\). For our purpose
the tilted axis cranking model (TAC) [11] represents the proper Hartree-Fock-Bogoliubov (HFB) theory which permits the calculations of the energies and intra band probabilities. As a residual interaction we consider the standard pairing field \( V = -GP^+P \). It is well known that the HFB theory does not provide an adequate description of the transition region where the pair field strongly fluctuates. Therefore we use the version of the TAC that includes the particle number projection (PNP) and improves the description of the pair correlations in high-K bands [12]. Fig.2 shows the results for different Routhian energies of the g-band calculated with the TAC alone, with the TAC which incorporates the PNP, and the TAC results which include the RPA correlation energy due to pairing vibrations, Eq.(4). On the whole region of a rotational frequency the RPA correlation energy lowers substantially the TAC Routhian energy and, consequently, improves the description of the g-band in comparison with the TAC combined with the PNP.

![Graph showing different Routhian energies for the g-band of 178W.](image)

FIG. 2. The g-band of \(^{178}\text{W}\). Different Routhian energies are presented: for the TAC (short-dashed line), for the TAC which includes the PNP (long-dashed line) and for the TAC with the RPA correlation energy (solid line).

Using the same method, we can evaluate the contribution of the RPA correlations to any physical quantity in the correlated ground state \( \delta Q_{RPA} = < Q >_{RPA} - < Q >_{MF} \) where \( \delta Q_{RPA} = \sum_{n>0} \sum_{ij} q_{ij} Y_{il}^n Y_{jl}^m \) [7,13]. For example, the aligned angular momentum calculated in the cranking HFB theory is larger than the experimental alignment. The consideration of the additional term arisen due to the RPA correlations leads to better agreement with experimental data. Notice that the strength function method [14] may be considered as an
alternative approach, however, it would treat the spurious contributions and $\varepsilon_{\text{corr}}$ separately. The comprehensive analysis of results obtained with different approaches will be discussed in the forthcoming paper [15].

In conclusion, the transparent practical method has been developed which drastically reduces the numerical efforts to calculate the integral characteristics renormalized by residual interactions in finite quantum systems. In particular, the correlation energy which arises in the RPA can be estimated with the necessary accuracy. In the considered example of $^{178}\text{W}$ the method demonstrates a remarkable improvement of the description of the g-band in comparison with the particle number projection approach.

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