Response Function Technique for Calculating the Random-Phase Approximation Correlation Energy

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We develop a scheme to exactly evaluate the correlation energy in the random-phase approximation, based on linear response theory [Y. R. Shimizu, J. D. Garrett, R. A. Broglia, M. Gallardo, and E. Vigezzi, Rev. Mod. Phys. **61**, 131 (1989)]. It is demonstrated that our formula is equivalent to a contour integral representation recently proposed [F. Dönau, D. Almehed, and R. G. Nazmitdinov, Phys. Rev. Lett. **83**, 280 (1999)] being numerically more efficient for realistic calculations. Examples are presented for pairing correlations in rapidly rotating nuclei.

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Mean-field theory provides a powerful approximation for describing many-particle systems. However, there are many situations where one is forced to go beyond mean field to include higher-order correlations, the random-phase approximation (RPA) being a widely used method for this purpose. One of the basic observables which requires one to go beyond mean-field approximation is the correlation energy, which in the quasiparticle basis takes the form (see, e.g., [6])

$$E_{\rm corr}^{\rm RPA} = \frac{1}{2}\left[\sum_n \omega_n - \sum_{\alpha<\beta} E_{\alpha\beta}\right], \tag{1}$$

where ω_n are the RPA eigenfrequencies, $E_{\alpha\beta} \equiv E_\alpha + E_\beta$ being the unperturbed two-quasiparticle energies. Because the different RPA modes contribute democratically to $E_{\rm corr}^{\rm RPA}$, to calculate this quantity one needs to determine very many, closely spaced, RPA eigenmodes. This is particularly true in the case where symmetries of the mean field are spontaneously broken, such as in the case of superfluid and deformed nuclei, where the detailed computation of the contribution of every single RPA root to $E_{\rm corr}^{\rm RPA}$ becomes unfeasible. To avoid this problem, we developed in [1] a method to calculate the correlation energy, making use of response function techniques, and applied it to the study of pairing correlations in rapidly rotating nuclei. The essence of the method consists in expressing the RPA correlation as an integral in terms of the RPA response function, which can be calculated without explicitly solving the RPA eigenvalue problem. These techniques have been recently extended to deal with the Nambu-Goldstone (NG) modes [2], and to calculate the nucleon effective mass in superfluid, deformed, rotating nuclei [3].

Recently, a contour integral representation for the RPA correlation energy has been proposed in [4]. It was claimed that this method is more efficient than that developed in [1]. The assertion was also made that the method of [1] did not take the contribution of the spurious modes into account. In this Letter we show that both methods are equivalent. Furthermore, using the property of meromorphic functions, we improve the original method of [1] to obtain the exact RPA correlation energy in a more efficient way than that proposed in [4].

Following [1], we start from the Hamiltonian,

$$H = H_0 + V\,, \tag{2}$$

where H_0 is the unperturbed one-body (mean-field) Hamiltonian and V is the residual two-body interaction, which is assumed to be of multiseparable form,

$$V = -\frac{1}{2}\sum_\rho \chi_\rho Q_\rho Q_\rho\,, \tag{3}$$

with Q_ρ being a one-body Hermitian operator while χ_ρ is the strength of the interaction in channel ρ. The associated ground state energies and state vectors of H_0 and H are denoted E_0, $|\Phi_0\rangle$ and E, $|\Psi\rangle$, respectively. Turning on the interaction adiabatically, the correlation energy can be written as [5]

$$E_{\rm corr} \equiv E - E_0 = \int_0^1 d\lambda \langle\Psi(\lambda)|V|\Psi(\lambda)\rangle\,. \tag{4}$$

In this equation, $|\Psi(\lambda)\rangle$ is the ground state of the λ-scaled Hamiltonian $H(\lambda) \equiv H_0 + \lambda V$. Within the RPA, the above expression can be rewritten by making use of a contour integration as

$$\begin{aligned} E_{\rm corr}^{\rm RPA} &= -\frac{1}{2}\int_0^1 d\lambda \sum_{\rho,n} \chi_\rho \mathcal{Q}_{\rho,n}^{(\lambda)*} \mathcal{Q}_{\rho,n}^{(\lambda)} \\ &= -\frac{1}{4\pi i}\int_0^1 d\lambda \oint_C dz \sum_\rho [\mathcal{R}_{\rho\rho}^{(\lambda)}(z)\chi_\rho], \end{aligned} \tag{5}$$

in terms of the λ-scaled RPA response function (matrix),

$$\mathcal{R}_{\rho\sigma}^{(\lambda)}(\omega) \equiv \sum_n \left[\frac{\mathcal{Q}_{\rho,n}^{(\lambda)*}\mathcal{Q}_{\sigma,n}^{(\lambda)}}{\omega_n^{(\lambda)} - \omega} + \frac{\mathcal{Q}_{\rho,n}^{(\lambda)}\mathcal{Q}_{\sigma,n}^{(\lambda)*}}{\omega_n^{(\lambda)} + \omega}\right], \tag{6}$$

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where $\mathcal{Q}^{(\lambda)}_{\rho,n} = \langle n(\lambda)|Q_\rho|\Psi(\lambda)\rangle_{\mathrm{RPA}}$, and the contour C encloses all the positive λ-scaled RPA eigenvalues $z = \omega^{(\lambda)}_n$ clockwise. Note that $\mathcal{R}^{(\lambda)}_{\rho\sigma}(\omega)$ can be calculated as

$$\mathcal{R}^{(\lambda)}(\omega) = [1 - R(\omega)\chi\lambda]^{-1}R(\omega), \tag{7}$$

in terms of $\chi = (\delta_{\rho\sigma}\chi_\rho)$ and the unperturbed response function (matrix), $R_{\rho\sigma}(\omega)$, which is defined by replacing $\mathcal{Q}^{(\lambda)}_{\rho,n}$ and $\omega^{(\lambda)}_n$ in Eq. (6) with unperturbed quantities, $q_{\rho,\alpha\beta} = \langle\alpha\beta|Q_\rho|0\rangle$ and $E_{\alpha\beta}$.

By choosing a common contour C for all values of $0 < \lambda < 1$, one may exchange the order of integration in Eq. (5) [7,8]. The selected path is the one shown in Fig. 1a passing through the origin of the complex z plane in keeping with the presence of spurious zero-energy modes (the symmetry-recovering or Nambu-Goldstone modes) in the RPA spectrum ($\omega_{n=\mathrm{NG}} \to 0$ as $\lambda \to 1$). In this case the λ integration in Eq. (5) converges because $|\mathcal{Q}^{(\lambda)}_{\rho,n=\mathrm{NG}}|^2 \propto 1/\sqrt{1-\lambda}$ as $\lambda \to 1$. After performing the λ integration analytically, we finally obtain

$$E^{\mathrm{RPA}}_{\mathrm{corr}} = \frac{1}{4\pi i}\oint_{C_{1a}} F(z)\,dz, \tag{8}$$

where

$$F(z) \equiv -\int_0^1 \mathrm{Tr}[\mathcal{R}^{(\lambda)}(z)\chi]\,d\lambda = \log\{\det[1 - R(z)\chi]\}. \tag{9}$$

Rewriting the determinant as a function of the RPA and unperturbed energies, one obtains

$$F(z) = \sum_n [\log(z - \omega_n) + \log(z + \omega_n)] - \sum_{\alpha<\beta} [\log(z - E_{\alpha\beta}) + \log(z + E_{\alpha\beta})]. \tag{10}$$

Thus, Eq. (8) is the sum of integrals of the complex multivalued logarithmic functions of type $\log(z - p)$, where

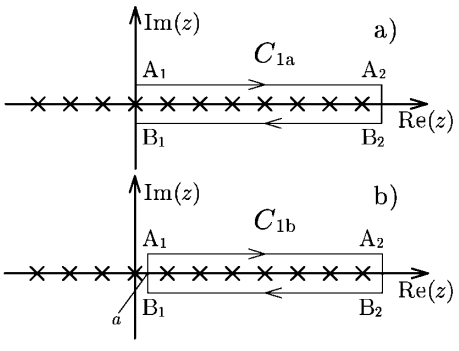

FIG. 1. An illustration of the integration contour in the complex z plane used in Eq. (8). Crosses denote the positions of all the λ-scaled RPA roots for arbitrary values of $0 < \lambda < 1$, i.e., $\mathrm{Re}(A_2) = \mathrm{Re}(B_2) > \max_{n,\lambda}\{\omega^{(\lambda)}_n\}$.

the real value p (in our case ω_n or $E_{\alpha\beta}$) indicates a branch point. Here the principal branch of the logarithmic function should be taken in accordance with the choice of path C_{1a}, that is $-\pi < \arg\log(z - p) \leq \pi$, and the segment of the real axis with $z < p$ is the branch cut. One can now integrate Eq. (8) around all the branch points within C_{1a} by deforming the path and using for each of them a clockwise circular path C_p centered at the point itself [9], that is,

$$\int_{C_p} \log(z - p)\,dz = 2\pi i R_p, \tag{11}$$

where R_p is the radius of the circle C_p. Considering that R_p is ω_n or $E_{\alpha\beta}$, it can be shown that Eq. (8) leads the original expression given in Eq. (1). The contribution associated with the zero mode vanishes in keeping with the fact that in this case the path of integration becomes a semicircle (cf. [9]). This can also be seen by direct evaluation of the integral in Eq. (11) in the case where C_p is a semicircle centered at zero with $R_{p=0} \to 0$.

Making use of a limiting procedure and the following properties of the function $F(z)$,

$$[F(z)]^* = F(-z^*), \qquad F(-z) = F(z), \tag{12}$$

$$F(z) \to o(1/z^2) \quad \text{as } |z| \to \infty, \tag{13}$$

it can be shown that Eq. (8) can be written as

$$E^{\mathrm{RPA}}_{\mathrm{corr}} = \frac{1}{2\pi}\lim_{\epsilon\to 0+}\int_0^\infty \mathrm{Im}[F(\omega + i\epsilon)]\,d\omega, \tag{14}$$

which is the formula utilized in [1]. To obtain this result, one deforms the path shown in Fig. 1a taking the part A_2 and B_2 to infinity and A_1B_1 infinitely close to the origin ($\epsilon \to 0$). In this case the contributions from segments A_2B_2 and A_1B_1 vanish, those arising from A_1A_2 and B_1B_2 being equal.

We now proceed to show that Eq. (8) is equivalent to the integral representation proposed in [4]. For this purpose, we use integration by parts obtaining

$$\oint_{C_{1a}} F(z)\,dz = -\oint_{C_{1a}} z\frac{d}{dz}F(z)\,dz = -\oint_{C_{1b}} z\frac{d}{dz}F(z)\,dz, \tag{15}$$

where the path C_{1b} is depicted in Fig. 1b, and the quantity a [$= \mathrm{Re}(A_1) = \mathrm{Re}(B_1) > 0$] is chosen to be smaller than the lowest nonzero singular point of $F(z)$. The validity of Eq. (15) arises from the equivalence of paths C_{1b} and C_{1a} for the integrand function $z\frac{d}{dz}F(z)$ which has no branch points. In fact, even if there are zero modes, $\frac{d}{dz}F(z) \sim 1/z$, the integrand in Eq. (15) (last equality) has no singularity at $z = 0$. Then,

$$E_{\rm corr}^{\rm RPA} = -\frac{1}{4\pi i}\oint_{C_{1b}} z\,\frac{d}{dz}F(z)\,dz\,, \qquad (16)$$

which is nothing else but the integral representation of $E_{\rm corr}^{\rm RPA}$ in [4] [cf. Eq. (6)].

In order to present a more efficient way to evaluate the RPA correlation energy, the integration path in Fig. 1a is modified to the one shown in Fig. 2a. Then the contribution from the semicircle vanishes as its radius goes to infinity because of the asymptotic property given in Eq. (13), which is in contrast with Eq. (16) proposed in [4], where $z\,\frac{d}{dz}F(z) \to o(1)$ as $|z| \to \infty$. Using also the properties given in Eq. (12), we obtain

$$E_{\rm corr}^{\rm RPA} = \frac{1}{2\pi}\int_0^\infty {\rm Re}[F(i\omega)]\,d\omega\,, \qquad (17)$$

Note that the modification of the path of integration from parallel to the real axis into one parallel to the imaginary axis is quite useful for making the numerical calculations efficient. This is because ${\rm Im}F(z)$ is an oscillating function of ${\rm Re}(z)$ on the path shown in Fig. 1a, while ${\rm Re}\,F(z)$ is a monotonically decreasing function along the imaginary axis on the path shown in Fig. 2a. Consequently, the number of mesh points needed in the calculation reduces dramatically after a suitable transformation of integration variable, e.g., the double exponential transformation [10], $\omega = \exp[2\sinh(t)]$, is made.

In [1,11], pairing correlations in rapidly rotating nuclei have been studied using the general method discussed above. In these references, in addition to the RPA correlation energy, another measure of pairing correlations was introduced, namely, the RPA pairing gap, $\Delta_{\rm RPA}$ [11] (called the "effective" pairing gap in [1]). It is defined as

$$\Delta_{\rm RPA} \equiv \sqrt{\Delta^2 + \frac{1}{2}G^2 S_0({\rm RPA})}\,, \qquad (18)$$

with

$$S_0({\rm RPA}) \equiv \sum_{n\neq{\rm NG}} [|\langle n|P|0\rangle|^2 + |\langle n|P^\dagger|0\rangle|^2]_{\rm RPA}\,, \qquad (19)$$

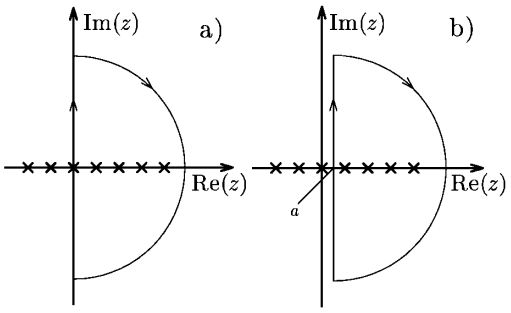

FIG. 2. Modified integration contour from Fig. 1 found to be more suitable to calculate the RPA correlation energy. Taking the limit of infinite radius of the semicircle, the corresponding contribution vanishes.

where $\Delta = G\langle 0|P^\dagger|0\rangle_{\rm HB}$ is the standard, static Hartree-Bogoliubov (BCS) pairing gap (the order parameter of mean field), while G is the pairing force strength. The nonenergy weighted sum rule $S_0({\rm RPA})$ describes the contribution of pairing fluctuations, associated with the monopole pair transfer operator, $P^\dagger = \sum_{i>0} c_i^\dagger c_{\bar{i}}^\dagger$, to the effective (RPA) gap [11]. Note that $\sum_{n\neq{\rm NG}}$ means that the divergent contribution from the spurious mode (pairing rotation) is to be excluded, in keeping with the fact that its contribution to Eq. (18) is included through the static (BCS) pairing gap Δ. In [1], $S_0({\rm RPA})$ was calculated making use of the expression

$$S_0({\rm RPA}) \approx \frac{1}{\pi}\int_{\omega_{\rm cut}}^\infty {\rm Im\,Tr}[\mathcal{R}(\omega + i\epsilon)]\,d\omega\,, \qquad (20)$$

where $\mathcal{R}(\omega) \equiv \mathcal{R}^{(\lambda=1)}(\omega)$ is the RPA response function, whose dimension is 2 corresponding to $Q_1 = (P^\dagger + P)/\sqrt{2}$ and $Q_2 = i(P^\dagger - P)/\sqrt{2}$. A finite value of ϵ and a low-energy cutoff $\omega_{\rm cut}$ are used to get rid of the NG mode contribution numerically. This is the same approximation as that used in calculating the RPA correlation energy [1], and can then be avoided in keeping with the discussion leading to Eqs. (14) and (17). In this case, the path in Fig. 2b is to be used in order to avoid the singularity associated with an eventual zero mode, as in this case $\mathcal{R}(z)$ has a second order pole at the origin (cf. [2]):

$$S_0({\rm RPA}) = \frac{1}{\pi}\int_0^\infty {\rm Re\,Tr}[\mathcal{R}(a + i\omega)]\,d\omega\,. \qquad (21)$$

Since the function ${\rm Tr}[\mathcal{R}(z)]$ has poles as singularities, the integral is independent of the choice of a. Summing up, making use of Eqs. (17) and (21), both the RPA correlation energy and the RPA pairing gap can be exactly evaluated in a numerically efficient way.

In what follows, we compare the results of the exact and approximate calculations of both $E_{\rm corr}^{\rm RPA}$ and $\Delta_{\rm RPA}$ in the case of deformed, superfluid nuclei as a function of the rotational frequency (cf. Fig. 3). Equations (17) and (21) were used to carry out the exact calculation, while Eqs. (14) and (20) [with $\epsilon \equiv {\rm Im}(\omega) = 100,\ 200$ keV] were used to obtain the approximate results, as was been done in [1,11] (where $\epsilon = 80$ keV was used). The nucleus 164Er has been chosen as a typical rotating nucleus and constant deformation parameters were used for simplicity. Only the monopole pairing force has been included with the smoothed pairing gap method being employed, which leads to a slightly different model space from that used in [1,11]. Note that the correlation energy given in Eq. (1) as well as the sum rule value of the pairing gap given in Eq. (19) include the exchange (Fock) contribution. In Fig. 3, this contribution is excluded for the RPA pairing gap in accordance with [11], while it is included for the RPA correlation energy as in [1]. The cusp behaviors are clearly visible in the correlation energy, which

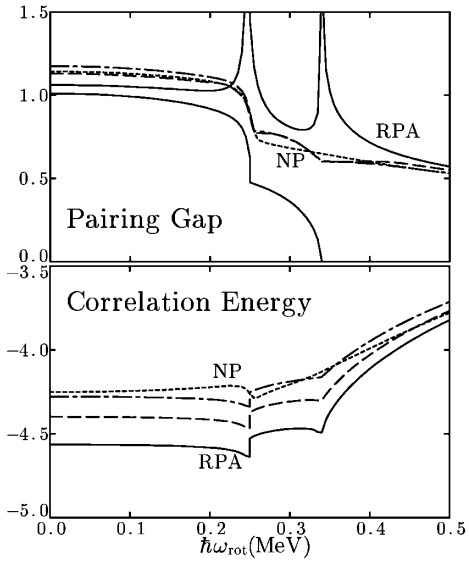

FIG. 3. RPA Pairing gap (upper panel) and RPA correlation energy (lower panel) for neutrons in 164Er as a function of the rotational frequency. Both quantities are in MeV. The solid, dashed and dash-dotted curves denote the results of calculations with $\epsilon = 0$ (exact), 100, and 200 keV, respectively. $\hbar\omega_{\rm cut} =$ 400 keV is used for the approximate (finite ϵ) calculations of the RPA pairing gap. The value of the static (mean-field) pairing gap Δ, which vanishes at $\hbar\omega_{\rm rot} = 0.34$ MeV, is also displayed in the upper panel. The results of the number-projection (NP) calculations are displayed in terms of dotted curves.

are caused by the sudden change of the mean field (static pairing gap); they are associated with the pairing phase transition at $\hbar\omega_{\rm rot} = 0.34$ MeV, and with the crossing of the g and s bands at $\hbar\omega_{\rm rot} = 0.25$ MeV. They are more evident in the RPA pairing gap, where the "exact" ($\epsilon = 0$) calculation diverges at these transition points. These divergences are due to a contribution of the lowest solution, which approaches zero energy at the transition points and brings about similar effects as those caused by the spurious mode, e.g., infinite strength. This is a well-known drawback of the RPA, connected with the fact that the small amplitude approximation breaks down near the transition points. The approximate results ($\epsilon \neq 0$) are very similar to the exact one ($\epsilon = 0$) and provide accurate estimates of the rotational frequency dependence of both the correlation energy and the pairing gap, except at the transition points. In particular, in the case of the pairing gap, the singular behavior at these points is smoothed out because of the low-energy cutoff $\hbar\omega_{\rm cut}$.

There is another method which allows one to go beyond mean-field approximation, namely, the number-projection (NP) (see, e.g., [6]). The results of both methods were compared in [11], where the RPA calculation was carried out approximately as in [1]. In Fig. 3 we also included the NP results for comparison. The NP correlation energy is defined as the energy difference between the NP and mean field (Hartree-Bogoliubov), $E_{\rm corr}^{\rm (NP)} \equiv E_{\rm NP} - E_{\rm HB}$ (the exchange energy is included in $E_{\rm NP}$). Although RPA leads to larger values of the correlations, especially in the superfluid phase, the rotational frequency dependences are quite similar as already found in [11]. The advantage of the NP method over the RPA is to lead to smooth functions for both the correlation energy and the pairing gap at the pairing phase-transition point. It is, however, noticed that the cusp behavior remains in the correlation energy at the gs crossing point.

In conclusion, a method to exactly deal with RPA correlations, based on that proposed in [1], has been developed. It is equivalent to a recently proposed integral representation in [4], and allows one to calculate the exact RPA correlation energy in a numerically efficient way, properly dealing with the contribution of the Nambu-Goldstone modes. Making use of this method, the pairing correlation in rapidly rotating nuclei can be studied in detail, providing the basis for an eventual analysis of the pairing phase-transition in strongly rotating nuclei.

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