Contour integral method for thermal and quantal fluctuations

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The partition function by means of the static path approximation (SPA) plus the random-phase approximation (RPA) treatment can be written as a contour integral form without solving the RPA equations for a separable interaction. This method is an efficient way to evaluate numerically the partition function for realistic calculations. As an illustration, we adopt the pairing model at finite temperature.

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Mean-field approximations, such as the finite temperature Hartree-Fock Bogolyubov (FTHFB) approach\textsuperscript{[1, 2, 3]}, are standard methods for describing nuclei at finite temperature, and the collective motions around the static HFB solution are obtained by solving the finite temperature random phase approximation (RPA). At zero temperature, the HF plus RPA method gives a good approximation to ground-state energy of the exact shell model calculation\textsuperscript{[2]}. However, the FTHFB+RPA method is not applicable to systems at high temperature because of large thermal fluctuations. The inclusion of fluctuations and correlations beyond thermal mean field can be done by use of the path integral representation of the partition function. The static path approximation (SPA)\textsuperscript{[4, 5, 6, 7]} is useful treatment to evaluate approximately the partition function in finite systems with separable interactions, and provides the exact result at high temperature. However, as temperature decreases the SPA becomes inaccurate because the quantal fluctuations around the mean fields can no longer be neglected. Small amplitude fluctuations around such a configuration give corrections to the partition function similar to the standard RPA around the mean field. The SPA+RPA method\textsuperscript{[8, 9, 10, 11]} can take the effects into account. It should, however, be pointed out that in the limit of zero temperature the formalism breaks down since it includes contributions of small-amplitude quantal fluctuations around unstable mean-fields.

In realistic calculations for deformed nuclei or heavy nuclei, the evaluation of the RPA partition function is difficult due to time-consuming computation, because a complete set of RPA frequencies and amplitudes must be known with high accuracy for each temperature and the number of the RPA eigenvalues is very large. Recently, a contour integral representation for the standard RPA correlation energy\textsuperscript{[12]} and more efficient way\textsuperscript{[13]} based on the linear response theory have been proposed. These methods are valuable and useful for evaluating the standard RPA correlation energy. In this letter, we present a contour integral method for the RPA partition function at finite temperature.

We consider the total Hamiltonian

\[ H = H_0 + V, \]

where \( H_0 \) and \( V \) are the single-particle Hamiltonian and a two-body residual interaction, respectively. Here, the two-body interaction is assumed to be of separable multipole-multipole form interaction:

\[ V = -\frac{1}{2} \sum_{\alpha} \chi_\alpha Q_\alpha^2, \]

where \( Q_\alpha \) is a one-body Hermitian operator

\[ Q_\alpha = \sum_{kl} q_{kl} c^\dagger_k c_l. \]

Using the Hubbard-Stratonovich transformation\textsuperscript{[14]}, the functional integral representation for the partition function is written as an auxiliary field path-integral

\[ Z = \text{Tr}(e^{-\beta H}) = \int \mathcal{D}[\sigma(\tau)] \exp \left( -\frac{1}{2} \sum_{\alpha} \chi_\alpha \int_0^\beta \sigma_\alpha(\tau)d\tau \right) \times \text{Tr}[\hat{T}\exp(-\int_0^\beta d\tau H'(\tau))], \]

where \( H'(\tau) = H_0 - \sum_{\alpha} \chi_\alpha \sigma_\alpha(\tau)Q_\alpha, \)

with the Matsubara frequencies \( \omega_n = 2\pi n/\beta \) and the static variables \( \bar{\sigma}_\alpha \). The SPA is obtained by considering only the static paths in the evolution operator. The Hamiltonian \( H'(\tau) \) can be divided into the static and fluctuation parts:

\[ H'(\tau) = H_s + \delta H(\tau), \]

where \( H_s \) and \( \delta H(\tau) \) are the static and fluctuation part as follows:

\[ H_s = H_0 - \sum_{\alpha} \chi_\alpha \bar{\sigma}_\alpha Q_\alpha, \]

\[ \delta H(\tau) = -\sum_{\alpha} \chi_\alpha \sum_{n \neq 0} \eta_{\alpha n} Q_\alpha e^{-i\omega_n \tau}. \]
Substituting Eqs. (6-9) into Eq. (4) and performing the Gauss integral over the coefficients \( \eta_{\alpha n} \), we obtain

\[
Z = \frac{\beta \chi_\alpha}{2\pi} \int d\sigma_\alpha \exp \left( -\frac{1}{2} \sum_\alpha \chi_\alpha \sigma_\alpha^2 \right) \times \prod_{k} (1 + e^{-\beta \varepsilon_k}) C_{\text{RPA}},
\]

\[
C_{\text{RPA}} = \prod_{n>0} \det(1 - \chi R(\omega_n))^{-1},
\]

where \( \varepsilon_k \) are the eigenenergies of \( H' \), and \( R(\omega_n) \) is the response function matrix given as

\[
R_{\alpha\alpha'}(\omega_n) = \sum_{kl} g_{kl}' g_{kl}'^* \frac{\varepsilon_{kl}(f_k - f_l)}{\varepsilon_{kl}^2 + \omega_n^2},
\]

with \( \varepsilon_{kl} = \varepsilon_k - \varepsilon_l \) and the Fermi occupation probability \( f_k = (1 + e^{\beta \varepsilon_k})^{-1} \). Solving the dispersion equation \( \det(1 - \chi R(i\omega_n)) = 0 \) or diagonalizing the finite temperature RPA equations, \( C_{\text{RPA}} \) can be written exactly in terms of the RPA frequencies \( \Omega_\nu \),

\[
C_{\text{RPA}} = \prod_{k<l} \frac{\sinh \frac{\beta \varepsilon_{kl}}{2}}{\sinh \frac{\beta \varepsilon_{kl} + \beta \Omega_\nu}{2}},
\]

where the prime in \( \prod' \) restricts the product to pairs \( (k,l) \) that satisfy \( k < l \) and \( \varepsilon_{kl} \neq 0 \). Note that for deformed nuclei or heavy nuclei there are many RPA frequencies \( \Omega_\nu \) in the numerator and \( \varepsilon_{kl} \) in the denominator. For arbitrary \( \sigma \), the lowest \( \Omega_\nu \)'s may become zero and imaginary (or complex) at low temperature. However, \( C_{\text{RPA}}(\sigma) \) remains finite and positive both for \( \Omega_\nu = 0 \) and for imaginary \( \Omega_\nu \) if \( \beta |\Omega| < 2\pi \). This condition will be violated at very low temperature.

Let us define the thermal RPA energy

\[
E_{\text{RPA}} = \frac{\partial \ln C_{\text{RPA}}}{\partial \beta} = \frac{1}{2} \left( \sum_\nu \Omega_\nu \coth \frac{\beta \Omega_\nu}{2} - \sum_{k<l} \varepsilon_{kl} \coth \frac{\beta \varepsilon_{kl}}{2} \right),
\]

\( \beta \rightarrow \infty \), the thermal RPA energy \( E_{\text{RPA}} \) reduces correctly the RPA correlation energy

\[
E_{\text{RPA}}(T=0) = \frac{1}{2} \left( \sum_\nu \Omega_\nu - \sum_{k<l} \varepsilon_{kl} \right).
\]

We now introduce the analytical function of the complex variable \( z \)

\[
f(z) = \det(1 - \chi R(iz)) = \prod_\nu \frac{\Omega_\nu^2 - z^2}{\varepsilon_{kl}^2 - z^2}.
\]
\[ Z_N^e = \frac{1}{4\pi} \int dz (z \coth \frac{\beta z}{2}) \ln f(z), \tag{20} \]

where the closed path for Eq. (19) is taken so that the function \( z \coth \beta z/2 \) is analytical in the closed region (see Fig. 1(a)). A modified contour integral for Eq. (20) is illustrated in Fig. 1(b), where the contribution from the semicircle vanishes in the limit of infinite radius. These are the extended form of the contour integral of the RPA correlation energy at zero temperature. Integrating \( E_{RPA} = -\partial \ln Z_{RPA}/\partial \beta \) over \( \beta \) in Eq. (14) provides the RPA partition function \( Z_{RPA} \)

\[ C_{RPA} = \exp \left( -\int_0^\beta E_{RPA} d\beta' \right). \tag{21} \]

In comparison with the usual RPA method of Eq. (14), the advantage of the contour integral form in Eqs. (19-20) is that one can choose the integration path so that the integrand is smooth enough and the mesh of numerical integration along such path can be much larger than the actual energy intervals of the FTRPA solutions \( \Omega_n \). The contour integral calculation reduces drastically the computation time without loss of precision. In practical calculations of the above method, we evaluated the contour integral (20) illustrated in Fig. 1(b) neglecting the RPA partition function \( Z_{RPA} \).

As an illustration, we consider a monopole pairing Hamiltonian

\[ H = \sum_k \varepsilon_k (c_k^\dagger c_k + c_k^\dagger c_\bar{k}) - GP^1 P, \tag{22} \]

with \( \bar{k} \) the time reversed states. Here, \( \varepsilon_k \) is a single-particle energy and \( P \) is the pairing operator \( P = \sum_k c_k^\dagger c_k \). By means of the SPA+RPA based on the Hubbard-Stratonovich transformation, the canonical partition function is given by

\[ Z_N^e = \text{Tr}[P^N e^{-H/T}]_{\text{SPA+RPA}} = \frac{2}{GT} \int_0^\infty \Delta d\Delta e^{-\Delta^2/GT} Z_N C_{RPA}. \tag{23} \]

\[ Z_N = \frac{1}{2} \prod_k e^{-\gamma_k/T} (1 + e^{-\lambda_k/T})^2 \times [1 + \sigma \prod_{k'} \tanh^2 (\lambda_k/T)], \tag{24} \]

\[ C_{RPA} = \prod_k \frac{\omega_k \sinh [\lambda_k/T]}{2 \lambda_k \sinh [\omega_k/2T]}, \tag{25} \]

where we introduced the number parity projection \( P_N = (1 + \sigma e^{i\pi N})/2 \) (\( \sigma \) means the even or odd number parity) instead of the exact number projection. Here use the notation \( \omega_k \) for the conventional thermal RPA energies and \( \lambda_k = \sqrt{\varepsilon_k^2 + \Delta^2} \), \( \varepsilon_k' = \varepsilon_k - \mu - G/2 \), and \( \gamma_k = \varepsilon_k - \mu - \lambda_k \). The SPA partition function is obtained by neglecting the RPA partition function \( C_{RPA} \). Then the thermal energy can be calculated from

\[ E = -\partial \ln Z_N^e/\partial \beta. \]

In this calculation, we use the single-particle energies \( \varepsilon_k \) given by an axially deformed Woods-Saxon potential with spin-orbit interaction. The Woods-Saxon parameters are chosen so as to approximately reproduce the experimental single-particle energies extracted from the energy levels of the odd nucleus \(^{133}\text{Sn} \) \((^{132}\text{Sn} \) core plus one neutron). The deformation parameter estimated from the experimental \( B(E2) \) value is \( \delta = 0.23 \) in the even-even nucleus \(^{184}\text{W} \). The 50 doubly degenerate single-particle levels are taken outside \(^{132}\text{Sn} \) core, and we fix the pairing force strength at \( G = 20/A \) MeV. As mentioned above, the SPA+RPA breaks down at low temperature. However, it has recently been shown that in the monopole pairing case the SPA+RPA with the number parity projection reproduces well exact results for low temperature. Thus, the number parity projection is essential to describe the thermal properties for low temperature.

For the partition function (23), we performed the three cases of numerical calculations; the SPA, the SPA plus contour integral representation (SPA+CIR) with
Eq. (19-20), and the SPA plus RPA (SPA+RPA) with Eq. (14) using the RPA frequencies. The thermal energies are calculated from $E = -\partial \ln Z_N^c / \partial \beta$. The thermal energy obtained in the SPA+CIR (SPA+RPA) deviates from that of the SPA. The energy difference between the SPA+CIR (SPA+RPA) and the SPA is the correlation energy $E_{\text{corr}} = E - E_{\text{SPA}}$. Figure 2 shows the thermal energy $E$ and the RPA correlation energy $E_{\text{corr}}$ as a function of $\beta$. We can see that the SPA+CIR results agree well with the SPA+RPA one. Thus, the contour integral method is useful for studying the thermal and quantal fluctuations. For comparison, we solved the Richardson equations [16, 17] and calculated exactly the ground-state energy $E_{gs}$. The obtained energy $E_{gs} = -74.48$ MeV is quite close to the SPA+CIR value, $E = -75.24$ MeV at $\beta = 10$ MeV$^{-1}$, supporting the SPA+CIR method.

Figure 4 depicts the natural logarithm of the level density (27) as a function of the thermal energy $E$. We can see that the SPA+CIR result agrees with the SPA+RPA one.

In conclusion, we developed the contour integral method which drastically reduces the computation time without loss of precision when evaluating the thermal and quantal fluctuations. This method is the extension of contour integral representation at zero temperature to the thermal system, and is numerically efficient. In this paper, we considered the simple pairing model as an illustration. The contour integral method is also applicable to more realistic interactions such as the pairing plus...
quadrupole-quadrupole interaction. This study is now in progress.

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