Self-Consistent RPA with Multilevel Pairing Model at Finite Temperature*

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Abstract—A self-consistent version of the thermal random phase approximation (TSCRPA) is developed within the Matsubara Green’s function formalism. The TSCRPA is applied to the many-level pairing model, and the normal phase of the system is considered. The TSCRPA results are compared with the exact ones calculated for the grand canonical ensemble. Advantages of the TSCRPA over the thermal mean-field approximation and the standard thermal random phase approximation are demonstrated. Results for correlation functions, excitation energies, etc., as a function of temperature are presented.

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1. INTRODUCTION

Almost all microscopic approximations used to describe excitations in hot finite Fermi systems such as the thermal Hartree–Fock and Hartree–Fock–Bogolyubov approximations or the thermal random phase approximation (TRPA) are based upon the single–particle or single–quasiparticle picture. Some approximations going beyond the TRPA were considered as well, but merely a coupling of thermal particle–hole or TRPA phonon excitations with more complex ones was studied [1]. Although these approaches are able to provide a qualitative description of some properties of highly excited nuclei, they have some drawbacks. The most evident difficulty is the description of the strongly correlated finite systems of fermions in the vicinity of the phase-transition point, where proper inclusion of two-body correlations is especially important.

There are different ways to construct a theory which can adequately treat two-body correlations. One of the greatest promising approaches providing such a consideration is the self-consistent RPA (SCRPA) theory [2], which grew out of the works by Ken-ji Hara and D. Rowe, who first suggested a way to generalize the RPA [3]. Recently, the SCRPA was successfully applied to various nontrivial models, where two-body correlations are of importance [4].

Extensions of the SCRPA to finite temperatures were studied as well. In [5], besides a general formulation of the new thermal approximation (TSCRPA) within the framework of thermofield dynamics, applications of TSCRPA to simple model systems with particle–hole correlations were considered. Advantages of TSCRPA over traditional approximations were found.

The main aim of this paper is an extension of SCRPA to finite temperature and investigation in this respect of the many-level pairing model [also known as the picket fence model (PFM)], which was initially introduced to describe deformed superfluid nuclei [6] and was recently used for investigation of ultrasmall superconducting metallic grains [7, 8].

We organize the paper in the following way. In Section 2, the approach is outlined in general. Then, in Section 3, the formalism is applied to the PFM. A comparison with the exact solutions as well as with the corresponding results of other approximations is made in Section 4. In Section 5, we summarize the results and draw some conclusions.

2. GENERAL FORMALISM

In treating a finite many–body system at finite temperature, it is convenient to use the grand canonical ensemble, although it violates number conservation. With the definition

\[ K = H - \mu N, \]

the grand partition function and statistical operator read

\[ Z_G = e^{-\beta\Omega} = \text{Tr}(e^{-\beta K}), \]

\[ \rho_G = Z_G^{-1} e^{-\beta K} = e^{\beta(\Omega - K)}, \]
where $\beta = 1/T$. Then, for any Schrödinger operator $A_\alpha$, the modified Heisenberg picture can be introduced,

$$A_\alpha(\tau) = e^{K_\tau} A_\alpha e^{-K_\tau},$$

and the temperature (or the Matsubara) Green’s function (GF) is defined as [9]

$$G_{\alpha\beta}^{\tau-\tau'} = -(T_\tau A_\alpha(\tau) A_\beta^+(\tau'))$$

$$= -\text{Tr}[e^{\beta(K - \Omega)} T_\tau e^{K_\tau} A_\alpha e^{-(\tau-\tau')K} A_\beta^+ e^{-\tau'K}]$$

$$= -\text{Tr}[\rho_T e^{r'K} A_\alpha e^{-(\tau-\tau')K} A_\beta^+ e^{-\tau'K}].$$

Here, the brackets $\langle \rangle$ mean the thermodynamic average; $T_\tau$ is a $\tau$ ordering operator, which arranges operators with the earliest $\tau$ (the closest to $-\beta$) to the right.

Let us consider a two-body Hamiltonian

$$H = \sum_{12} t_{12} a_1^+ a_2 + \frac{1}{4} \sum_{1234} \bar{v}_{1234} a_1^+ a_2^+ a_3 a_4,$$  (2)

where $a$ and $a^+$ are fermion annihilation and creation operators, and $t_{12}$ and $\bar{v}_{1234} = v_{1234} - v_{1243}$ are the kinetic energy and the antisymmetrized matrix element of the two-body interaction. The GF $G_{\alpha\beta}^{\tau-\tau'}$ for an arbitrary operator $A_\alpha^+$ obeys the following equation of motion:

$$-\frac{\partial}{\partial \tau} G_{\alpha\beta}^{\tau-\tau'} = \delta_{\tau-\tau'} \langle [A_\alpha, A_\beta^+] \rangle$$

$$- \langle T_\tau [A_\alpha, K]^\tau A_\beta^+(\tau') \rangle = \delta_{\tau-\tau'} \delta_{\alpha\beta}$$

$$+ \sum_{\gamma} \int d\tau' \mathcal{H}_{\alpha\gamma}^{\tau-\tau'} G_{\gamma\beta}^{\tau-\tau'}.$$  

In this expression, it is possible to split the effective Hamiltonian $\mathcal{H}_{\alpha\beta}^{\tau-\tau'}$ into an instantaneous and a dynamic (frequency dependent) part [2]:

$$\mathcal{H}_{\alpha\beta}^{\tau-\tau'} = \sum_{\beta'} \{ \delta_{\tau-\tau'} \langle [A_\alpha, K], A_\beta^+ \rangle \}$$

$$- \langle T_\tau [A_\alpha, K]^\tau [K, A_\beta^+]^\tau \rangle_{\text{irr}} N_{\beta\beta}^{-1}$$

$$= \mathcal{H}_{\alpha\beta}^{(0)} \delta_{\tau-\tau'} + \mathcal{H}_{\alpha\beta}^{(r)} \delta_{\tau-\tau'}.$$  

In the approximation of the instantaneous effective Hamiltonian, i.e., neglecting $\mathcal{H}_{\alpha\beta}^{(r)}$, the Dyson equation for the two-body Matsubara GF $G_{\alpha\beta}^{\tau-\tau'}$ can be written as

$$-\frac{\partial}{\partial \tau} G_{\alpha\beta}^{(0)}(\tau-\tau') = \delta_{\tau-\tau'} \delta_{\alpha\beta} + \sum_{\gamma} \mathcal{H}_{\alpha\gamma}^{(0)} G_{\gamma\beta}^{(0)}(\tau-\tau').$$  (3)

3. APPLICATION TO THE PICKET FENCE MODEL

The so-called PFM consists of an equidistant multilevel pairing Hamiltonian. Each level is twofold degenerate; i.e., only spin up/down fermions of one kind can occupy it. The corresponding Hamiltonian is given by

$$H = \sum_{k=1}^{\Omega} e_k N_k - G \sum_{i,k=1}^{\Omega} P_i^+ P_k,$$  (4)

where $N_k = c_k^+ c_k + c_k^+ c_k^+$, $P_k^+ = c_k^+ c_k^+$; $\bar{k}$ means the time reversal of $k$; single-particle energies are $e_k = k \varepsilon - \lambda$, with level spacing $\varepsilon$ chosen to be equal to 1; and $\Omega$ stands for the number of levels. The chemical potential $\lambda$ will be chosen such as to conserve the average number of particles $N = \Omega$ of the system.

To study the model at finite temperature, we define in analogy to (1) the following set of two-body Matsubara GFs: $G_{ji}^{\tau} = -\langle T_\tau \tilde{P}_j(\tau) \tilde{P}_i^+(0) \rangle$, where $\tilde{P}_j = P_j / \sqrt{[1 - N_j]}$. Applying the instantaneous approximation for a mass operator, we obtain expressions for the two-body SCRPA GFs:

$$i \omega_n G_{ji}^{\text{SCRPA}} = \delta_{ji} + \sum_k \mathcal{H}_{jk}^{(0)} G_{ki}^{\text{SCRPA}},$$  (5)

with

$$\mathcal{H}_{jk}^{(0)} = 2\delta_{jk} \left( e_j + \frac{G}{\langle 1 - N_j \rangle} \sum_{j'} \langle P_j^+ P_{j'} \rangle \right)$$

$$- G \frac{\langle (1 - N_j)(1 - N_k) \rangle}{\sqrt{[1 - N_j](1 - N_k)}}.$$  

To find the correlation functions of the form $\langle (1 - N_j)(1 - N_k) \rangle$, we use the following approximation.

When $j \neq k$, we apply a simple factorization procedure, which has turned out to be accurate in the zero temperature limit,

$$\langle (1 - N_j)(1 - N_k) \rangle = \langle 1 - N_j \rangle \langle 1 - N_k \rangle,$$  (7a)

but when $j = k$, we use the exact relation

$$\langle (1 - N_j)^2 \rangle = \langle 1 - N_j \rangle + \langle P_j^+ P_j \rangle.$$  (7b)

With this ansatz, a particle–particle RPA-like equation is obtained in the form

$$G_{ji}^{\text{SCRPA}} = \delta_{ji} \frac{1}{z - C_j} - \frac{G \sqrt{D_j D_i}}{(z - C_j)(z - C_i)}$$

$$\times \left[ 1 + G \sum_k \frac{D_k}{z - C_k} \right]^{-1},$$

where $D_j = \frac{1}{2} \sum_{\varepsilon} e^{\beta \varepsilon} G_{ji}^{\text{SCRPA}}(|e_j + \varepsilon|)$.