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RENORMALIZED **RPA** AT FINITE TEMPERATURE

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One of the main assumptions of the random phase approximation (RPA) is the negligible number of virtual particle-hole excitations (or multi-quasiparticle excitations) in the RPA vacuum state. The validity of this assumption and ways going beyond it have been discussed by many authors [1-9]. Recently [5, 6] it has been shown that the presence of a finite number of quasiparticles in the RPA vacuum produces noticeable and nontrivial changes in some nuclear observables. An intrinsic reason for these changes is a violation of the Pauli principle when a nuclear ground state is constructed by using a simplest boson representation of bifermion operators, and a phonon state which is a coherent superposition of one-particle – one-hole components is created from this state as a vacuum state. Nonvanishing number of quasiparticles in the RPA vacuum affects the RPA state occupation numbers [7] and suppresses a contribution of valence two-quasiparticle states to the one-phonon wave function [5].

At first sight, the violation of the Pauli principle in the RPA should affect properties of hot nuclei even more strongly because of the appearance of a great number of multi-quasiparticle excitations in compound state. To check the validity of the thermal RPA and consequences of the violation of the Pauli principle in hot nuclei, we elaborated a method taking account of the deviation of state occupation numbers from the thermal RPA prescriptions. We call the corresponding approximation scheme as the Thermal Renormalized Random Phase Approximation (TRRPA). The main idea of the TRRPA goes back to papers of Ken-ji Hara [1] and D.J. Rowe [2]. In developing TRRPA we use a formalism of the thermofield dynamics (TFD)[11]. Some numerical results are given for the SU(2) model [10].

We start with the model nuclear Hamiltonian that consists of a mean field and an effective particle-hole separable interaction:

$$H = \sum_i (\varepsilon_i - \lambda) a_i^+ a_i + \frac{\kappa}{2} \left(\sum_{kl} f_{kl} a_k^+ a_l \right)^2 \tag{1}$$

By ε_i we denote the single-particle energy and by f_{kl} - the single-particle matrix element of a one-body operator (e.g. a quadrupole one).

First, following the TFD prescriptions, let us construct the thermal Hamiltonian of the system [12, 13].

It is known that the extension of quantum field theory to finite temperature requires a doubling of the field degrees of freedom. In the TFD, a tilde conjugate operator $\tilde{A}$ is associated to any operator A acting in ordinary space through the tilde conjugation rules

$$(\tilde{AB}) = \tilde{A}\tilde{B}\ ; (aA + bB)^{\sim} = a^{*}\tilde{A} + b^{*}\tilde{B}\ ,$$

where A and B stand for any operators and a , b are c-numbers. The asterisk denotes the complex conjugate. The tilde operation commutes with the hermitian conjugation operation and any tilde and nontilde operators are assumed to commute or anticommute with each other. For any system governed by the Hamiltonian H the whole Hilbert space at $T \neq 0$ is spanned by the direct product of the eigenstates of H and those of the tilde Hamiltonian $\tilde{H}$ which has the same eigenvalues as H. The thermal Hamiltonian $\mathcal{H} = H - \tilde{H}$ is the time - translation operator and the properties of the system excitations are obtained by the diagonalization of $\mathcal{H}$.

The thermal Hartree-Fock ground state $|0(T)\rangle_{HF}$ of a heated system is treated to be the so-called thermal vacuum state. The latter is defined so that the expectation value of any operator A over it equals to a thermal average of this operator over the grand canonical ensemble [11]:

$$\ll A \gg = \frac{1}{Tr(\exp(-\frac{H}{T}))} Tr[A\ exp(-\beta H)] =_{HF} \langle 0(T)|A|0(T)\rangle_{HF}$$

The wave function $|0(T)\rangle_{HF}$ is a vacuum for the so-called thermal quasiparticles $\beta_i, \tilde{\beta}_i$ [12, 13]:

$$\begin{aligned} \beta_i &= x_i a_i - y_i \tilde{a}_i^{+} \\ \tilde{\beta}_i &= x_i \tilde{a}_i + y_i a_i^{+} \end{aligned} \tag{2}$$

$$\beta_i|0(T)\rangle_{HF} = \tilde{\beta}_i|0(T)\rangle_{HF} = 0$$

where the coefficients x_i, y_i are the thermal Fermi occupation numbers of the states $|n_i\rangle$:

$$x_i = \sqrt{1 - n_i}\ ,\ y_i = \sqrt{n_i} \tag{3}$$

$$n_i = \frac{1}{1 + exp[(\varepsilon_i - \lambda)/T]}$$

A chemical potential λ is adjusted to keep constant an average number of particles in a system.

The transformation $\{x, y\}$ is unitary, and thus, the standard anticommutation rules are valid for creation and annihilation operators of thermal quasiparticles β^{+}, β and their tilde counterparts $\tilde{\beta}^{+}, \tilde{\beta}$.

After transformation (2) to the thermal quasiparticles the RPA part of the thermal Hamiltonian $\mathcal{H}$ takes the form:

$$\mathcal{H} = \sum_i \varepsilon_i(\beta_i^+\beta_i - \tilde{\beta}_i^+\tilde{\beta}_i) -$$

$$-\frac{\kappa}{2}\sum_{klmn} f_{kl} f_{mn}(x_k y_l x_m y_n - y_l x_k y_m x_n)(\beta_k^+\tilde{\beta}_l^+ + \tilde{\beta}_l\beta_k)(\beta_m^+\tilde{\beta}_n^+ + \tilde{\beta}_n\beta_m) \quad (4)$$

Note that although the initial Hamiltonian (1) has a separable form, the thermal Hamiltonian cannot be factorized.

The following commutation rules are valid for the thermal biquasiparticle operators $\tilde{\beta}_l\beta_k, \beta_i^+\tilde{\beta}_j^+$:

$$[\tilde{\beta}_l\beta_k, \beta_i^+\tilde{\beta}_j^+] = \delta_{jl}\delta_{ik} - \delta_{jl}\beta_i^+\beta_k - \delta_{ik}\tilde{\beta}_j^+\tilde{\beta}_l$$

$$(6)$$

$$[\tilde{\beta}_j\beta_i, \tilde{\beta}_l\beta_k] = [\beta_j^+\tilde{\beta}_i^+, \tilde{\beta}_l\beta_k] = 0$$

If we wish to follow the quasiboson approximation, we have to assume that the new biquasiparticle operators are pure boson ones. This means that in the right-hand side of (6) the terms $\sim \beta_l^+\beta_k$ and $\sim \tilde{\beta}^+{}_l\tilde{\beta}_k$ have to be omitted, which is equivalent to the assumption that the number of thermal quasiparticles in the thermal ground state vanishes.

In cold nuclei, as a first step going beyond the RPA, it has been proposed [1, 2] to approximate the commutators (6) by c - numbers. We follow the same idea at $T \neq 0$ and assume the following form of the commutator (6):

$$[\tilde{\beta}_l\beta_k, \beta_i^+\tilde{\beta}_j^+] = \delta_{jl}\delta_{ik}(1 - \rho_i - \rho_j) \quad (7)$$

where

$$\rho_i = \langle\Psi_0(T)|\beta_i^+\beta_i|\Psi_0(T)\rangle = \langle\Psi_0(T)|\tilde{\beta}_i^+\tilde{\beta}_i|\Psi_0(T)\rangle$$

and $|\Psi_0(T)\rangle$ is the wave function of the ground state of a hot nucleus which to be defined below. Note that the expectation numbers for ordinary and tilde thermal quasiparticles are the same. Equation (7) allows one to introduce the pure bosonic operators

$$b_{ik}^+ = \frac{1}{\sqrt{1-\rho_i-\rho_k}}\beta_i^+\tilde{\beta}_k^+ \qquad b_{ik} = \frac{1}{\sqrt{1-\rho_i-\rho_k}}\tilde{\beta}_k\beta_i$$

which obey the standard boson commutation rules:

$$[b_{lk}, b_{ij}^+] = \delta_{li}\delta_{kj} \quad (8)$$

The thermal RPA Hamiltonian (4) can be diagonalized in terms of thermal phonon operators which are constructed from the boson operators as follows:

$$Q^+_{\sigma\nu} = \sum_{kk'} \psi^{\sigma\nu}_{kk'} b^+_{kk'} - \phi^{\sigma\nu}_{kk'} b_{kk'} \tag{9}$$

$$Q_{\sigma\nu}|\Psi_0(T)\rangle = 0 \tag{10}$$

We label phonon states by two indices for convenience. The index ν denotes usual quantum numbers like the angular momentum, $\sigma = \pm$. The meaning of σ will be discussed below. The amplitudes $\psi^{\sigma\nu}_{kk'}$ and $\phi^{\sigma\nu}_{kk'}$ obey the usual orthogonality relations:

$$\sum_{ik} (\psi^{\sigma\nu}_{ik} \psi^{\sigma'\mu}_{ik} - \phi^{\sigma\nu}_{ik} \phi^{\sigma'\mu}_{ik}) = \delta_{\nu\mu}\delta_{\sigma\sigma'} , \tag{11}$$

as one can easily check using eq.(8). The system of equations for the amplitudes ψ, ϕ and phonon frequencies $\omega_{\sigma\nu}$ can be obtained by the equation-of-motion method and appears to be nonlinear. The system has a nontrivial solution if ω_ν is a root of the following secular equation:

$$1 = \kappa \sum_{ik} \frac{(f_{ik})^2 (1 - \rho_i - \rho_k)(n_k - n_i)(E_i - E_k)}{(E_i - E_k)^2 - \omega^2} \tag{12}$$

Since the right-hand side of eq.(12) is a function of ω^2, the number of the solutions is twice the number of matrix elements f_{ik}. So, the index σ differentiates roots with positive and negative values of ω. Solving equations separately for positive and negative energies:

$$\omega_{+\nu} = \omega_\nu \qquad \omega_{-\nu} = -\omega_\nu \qquad \omega_\nu > 0$$

one obtains the following expressions for phonon amplitudes:

$$\psi^{+\nu}_{ik} = \frac{1}{\sqrt{N}} \frac{\kappa f_{ki} \sqrt{1 - \rho_k - \rho_i} x_i y_k}{E_i - E_k - \omega_\nu}, \quad \phi^{+\nu}_{ik} = \frac{1}{\sqrt{N}} \frac{\kappa f_{ki} \sqrt{1 - \rho_k - \rho_i} x_i y_k}{E_i - E_k + \omega_\nu} \tag{13}$$

$$\psi^{-\nu}_{ik} = \psi^{+\nu}_{ki}, \qquad \phi^{-\nu}_{ik} = \phi^{+\nu}_{ki} \tag{14}$$

Due to the relation (14) which connects amplitudes of wave functions corresponding to solutions with positive and negative energies, the following relationship between ordinary and tilde phonons:

$$Q^+_{-\nu} = \tilde{Q}^+_{+\nu}$$

is valid. So, tilde phonons correspond to the solutions with negative energies, in agreement with the general principles of TFD [11].

Now the Hamiltonian (4) is diagonal in terms of phonon operators:

$$\mathcal{H} = \sum_{\nu} \omega_{\nu}(Q^{+}_{+\nu}Q_{+\nu} - Q^{+}_{-\nu}Q_{-\nu}) = \sum_{\nu} \omega_{\nu}(Q^{+}_{+\nu}Q_{+\nu} - \tilde{Q}^{+}_{+\nu}\tilde{Q}_{+\nu})$$

The system of equations (12-13) is still not complete, since the number of thermal quasiparticles ρ_k in the phonon vacuum state is unknown. To evaluate ρ_k, we use the explicit expression of the thermal ground state $|\Psi_0(T)\rangle$ in terms of the bosonic operators b^{+}_{ij}, b^{+}_{kl}. This expression can be obtained by using the commutation (8) and the orthogonality (11) relations and has the form:

$$|\Psi_0(T)\rangle = \frac{1}{\sqrt{N}} \exp S|0(T)\rangle_{HF}$$

$$S = \frac{1}{2}\sum_{ijkl} C_{ijkl} b^{+}_{ij} b^{+}_{kl}$$

where the matrix C_{ijkl} is defined through the following set of equations:

$$\sum_{ij} \psi^{\sigma\nu}_{ij} C_{ijkl} = \phi^{\sigma\nu}_{kl}$$

Then we get the following equations for ρ_i:

$$\rho_i = \langle\Psi_0(T)|\beta^{+}_i\beta_i|\Psi_0(T)\rangle = \langle\Psi_0(T)|\tilde{\beta}^{+}_i\tilde{\beta}_i|\Psi_0(T)\rangle = \sum_{i'\sigma\nu}(\phi^{\sigma\nu}_{i'i})^2 \qquad (15)$$

Thus, to determine the properties of one-phonon states in hot nucleus within TRRPA one has to solve the system of nonlinear equations (12-15).

Putting in these equations $\rho_i = 0$, one gets the standard TRPA equations [14, 15]. On the other hand, at $n_i, n_k = 0$ or 1 one gets the equations of renormalized RPA in cold nuclei [1, 2].

To demonstrate how the TRRPA works, we apply it to a simple SU(2) model [10] widely used to test various kinds of nuclear many-body theories. The model consists of two single particle levels with the same degeneracy Ω and a distance between the levels ε. At $T = 0$ the low level is fully occupied by N nucleons (i.e. $N = \Omega$), the high level is empty. The effective interaction is independent of the state and is characterized by a coupling constant V. For this model the set of the TRRPA equations is reduced to the algebraic fourth-order equation for ω. The equation for the absolute value of energy of the thermal phonon ω is the following:

$$\omega^4 + \left\{[V(n_- - n_+)(N+1)]^2 - \varepsilon^2\right\}\omega^2 - 2\,[V(n_- - n_+)]^2\,(N+1)\varepsilon\omega$$
$$+\,[V(n_- - n_+)\varepsilon]^2 = 0 \qquad (16)$$

where $n_\mp$ is the thermal occupation number of the low (high) level.

Equation (16) has four roots, but we are interested only in positive roots. There are two of them: one corresponds to a value of $\rho > 1$ and the other, to $\rho < 1$. Obviously only the latter root has physical meaning. In fig. 1 we show the dependence of the energy ω of the phonon state on the interaction strength V at different temperatures T and the same function calculated within the standard thermal RPA. In a cold nucleus, a collapse of the lowest RPA state takes place at some critical value of the attractive particle-hole interaction strength V and this collapse disappears in the renormalized RPA [1, 2]. As one can see from fig. 1, the same situation takes place in a hot nucleus. With increasing T the function $\omega(V)$ appears to be smoother. This means that increasing of T effectively weakens a particle-hole interaction. The reason for this can be easily seen from eq.(16) where the interaction strength V appears multiplied by the difference of thermal occupation numbers of the two single-particle levels $(n_- - n_+)$. The difference is less than unity at $T \neq 0$ and decreases with increasing T. So, in a hot nucleus the main RPA assumption is valid even for a wider range of the effective interaction strength than in a cold one.

In summary, using the formalism of the thermo field dynamics we extended the renormalized RPA of refs.[1, 2] to finite temperature thus formulating the Thermal Renormalized Random Phase Approximation. Then the equations of TRRPA were solved for the simple $SU(2)$ model to demonstrate the influence of ground state correlations beyond TRPA on the collective state in a hot system. Strictly speaking, the $SU(2)$ model is too simple to reflect a variety of changes introducing by temperature to the nuclear structure. For example, in a heated nucleus the number of two-quasiparticle states appears to be much larger than in a cold one. This enlarging of excitation spectra is not reproduced by the $SU(2)$ model. Thus, to understand more deeply the influence of the new type of ground state correlations on properties of collective excitations in hot nuclei, calculations within a more realistic model are needed. This work is in progress.

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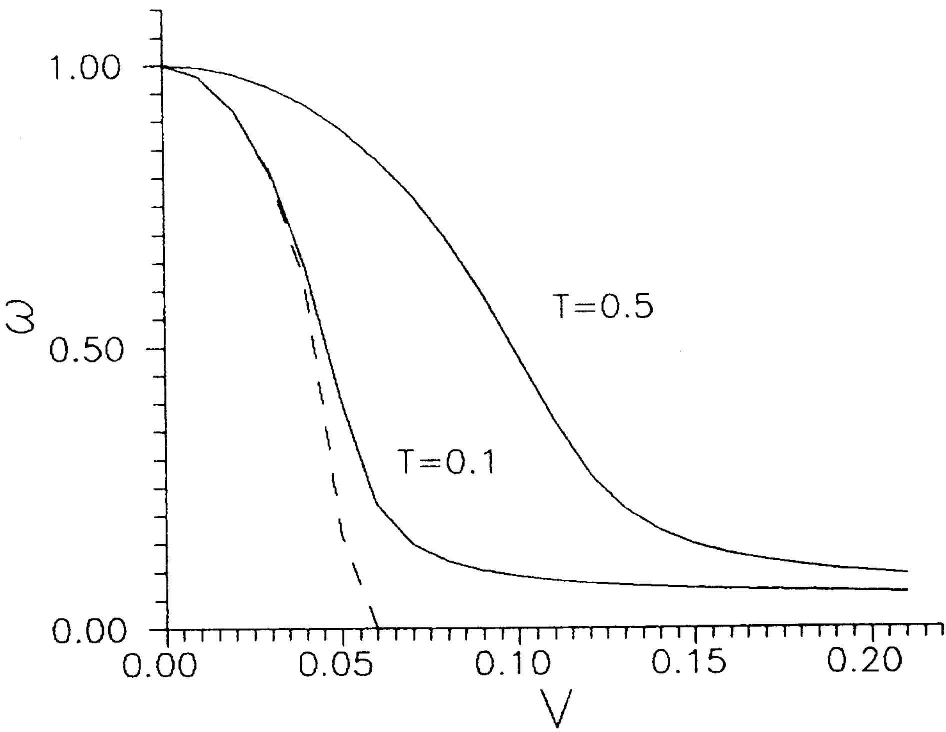

Fig.1 The dependence of the energy ω of the phonon state in $SU(2)$ model on the interaction strength V at different temperatures T. Solid lines – the TRRPA results, dashed line – the standard TRPA result at $T = 0.1$.

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Перенормированное ПСФ при конечной температуре

Для изучения коллективных возбуждений в нагретых ядрах разработан метод, учитывающий отклонение чисел заполнения от значений, предсказываемых температурным приближением случайной фазы. Идея введения перенормированных бозонов взята из работ К.Хары и Д.Роу. Основные уравнения перенормированного теплового приближения случайной фазы получены с использованием термополевой динамики. Численные результаты продемонстрированы на примере $SU(2)$ модели.

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Renormalized RPA at Finite Temperature

A method taking account of a deviation of state occupation numbers from the thermal RPA prescriptions is elaborated to study collective excitations in hot nuclei. The main idea of this Thermal Renormalized Random Phase Approximation goes back to Ken-Ji Hara and D.J.Rowe. In developing the TRRPA, a formalism of the thermo field dynamics (TFD) is used. Some numerical results are given for the $SU(2)$ model.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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