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LIPKIN — MESHKOV — GLICK MODEL AT FINITE TEMPERATURE

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Стороженко А.Н., Косов Д.С., Вдовин А.И. Е4-97-352 Модель Липкина — Мешкова — Глика при конечной температуре

На примере двухуровневой модели Липкина — Мешкова — Глика исследована точность приближенных методов теории многих тел при конечной температуре. Рассмотрены тепловое приближение случайной фазы (ТПСФ) и тепловое перенормированное приближение случайной фазы (ТППСФ). Рассчитанные в этих приближениях средняя энергия, среднее значение проекции квазиспина и дисперсия числа частиц сравниваются с результатами точного расчета для большого канонического ансамбля. Результаты ТППСФ в целом ближе к точным. С ростом температуры и/или числа частиц в системе точность обоих приближений улучшается.

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The Lipkin — Meshkov — Glick model is used to examine the validity of some approximate methods in a many-body theory at finite temperature. Namely, the thermal random phase approximation (TRPA) and the thermal renormalised random phase approximation (TRRPA) are studied. An average energy of the system, an average quasispin projection and a particle number variance are calculated within these approximations and exactly with the grand canonical ensemble partition function. On the whole the results of TRRPA are found to be in better agreement with the exact ones. The validity of the both approximations becomes better with increasing temperature as well as particle number.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR and at the Institute for Theoretical Physics of the University of Tuebingen (Germany).

1. Introduction

New approximate methods of nuclear structure theory are usually examined by applying them to simple exactly soluble models in order to gain some insights on a range of their validity. One of the widely used models is the two level schematic shell model which possess the SU(2) symmetry and is often called SU(2) or Lipkin – Meshkov (lick (LMG) model [1]. Numerous applications of the LMG- model can be found in [2].

During the last years the model has been used many times to justify approximate methods of the many-body theory at finite temperature [3-9]. These methods are especially interesting in view of current intensive studies of hot nuclear systems. Previous works on the LMG- model at finite temperature [3, 4] have focused on boson expansion methods and symmetry breaking in hot nuclei. The mixed state representation has been formulated and then applied to the LMG- model in refs. [5-8]. In particular, the thermal Hartree - Fock approximation as well as the thermal random phase approximation (TRPA) were studied within the approach [8]. The thermal llartree - Fock approximation and the static path-approximation were analyzed within the model in ref. [9].

A-new approximate method has been recently proposed [10] to describe collective, excitations in hot finite Fermi systems. This method, the so-called renormalized TRPA (TRPA), is an extension of the renormalized RPA of Ken-ji Hara [11] and D. Rowe [12] to finite temperatures. Within TRRPA vibrational excitations are supposed to be harmonic like in TRPA but a temperature - dependent ground state is treated in a more consistent manner. Namely, a finite number of thermal quasiparticles are presented in this ground state.

In the present paper, we investigate the accuracy of the thermal renormalized random phase approximation by comparing it with the exact calculations for the grand canonical ensemble for the LMG- model. Moreover, a comparison with the thermal mean field approximation (TMFA) and TRPA is also done.

2. The LMG- model and the grand canonical ensemble calculations

The following version of the LMG- model is used: N fermions are distributed over two levels. each having a degeneracy Ω . The distance between the levels is ε , the coupling constant V does not depend on any quantum number. At T = 0 and V = 0 the lower level is full, the upper - empty, i.e. $N = \Omega$. The model Hamiltonian has the form

$$H = \varepsilon \hat{J}_{z} - \frac{1}{2} V \left(\hat{J}_{+} \hat{J}_{+} + \hat{J}_{-} \hat{J}_{-} \right) , \qquad (1)$$

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where the operators of quasispin \hat{J} and its projections $\hat{J}_+, \hat{J}_-, \hat{J}_z$ are defined as follows:

$$\hat{J}^2 = \frac{1}{2} \left(\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_- \right) + \hat{J}_z^2 ,$$

$$J_z = \frac{1}{2} \sum_{p=1}^{\Omega} \left(a_{2p}^+ a_{2p} - a_{1p}^+ a_{1p} \right) , \quad \hat{J}_+ = \sum_{p=1}^{\Omega} a_{2p}^+ a_{1p} , \quad \hat{J}_- = \left(\hat{J}_+ \right)^+ .$$

Here a_{ip}^+ and a_{ip} are particle creation and annihilation operators on the lower (i = 1) or the upper (i = 2) level.

The operators \hat{J}_{\pm} and \hat{J}_z form SU(2) algebra, and the quasispin operator commutes with H. So the Hamiltonian matrix breaks up into submatrices Θ_J of dimension 2J + 1. The Hamiltonian can be diagonalized in each of these subspaces independently. The corresponding eigenvalues are denoted by $E_1^J, E_2^J, \dots E_{2J+1}^J$.

To calculate the grand canonical partition function, one needs the eigenvalues E_k^J and the degeneracies of irreducible quasispin representations Θ_J for different particle numbers from the range $0 < N \leq 2\Omega$. The latter have been determined in ref. [7], and here we use this result. The whole number of the ensemble states, i.e., the whole number of the eigenstates of the LMG- systems formed by two Ω - degenerated levels with a number of particles varying from 1 to 2Ω is equal to $2^{2\Omega}$. Any state of the ensemble can be written in the following form:

$$|g_1p_1, g_2p_2, ..., g_np_n\rangle = a^+_{g_1p_1}a^+_{g_2p_2}, ..., a^+_{g_np_n}|0\rangle, \qquad a_{g_p}|0\rangle = 0.$$

The indices g_i, p_i, n have the following meanings:

 $g_i \in \{1, 2\}, p_i \in \{1, ..., \Omega\}, i \in \{1, ..., n\}, n \in \{1, ..., 2\Omega\},$

i.e., g marks the lower and the upper levels, p - sublevels, i is an index of a particle and n is the particle number in the particular LMG- system from the grand canonical ensemble. If n = 0, $|g_1p_1, g_2p_2, ..., g_np_n\rangle = |0\rangle$. A particular distribution of the given number of particles over two degenerate levels can be characterized by numbers ν_1 and ν_2 : ν_1 is a number of sublevels which are occupied by particles for both the lower and upper levels; ν_2 is a number of sublevels which are occupied for neither the lower nor the upper level. The quasispin J of the state is determined by the distribution of the rest of particles over 2τ sublevels where $2\tau = \Omega - \nu_1 - \nu_2$. The number $2(\tau + \nu_1)$ is equal to the number of particles. We denote by $\Gamma_{p_1,p_2,...,p_{2\tau+\nu_1}}$ the subspace of states with ν_1 occupied and ν_2 empty sublevels. Its dimension is $2^{2\tau}$. There exist $\Omega!/(2\tau)!\nu_1!\nu_2!$ distinct subspaces $\Gamma_{p_1,p_2,...,p_{2\tau+\nu_1}}$ for fixed τ and ν_1 . Each of them may be decomposed into irreducible subspaces with fixed quasispin values Θ_{τ} (appearing once), $\Theta_{\tau-1}$ (appearing g_{τ}^{τ} times), $\Theta_{\tau-2}$ (appearing g_{τ}^{τ} times), ..., $\Theta_{\tau-k}$ (appearing g_{τ}^{τ} times),..., $\Theta_{\tau-[\tau]}$ (appearing $g_{\tau-1}^{\tau}$ times). Here

$$g_k^{\tau} = \frac{(2\tau)!}{k!(2\tau-k)!} - \frac{(2\tau)!}{(k-1)!(2\tau-k+1)!}$$

and $[\tau] = \tau$, if τ is integer, $[\tau] = \tau - 1/2$ if τ is half-integer.

Then, the exact grand partition function is

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$$Z(T) = \sum_{\tau\nu_1\nu_2} \frac{\Omega!}{(2\tau)!\nu_1!\nu_2!} \sum_k g_k^{\tau} \sum_m \exp\left[-\frac{E_m^{\tau-k} - 2(\tau+\nu_1)\lambda}{T}\right]$$

The expressions for average energy, quasispin z-projection and the total fermion number are

3. Thermo field dynamics: basic elements

To be more understandable while describing approximate methods, we briefly recapitulate the formalism of thermo field dynamics (TFD) (see, [3, 13-15]).

The extension of quantum field theory to finite temperature requires the field degrees of freedom to be doubled. In TFD, this doubling is achieved by introducing an additional tilde space. A tilde conjugate operator \tilde{A} is assigned to an operator A (acting in ordinary space) through the tilde conjugation rules

$$(\widetilde{AB}) = \widetilde{AB}; \quad (a\widetilde{A+bB}) = a^*\widetilde{A} + b^*\widetilde{B},$$

where A and B represent ordinary operators and a and b are c-numbers. The asterisk denotes the complex conjugation. The tilde operation commutes with hermitian conjugation and any tilde and non-tilde operators are assumed to commute or anticommute with each other. A double application of tilde operation changes a sign of a fermionic operator and saves it for a bosonic one. The whole Hilbert space of a heated system is a direct product of ordinary and tilde spaces. A formal quantity playing a central role in the present discussion is the so-called thermal Hamiltonian:

 $\mathcal{H} = H - \tilde{H}$

The operator \mathcal{H} serves to translate temperature dependent wave functions along the time axis. It means that an "excitation spectrum" of a hot system (or, in other words, a set of energies corresponding to the thermal equilibrium states) should be obtained by the diagonalization of \mathcal{H} .

The temperature-dependent vacuum $|\Psi_0(T)\rangle$ is the eigenvector of \mathcal{H} with eigenvalue 0

$$\mathcal{H}|\Psi_0(T)\rangle=0$$

If one determines the thermal vacuum state as

$$|\Psi_0(T)\rangle = \frac{1}{\sqrt{Tr(\exp(-H/T))}} \sum_n \exp(-\frac{E_n}{2T})|n\rangle \otimes |\tilde{n}\rangle$$

where $E_n, |n\rangle$ and $|\tilde{n}\rangle$ are eigenvalues, eigenvectors and their tilde counterparts of the Hamiltonian H, respectively, the expectation value $\langle \Psi_0(T)|O|\Psi_0(T)\rangle$ will exactly correspond to the grand canonical ensemble average $\ll O \gg$ of a given observable O.

In practice, it is impossible to find the exact thermal vacuum for a full Hamiltonian of a many-body system. In setting up approximate schemes, the usual starting point is the thermal mean-field approximation. In this case, the thermal vacuum $|\Psi_0(T)\rangle$ is an eigenvector of the uncorrelated thermal Hamiltonian

$$\mathcal{H}_{MF}|0(T)\rangle = (H_{MF} - \tilde{H}_{MF})|0(T)\rangle = \sum_{i} \varepsilon_{i}(a_{i}^{+}a_{i} - \tilde{a}_{i}^{+}\tilde{a}_{i})|0(T)\rangle = 0.$$
(2)

The solutions of eq. (2) define the vacuum $|0(T)\rangle$ for so-called thermal quasiparticles $\beta, \tilde{\beta}$:

$$\begin{split} \beta_i &= x_i a_i - y_i \tilde{a}_i^+ \\ \tilde{\beta}_i &= x_i \tilde{a}_i + y_i a_i^+ \\ \beta_i &|0(T)\rangle = \tilde{\beta}_i &|0(T)\rangle = 0 \,, \end{split}$$

where the coefficients x_i, y_i denote the thermal Fermi occupation probabilities of the states $a_i^+|0\rangle$ ($|0\rangle$ is a vacuum for a_i)

$$x_i = \sqrt{1 - f_i}, y_i = \sqrt{f_i}$$

 $f_i = rac{1}{1 + \exp(\varepsilon_i/T)}$.

Sometimes the $\{x, y\}$ transformation is called the thermal Bogoliubov transformation. It is a unitary transformation and thus conserves the commutation relations.

4. Approximate methods

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Now we apply the TFD formalism to the LMG- model and derive the corresponding equations of TRRPA. A more general formulation of the thermal renormalized random phase approximation can be found in refs. [10, 16, 17]. Moreover, within the Hartree – Fock method, depending on the value of the coupling constant V two different phases of

the LMG- system exist – a normal phase and a deformed one. The present consideration is restricted to a normal phase. So we do not take into account the mean field rearrangement which occurs if the value of the effective coupling constant $\chi = V(N-1)/\varepsilon$ becomes more than unity.

The model thermal Hamiltonian $\mathcal{H} = H - \tilde{H}$, where H has the form (1), has to be written in terms of the thermal quasiparticle operators. The first item in (1) conserves the diagonal form. The interaction operator becomes more complicated. For further studies we need only that part of \mathcal{H} which consists of the terms with even numbers of both creation and annihilation thermal quasiparticle operators. Namely,

$$\mathcal{H}' = \varepsilon \left(B - \tilde{B} \right) - \frac{V(f_1 - f_2)}{2} \left[\left(A^{+2} + A^2 \right) - \left(\tilde{A}^{+2} + \tilde{A}^2 \right) \right], \tag{3}$$

where

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$$B = \frac{1}{2} \sum_{p=1}^{\Omega} \left(\beta_{2p}^{+} \beta_{2p} - \beta_{1p}^{+} \beta_{1p} \right), \quad A^{+} = \sum_{p=1}^{\Omega} \beta_{2p}^{+} \tilde{\beta}_{1p}^{+}, \quad \tilde{A}^{+} = \sum_{p=1}^{\Omega} \beta_{1p}^{+} \tilde{\beta}_{2p}^{+}$$

The following exact commutation rules are valid for the thermal biquasiparticle operators A, A^+, \tilde{A} and \tilde{A}^+ :

$$[A, A^{+}] = N - \sum_{p=1}^{\Omega} \tilde{\beta}_{1p}^{+} \tilde{\beta}_{1p} - \sum_{p=1}^{\Omega} \beta_{2p}^{+} \beta_{2p}, \quad \left[\tilde{A}, \tilde{A}^{+}\right] = N - \sum_{p=1}^{\Omega} \beta_{1p}^{+} \beta_{1p} - \sum_{p=1}^{\Omega} \tilde{\beta}_{2p}^{+} \tilde{\beta}_{2p}. \quad (4)$$

All other commutators between the operators A, A^+, \tilde{A} and \tilde{A}^+ vanish.

By the use of the Wick theorem one can approximate [10, 16] the r.h.s. of (4) by c-numbers neglecting an influence of the pairs of normal ordered operators : $\beta^+\beta$: and : $\hat{\beta}^+\hat{\beta}$:. Namely,

$$[A, A^+] = \left[\tilde{A}, \tilde{A}^+\right] = N(1 - \rho_1 - \rho_2) \equiv N(1 - 2\rho) .$$
(5)

Here ρ_i are the numbers of thermal quasiparticles in the temperature - dependent ground state $|\Psi_0(T)\rangle$ that will be defined later on. That is

$$\rho_i = \frac{1}{N} \langle \Psi_0(T) | N_i^\beta | \Psi_0(T) \rangle = \frac{1}{N} \langle \Psi_0(T) | \tilde{N}_i^\beta | \Psi_0(T) \rangle$$

where N_i^{β} is the operator of the number of thermal quasiparticles $N_i^{\beta} = \sum_{p=1}^{\Omega} \beta_{ip}^+ \beta_{ip}$.

The thermal Hamiltonian (3) can be diagonalized in the space of two one-phonon states constructed as bilinear forms of the thermal biquasiparticle operators:

$$Q_{1}^{+}[\Psi_{0}(T)] = (\psi_{1}A^{+} - \phi_{1}A) |\Psi_{0}(T)\rangle$$

$$Q_{n}^{+}[\Psi_{0}(T)] = (\psi_{2}\hat{A}^{+} - \phi_{2}\hat{A}) |\Psi_{0}(T)\rangle.$$
(6)

Now we define the wave function of the temperature - dependent ground state $|\Psi_0(T)\rangle$ as the thermal phonon vacuum, i.e. $Q_{1,2}|\Psi_0(T)\rangle = 0$.

The states (6) have to be orthonormal. Thus, taking account of eq. (5) the following constraints on the amplitudes ψ and ϕ are derived

$$\psi_i^2 - \phi_i^2 = [N(1-2\rho)]^{-1}, \quad i = 1, 2.$$

The system of equations for ψ_i , ϕ_i and the phonon frequencies ω_i is easily obtained by the equation of motion method. It appears that only a positive value of ω_1 and a negative value of ω_2 is allowed under a requirement that the wave functions $Q_1^+|\Psi_0(T)\rangle$ and $Q_2^+|\Psi_0(T)\rangle$ are vectors of the Hilbert space. The eigenvalue - eigenvector problem has the following solution:

$$\begin{split} \mu_{1} &= \omega \equiv \sqrt{\varepsilon^{2} - V^{2} \left(f_{2} - f_{1}\right)^{2} \left(1 - 2\rho\right)^{2} \left(N - 1\right)^{2},} \\ \psi_{1}^{2} &= \frac{\varepsilon + \omega}{2N\omega(1 - 2\rho)}, \quad \phi_{1}^{2} = \frac{\varepsilon - \omega}{2N\omega(1 - 2\rho)}, \\ \omega_{2} &= -\omega, \quad \psi_{2}^{2} = \psi_{1}^{2}, \quad \phi_{2}^{2} = \phi_{1}^{2}. \end{split}$$

One more equation has to be added to the above system – the equation for ρ . To evaluate this equation we need an expression for the thermal phonon vacuum state. The latter can be derived from the thermal quasiparticle vacuum state $|0(T)\rangle$ by a unitary transformation

$$|\Psi_0(T)\rangle = \sqrt{R}e^{S}|0(T)\rangle, \quad S = \frac{1}{2(1-2\rho)}\frac{\phi_1}{\psi_1}\left(A^+A^+ + \tilde{A}^+\tilde{A}^+\right)$$

By the use of standard techniques of the operator calculus [?] we get

$$\rho = \frac{1}{2} \frac{\varepsilon - \omega}{N\omega} \quad (7)$$

It is interesting to note that in the thermodynamic limit, i.e. at $N \to \infty$, ρ vanishes and the TRRPA equations are reduced to the TRPA ones.

Let us display the expressions for the average energy, the average quasispin z-projection and the variance of the particle number

$$\langle \hat{H}' \rangle_{TRRPA} = \frac{N\varepsilon(f_2 - f_1)}{2} (1 - 2\rho) + \frac{\varepsilon^2 - \omega^2}{2\omega} \times \frac{(f_2 - f_1)^2 + 2\rho}{2(f_2 - f_1)}$$

$$\langle \hat{J}_z \rangle_{TRRPA} = \frac{N(f_2 - f_1)}{2} (1 - 2\rho)$$

$$\Delta N_{TRRPA} = \sqrt{N(1 - 2\rho) [f_1(1 - f_1) + f_2(1 - f_2)]}.$$

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The above expectation values were taken over the TRRPA vacuum state.

It seems appropriate to give expressions for the same quantities within other approximations – TRPA and TMFA. The TRPA expressions are obtained from the TRRPA ones by putting $\rho = 0$. In this case, the commutator $[A, A^+]$ is equal to N and the expectation values are taken over the TRPA vacuum

$$\langle \hat{H}' \rangle_{TRPA} = \frac{N\varepsilon(f_2 - f_1)}{2} + \frac{\varepsilon^2 - \omega^2}{2\omega} \times \frac{(f_2 - f_1)^2 + 1}{2(f_2 - f_1)} ,$$

$$\langle \hat{J}_z \rangle_{TRPA} = \frac{N(f_2 - f_1)}{2} ,$$

$$\Delta N_{TRPA} = \sqrt{N[f_1(1 - f_1) + f_2(1 - f_2)]} .$$

Within TMFA the interaction between particles is omitted and one has to evaluate the expectation values over the thermal quasiparticle vacuum $|0(T)\rangle$. The TMFA expressions for $\langle \hat{J}_z \rangle_{TMFA}$ and ΔN_{TMFA} are the same as in TRPA. For $\langle \hat{H} \rangle_{TMFA}$ one gets

$$\langle \hat{H} \rangle_{TMFA} = \frac{N \varepsilon (f_2 - f_1)}{2} .$$

5. Results and discussion

The numerical calculations are done for the LMG- system with $N = \Omega = 10$ particles and $\varepsilon = 2$. The results are displayed in Figs. 1-6.

Firstly, we discuss a dependence of some characteristics of the system on the effective coupling constant χ . The energy of the collective state ω as a function of χ at T = 0 and 0.25ε is displayed in Fig. 1. Besides the results of the TRPA and TRRPA calculations the exact solution at T = 0 is also shown. As it should be, with increasing χ the energy ω goes down. Within TRPA ω vanishes at $\chi = 1$. This collapse does not take place for the exact solution as well as for the TRRPA result. This last feature of the RRPA solution is well known in the case of a cold nucleus and is actively used in some recent nuclear structure calculations [18]. As it has been demonstrated for the first time in ref. [10], the same is valid at $T \neq 0$. In the present version of the LMG- model heating effectively weakens the interaction of particles (the effective coupling constant χ is multiplied by a factor of $f_1 - f_2 < 1$) and the TRPA collapse occurs at larger χ -values. In TRPA when $\chi \rightarrow \chi_{collapse}$ (\hat{H})_{TRPA} $\sim -\omega^{-1} \rightarrow -\infty$. It is not the case for TRRPA (see Fig. 2). The value (\hat{H})_{TRRPA} goes down much slower and remains even greater than the exact value $\langle \hat{H} \rangle_{GCE}$. At large values of χ the strong difference between (\hat{H})_{TRRPA} and (\hat{H})_{GCE} is due to neglecting the mean field rearranging.

In Figs. 3-5, the average energy of the system, the average \hat{J}_z value and the variance of the particle number as functions of T are displayed ($\chi = 0.95$). The noticeable difference



TRPA results - dashed line; the TRRPA results - solid line.









between the exact and the approximate values is only at moderate $T \leq 0, 3\varepsilon$. Here TRRPA works evidently better than TRPA and TMFA. The absolute values $\langle H \rangle_{TRPA}$ and $\langle \hat{J}_z \rangle_{TRPA}$ are greater than $\langle H \rangle_{GCE}$ and $\langle \hat{J}_z \rangle_{GCE}$, respectively. At the same time, $|\langle H \rangle_{TRRPA}| < |\langle H \rangle_{GCE}|$. The relation $|\langle \hat{J}_z \rangle_{TRRPA}| < |\langle \hat{J}_z \rangle_{GCE}|$ is valid only at $T < 0, 8\varepsilon$ but then $|\langle \hat{J}_z \rangle_{TRRPA}|$ appears to be slightly greater than $|\langle \hat{J}_z \rangle_{GCE}|$. At $T > 0, 5\varepsilon$ the differences between the exact and the approximate results is negligible. The difference between exact and approximate values of the particle number variance is only 2-3%, i.e. even less than for other variables. Decreasing in the difference with raising up T is a result of effective weakening of the interaction.

The value $\Delta N/N$ as a function of N is shown in Fig. 6. It decreases slowly when T increases, and its typical value at N = 10-30 is around 10%. The approximate methods disturb ΔN only slightly. The difference between different approximations is of minor importance although formally TRRPA seems to be better.

6. Summary

Taking the Lipkin – Meshkov – Glick model as an example we have studied a validity of some approximate methods of many-body theory at finite temperature. The average energy, the average quasispin z-projection and the particle number variance as functions of temperature and particle number have been calculated in different approximations as well as exactly with the grand canonical partition function. On the whole, TRRPA gives better results than other approximations. Its advantages are especially evident at moderate temperatures $T \leq 0.5\epsilon$. With increasing T and N, results of approximate methods improve rapidly and at $T \gg \epsilon$ the difference between exact and approximate results is invisible.

In the present paper, we have studied only the case with not too strong particle interaction ($\chi < 1$). Investigations of the deformed phase of the LMG- model are in progress.

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