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D.S.Kosov, A.I.Vdovin

APPROXIMATE NUMBER PROJECTION  
AT FINITE TEMPERATURE

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Приближенное проектирование по числу частиц  
при конечной температуре

В рамках термодинамики разработан метод приближенного проектирования по числу частиц в нагретых ядрах.

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Approximate Number Projection at Finite Temperature

The approximate particle number projection method is developed in the framework of the thermo field dynamics.

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

# 1 Introduction

For a finite hot system like an atomic nucleus the number of particles in the system is fixed and any statistical calculations should be performed in the canonical ensemble. Since it is simpler to do these calculations with the partition function of the grand canonical ensemble, this way is used in practice as a rule. So, the results of the calculations are disturbed by thermal fluctuations of the number of particles.

In addition to these purely statistical effects in interacting systems, the use of approximate uncorrelated statistical operators generally requires the violation of relevant symmetries and this introduces additional quantum fluctuations in quantities which should in principle be conserved. In particular standard approaches treating heated nuclear systems with pairing (the thermal Hartree - Fock - Bogoliubov method or finite temperature BCS method) violate the particle number conservation law and introduce the particle number fluctuations [1].

That is why so many attempts were made to construct exact or approximate projection methods [2-5] to suppress these fluctuations.

In the present work, we formulate a new approximate particle number projection method for hot finite systems based on the ideas of a quite old although famous Lipkin - Nogami method [6-8]. Until now the Lipkin - Nogami approximation has widely been used for an approximate number projection in cold nuclei with strong pairing. To extend this method to finite temperature, we explore the formalism of the thermo field dynamics [9].

## 2 Formalism of TFD

Let us assume that a hot nuclear system in the thermal equilibrium is described by the partition function of the grand canonical ensemble. The main idea behind the TFD [9] is to define a thermal vacuum  $|0(T)\rangle$  such that the thermal expectation value of any operator

$$\langle\langle A \rangle\rangle = \frac{1}{Tr(\exp(-H/T))} Tr[A \exp(-H/T)]$$

equals the expectation value over the thermal vacuum state

$$\langle\langle A \rangle\rangle = \langle 0(T) | A | 0(T) \rangle$$

To this aim the TFD requires a doubling of the system degrees of freedom. The new Hilbert space of states is defined through tilde conjugation rules for

linear operators and by means of an appropriate choice of the wave function of the thermal ground state. A tilde conjugate operator  $\tilde{A}$  is associated with any operator  $A$  acting in the ordinary space through the tilde conjugation rules

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

where  $A$  and  $B$  stand for any operators and  $a$  and  $b$  are c-numbers. The asterisk denotes the complex conjugation. The tilde operation commutes with the hermitian conjugation operation and any tilde and non-tilde operators are assumed to commute or anticommute with each other. For any system governed by the Hamiltonian  $H$  the whole Hilbert space is now spanned by the direct product of the eigenstates of  $H$  and those of the tilde Hamiltonian  $\tilde{H}$  having the same eigenvalues. The time - translation operator is not the energy operator  $H$  but the thermal Hamiltonian  $\mathcal{H} = H - \tilde{H}$ . This means that the properties of the system excitations are obtained by the diagonalization of  $\mathcal{H}$ .

It is easy to see that with the doubling of the Hilbert space the temperature - dependent vacuum  $|0(T)\rangle$  has to be defined as follows:

$$|0(T)\rangle = \frac{1}{\sqrt{\text{Tr}(\exp(-H/T))}} \sum_k \exp(-\frac{E_k}{2T}) \phi_k \otimes \tilde{\phi}_k,$$

where  $H\phi_k = E_k\phi_k$  and  $\tilde{H}\tilde{\phi}_k = E_k\tilde{\phi}_k$ .

The Heisenberg equation, equal-time commutation relations, the tilde-conjugation rules and the temperature dependent thermal vacuum form the basic relations of the TFD.

### 3 TFD for number projection

The wave function of the thermal ground state represents a mixture of the state with a different number of particles in the tilde and in the ordinary space:

$$|0(T)\rangle = \sum_{nm} C_{nm} |n\rangle \otimes |\tilde{n}\rangle = \sum_{nm} C_{nm} |n\tilde{n}\rangle.$$

The expectation value over the thermal vacuum corresponds to averaging within the grand canonical ensemble. However since in atomic nucleus the nucleon number is fixed, one has to work within the TFD formalism only with the eigenfunction of the particle number operators  $N$  and  $\tilde{N}$  with a

certain eigenvalue  $n$  instead of averaging over the wave function in the whole Hilbert space:

$$N|n\tilde{n}\rangle = n|n\tilde{n}\rangle$$

$$\tilde{N}|n\tilde{n}\rangle = \tilde{n}|n\tilde{n}\rangle$$

To separate the required states the projection operator that "cuts" the wave function with given number of particles from the whole Hilbert space, should be constructed.

$$P_n = \frac{1}{2\pi} \int_0^{2\pi} \exp(i\phi(N - n)) d\phi \otimes \frac{1}{2\pi} \int_0^{2\pi} \exp(i\phi(\tilde{N} - \tilde{n})) d\phi$$

$$NP_n|0(T)\rangle = nP_n|0(T)\rangle$$

$$\tilde{N}P_n|0(T)\rangle = \tilde{n}P_n|0(T)\rangle$$

With this projector one can obtain the canonical averaged value of any operator in the following form:

$$\langle n\tilde{n}|A|n\tilde{n}\rangle = \frac{\langle 0(T)|P_n A P_n|0(T)\rangle}{\langle 0(T)|P_n|0(T)\rangle}$$

The elaboration of an approximate particle number projection method seems natural since the exact projection is a very hard task already in cold nuclei [10]. This approximate particle number projection method should be simple enough for practical realization and at the same time has to suppress noticeably the influence of the particle number fluctuations on calculated variables.

To formulate the method, we followed the idea of the Lipkin-Nogami approximation [6-8].

Let us consider any operator  $Q$  defined in the initial Hilbert space of a nuclear system. After placing our system into the thermal bath this operator can be rewritten as  $Q = Q \otimes \tilde{I}$ , where  $\tilde{I}$  is a unit operator in the space of tilde states. One can consider a matrix element  $\langle n\tilde{n}|Q|n\tilde{n}\rangle$  as a function  $q(n)$  of the number of particles and write the following power expansion for it:

$$\langle n\tilde{n}|Q|n\tilde{n}\rangle = \langle n|Q|n\rangle = q(n) = \sum_{k=0}^{\infty} q_k n^k, \quad (1)$$

Then

$$\langle 0(T)|Q|0(T)\rangle = \langle 0(T)|\sum_{k=0}^{\infty} q_k N^k|0(T)\rangle$$

Using the last equation one can rewrite (1) in the form:

$$\begin{aligned} \langle n\bar{n}|Q|n\bar{n}\rangle &= \langle 0(T)|Q|0(T)\rangle - \langle 0(T)|\sum_{k=0}^{\infty} q_k N^k|0(T)\rangle + \sum_{k=0}^{\infty} q_k n^k = \quad (2) \\ &= \langle 0(T)|Q - \sum_{k=1}^{\infty} q_k N^k|0(T)\rangle + \sum_{k=1}^{\infty} q_k n^k \end{aligned}$$

An important point is that the above manipulation yields the expectation value of the operator  $Q$  over the projected states  $|n\bar{n}\rangle$  in terms of the thermal vacuum. Formula (2) allows one to obtain the canonical average value  $\langle n\bar{n}|Q|n\bar{n}\rangle$  without explicit involving  $|n\bar{n}\rangle$ . However the coefficients  $q_k$  are still unknown. To find them, let us introduce the operator

$$\bar{Q} = Q - \sum_{k=1}^{\infty} q_k N^k$$

The operator  $\bar{Q}$  and an arbitrary function of the particle number operator  $f(N)$  obey the following relation:

$$\langle 0(T)|\bar{Q}f(N)|0(T)\rangle = \langle 0(T)|\bar{Q}|0(T)\rangle \langle 0(T)|f(N)|0(T)\rangle$$

that holds valid iff the following set of equations is valid:

$$\langle 0(T)|\bar{Q}N|0(T)\rangle = \langle 0(T)|\bar{Q}|0(T)\rangle \langle 0(T)|N|0(T)\rangle$$

$$\langle 0(T)|\bar{Q}N^2|0(T)\rangle = \langle 0(T)|\bar{Q}|0(T)\rangle \langle 0(T)|N^2|0(T)\rangle$$

....

$$\langle 0(T)|\bar{Q}N^m|0(T)\rangle = \langle 0(T)|\bar{Q}|0(T)\rangle \langle 0(T)|N^m|0(T)\rangle$$

....

One can rewrite this set of equations in the form of a linear system by returning from the operator  $\bar{Q}$  to  $Q$ .

$$\begin{pmatrix} \langle QN \rangle - \langle Q \rangle \langle N \rangle \\ \langle QN^2 \rangle - \langle Q \rangle \langle N^2 \rangle \\ \dots \\ \langle QN^m \rangle - \langle Q \rangle \langle N^m \rangle \\ \dots \end{pmatrix} = A \begin{pmatrix} q_1 \\ q_2 \\ \dots \\ q_m \\ \dots \end{pmatrix} \quad (3)$$

The element  $A_{ij}$  of the matrix  $A$  has the form  $A_{ij} = \langle N^{i+j} \rangle - \langle N^i \rangle \langle N^j \rangle$ , where  $\langle \dots \rangle$  means averaging over the thermal vacuum  $|0(T)\rangle$ .

So far our consideration was exact. For practical calculations one has to truncate expansion (1) retaining a finite number of terms. We retain the first 3 terms (this is the usual Lipkin-Nogami approximation). In this approximation the dispersion of  $N$ , i.e.  $\langle N \rangle^2 - \langle N^2 \rangle$ , vanishes. The following expressions for the coefficients  $q_1$  and  $q_2$  are valid:

$$q_1 = \frac{1}{\det(A)} \begin{vmatrix} \langle QN \rangle - \langle Q \rangle \langle N \rangle & \langle N^3 \rangle - \langle N^2 \rangle \langle N \rangle \\ \langle QN^2 \rangle - \langle Q \rangle \langle N^2 \rangle & \langle N^4 \rangle - \langle N^2 \rangle \langle N^2 \rangle \end{vmatrix} \quad (4)$$

$$q_2 = \frac{1}{\det(A)} \begin{vmatrix} \langle N^2 \rangle - \langle N \rangle \langle N \rangle & \langle QN \rangle - \langle Q \rangle \langle N \rangle \\ \langle N^3 \rangle - \langle N^2 \rangle \langle N \rangle & \langle QN^2 \rangle - \langle Q \rangle \langle N^2 \rangle \end{vmatrix}$$

where

$$\det(A) = \begin{vmatrix} \langle N^2 \rangle - \langle N \rangle \langle N \rangle & \langle N^3 \rangle - \langle N^2 \rangle \langle N \rangle \\ \langle N^3 \rangle - \langle N^2 \rangle \langle N \rangle & \langle N^4 \rangle - \langle N^2 \rangle \langle N^2 \rangle \end{vmatrix}$$

It is noteworthy that there is another method to calculate the coefficients  $q_k$ , more appropriate to project the operator  $Q$  of complicated structure. The use of expansion (1) allows one to get for  $q_k$  the following relation:

$$q_k = \frac{1}{k!} \left. \frac{d^k q(n)}{dn^k} \right|_{n=0} \quad (5)$$

## 4 The degenerate single $j$ -shell model

Let us consider the system of  $n$  (even) nucleons with the BCS pairing interaction in a degenerate  $j$ -shell. This model has been used often in the literature as a test of many body theories because it is an exactly soluble. If one places the energy of the shell equal to zero, the model Hamiltonian reads

$$H = -\frac{G}{4} \sum_{mm'} a_m^+ a_m^+ a_{m'}^- a_{m'}^- \quad (6)$$

The exact solution is a set of the energy levels labelled by the seniority number  $s$  which may take any even integer value from 0 to  $n$ :  $s = 0, 2, 4, \dots, n$ . The exact eigenvalues of the Hamiltonian (6) are

$$E_s = -\frac{1}{4} G(n-s)(2\Omega + 2 - n - s). \quad (7)$$

The degeneracy  $d_s$  of each level is

$$d_s = \binom{2\Omega}{s} - \binom{2\Omega}{s-2}, \quad (8)$$

where  $2\Omega = 2j + 1$  is the degeneracy of the shell.

Equations (7) and (8) allow one to compute exactly, within the canonical ensemble, all the thermodynamical functions. The partition function is given by

$$Z_c = \sum_{s=0}^n d_s \exp\left(-\frac{E_s}{T}\right)$$

and the ground state energy is

$$E_c = \frac{1}{Z_c} \sum_{s=0}^n d_s E_s \exp\left(-\frac{E_s}{T}\right)$$

The finite - temperature BCS approach can be also applied to the model. Following the prescriptions of TFD, we write the Hamiltonian of the hot system as the thermal Hamiltonian  $\mathcal{H} = H - \tilde{H}$ . It is possible to diagonalize this Hamiltonian by means of the thermofield transformation [11, 12]. The thermofield transformation is constructed as two successive canonical transformations: the standard Bogoliubov  $\{u, v\}$  transformation from particles to quasiparticles and the thermal canonical  $\{\sqrt{f}, \sqrt{1-f}\}$  one from quasiparticles to thermal quasiparticles:

$$\begin{pmatrix} a_m \\ a_m^+ \\ \tilde{a}_m^+ \\ \tilde{a}_m^- \end{pmatrix} = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} \begin{pmatrix} \beta_m \\ \beta_m^+ \\ \tilde{\beta}_m^+ \\ \tilde{\beta}_m^- \end{pmatrix}$$

$$A = \sqrt{1-f} \begin{pmatrix} u & v \\ -v & u \end{pmatrix}, \quad B = \sqrt{f} \begin{pmatrix} u & v \\ -v & u \end{pmatrix}$$

The temperature - dependent ground state of the system is the thermal vacuum  $|0(T)\rangle$  for thermal quasiparticles  $\beta$  and  $\tilde{\beta}$ :

$$\beta|0(T)\rangle = 0, \quad \tilde{\beta}|0(T)\rangle = 0.$$

As we have written before, the matrix element of any operator over  $|0(T)\rangle$  equals the grand canonical average of this operator.

To find the coefficients  $u, v, f$ , we suppose that the system is in the thermal equilibrium. It means that we have to find a minimum of the grand thermodynamic potential  $F = \langle 0(T)|H - \lambda N|0(T)\rangle - TS$ . Then for  $u, v, f$  the following standard FT BCS relations are valid:

$$u^2 = \frac{1}{2} \left(1 - \frac{\lambda}{\varepsilon}\right), \quad v^2 = \frac{1}{2} \left(1 + \frac{\lambda}{\varepsilon}\right)$$

$$\varepsilon = \sqrt{\lambda^2 + \Delta^2}, \quad f = \frac{1}{1 + \exp(\varepsilon/T)}$$

In turn, the correlation function (energy gap)  $\Delta$  and the chemical potential  $\lambda$  are found from the FT BCS equations. In this approach we have in our hot system both quantal and statistical fluctuations, the quantal ones being more important at low temperature and the statistical ones at higher temperature.

As an illustrative example, we find the projected ground state energy  $E_{pr}$  and compare it with the exact result (i.e. with results obtained with the partition function of the canonical ensemble) and with the result of the FT BCS approximation.

To this aim we use formula (2), where we place the Hamiltonian  $H$  (6) instead of the operator  $Q$ .

$$E_{pr} = -G\Omega [u^2 f + v^2(1-f)]^2 - G[\Omega uv(1-2f)]^2 - 2\lambda_2 \Omega \{ [uv(1-2f)]^2 + (u^2 f + v^2(1-f))(u^2(1-f) + v^2 f) \}$$

The first two terms in the above formula is the ground state energy within the FT BCS approximation  $E_{BCS}$ , i.e.

$$E_{BCS} = -G\Omega [u^2f + v^2(1-f)]^2 - G[\Omega uv(1-2f)]^2$$

Strictly speaking this expression for  $E_{BCS}$  cannot be obtained from the standard formula of FT BCS (see, e.g. [13, 14, 11]) because it takes into account the renormalization of the  $j^-$  shell energy due to the pairing interaction. The corresponding term is proportional to  $G[u^2f + v^2(1-f)]$  and is omitted usually within the standard approach.

The calculations are performed for  $j = 13/2$  and  $n = 6$ , the constant  $G$  is adjusted so, that  $\Delta = 1$  at  $T = 0$ . The values of  $E_{BCS}$ ,  $E_{pr}$  and  $E_c$  for different  $T$  are given in table (all variables are in arbitrary units).

One can see from the table that at temperatures well below  $T \sim 0.5$  the projected energy is quite close to  $E_c$  and the projection strongly improves the result of the FT BCS approximation. With increasing  $T$ , the deviation of  $E_{pr}$  from  $E_c$  rapidly increases and at the same time the difference between  $E_{pr}$  and  $E_{BCS}$  becomes still smaller and smaller. Only at  $T \rightarrow \infty$   $E_{pr}$  again becomes equal to  $E_c$ .

The reason for this behavior of  $E_{pr}$  is the phase transition from the superconducting to the normal phase which takes place in our system at  $T = T_{cr} \simeq 0.5$  within the FT BCS approximation. As it is well known [4] and as one can see from the behavior of  $E_c$  as the function of  $T$ , the exact solution doesn't show such a phase transition. The energy  $E_c$  only sharply decreases within the temperature range  $0.3 \leq T \leq 0.7$  and then goes quite smoothly to its asymptotic value. The exact projection [4] washes out the phase transition as well. We can't avoid it with our projection method because the method is of the so called "projection after variation" type. At  $T < T_{cr}$  the quantal and thermal fluctuations introduced by the FT BCS approximation are well suppressed by our method. To calculate the projected matrix elements of operator  $H$ , we use the pairing characteristics of the system calculated from the FT BCS equations which give rapidly decreasing  $\Delta$  with  $T$  and  $\Delta = 0$  at  $T \geq T_{cr}$ . As a result,  $E_{pr}$  and  $E_{BCS}$  decrease with increasing  $T$  in the interval  $0.3 \leq T \leq T_{cr}$  faster than  $E_c$  and become constant just after  $T_{cr}$ . The coefficient  $\lambda_2$  that determines the projection correction to  $E_{BCS}$  has a stepwise discontinuity at  $T = T_{cr}$ :  $\lambda_2 = \frac{G}{4}$  at  $T < T_{cr}$  and  $\lambda_2 = -\frac{G}{2(2\Omega-1)}$  at  $T > T_{cr}$ .

The constancy of  $E_{pr}$  and  $E_{BCS}$  after the phase transition is an intrinsic feature of the model of a degenerate  $j^-$  shell. At  $T > T_{cr}$  both functions depend on temperature only through the thermal occupation number  $f$ , but, as

it follows from the above equations, if  $\Delta = 0$ ,  $f = n/2\Omega$ , i.e.  $f$  is independent of  $T$ . This phenomenon doesn't occur in more realistic systems.

At  $T > T_{cr}$  only the thermal particle number fluctuations remain in the system. From the comparison of  $E_{pr}$  and  $E_{BCS}$  it is evident that the influence of the fluctuations on the ground state energy isn't strong, the difference between these two quantities is slightly higher than 10%. An important feature of the projected energy is that its value at  $T = 0$  and  $T \rightarrow \infty$  coincides with the asymptotic value of  $E_c$  as it should be [4]. Moreover, when  $T \rightarrow \infty$ ,  $E_{pr} > E_{BCS}$ , which is also in agreement with the result of the exact number projection.

It is quite obvious from the above formulas for the ground state energy in different approximations that the qualitative results don't depend on the coupling strength  $G$  and number of particles  $n$ .

## 5 Conclusion

We formulate the approximate number projection method for hot finite systems and hope that because of its relative simplicity the method can be widely applied in the studies of hot nuclear systems to suppress the thermal fluctuations of the particle number. If pairing plays an important role in the system, the method can be used at  $T$  well below the phase transition temperature (it means that for atomic nuclei it works for  $T \leq 0.3 MeV$ ).

It is noteworthy that the method can be used in the framework of other approaches, not only within the thermo field dynamics. To do this one should calculate the ensemble average of the operators  $N^k$  and  $Q$  by any convenient method and then use formulas (4) for the  $g_k$  coefficients.

It is quite easy to extend the method to the angular momentum projection in hot nuclei or to the projection of matrix elements of an operator given in both ordinary and tilde spaces. The latter example is especially interesting for studying the giant dipole resonance  $\gamma$  decay in hot nuclei.

Of course, it is quite desirable to formulate, within the framework of TFD, a method of the "projection before variation" type but on this way one has to resolve a longstanding problem how to project the operator of entropy.

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Table

The FT BCS ground state energy  $E_{BCS}$ , the projected ground state energy  $E_{pr}$  and the exact ground state energy  $E_c$  calculated within the canonical ensemble as functions of the temperature  $T$ . ( $T, E_{pr}, E_{BCS}, E_c$  and  $T$  - in arbitrary units.)

$T$	$E_{BCS}$	$E_{pr}$	$E_c$
0	-3.840	-4.335	-4.335
0.1	-3.839	-4.334	-4.335
0.2	-3.744	-4.233	-4.327
0.3	-3.241	-3.694	-4.112
0.4	-2.151	-2.256	-3.277
0.5	-0.419	-0.670	-2.299
0.6	-0.371	-0.333	-1.665
0.7	-0.371	-0.333	-1.299
...	...	...	...
1.0	-0.371	-0.333	-0.836
...	...	...	...
1.5	-0.371	-0.333	-0.605
...	...	...	...
30.0	-0.371	-0.333	-0.343
...	...	...	...
$\infty$	-0.371	-0.333	-0.333

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