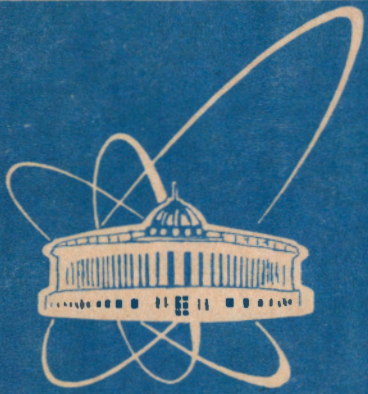

ОБЪЕДИНЕННЫЙ
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APPROXIMATE PARTICLE NUMBER PROJECTION IN HOT NUCLEI

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Приближённое проектирование по числу частиц в нагретых ядрах

Нагретые системы конечного числа частиц, каковыми являются ядра, следует описывать функцией распределения канонического ансамбля. Но из-за технических сложностей для этого чаще используют большой канонический ансамбль, в результате чего возникают погрешности, связанные с тепловыми флуктуациями числа частиц. В ядрах со спариванием к ним добавляются квантовые флуктуации числа частиц, вносимые приближенными методами типа БКШ. Т.к. точное проектирование по числу частиц трудоёмкая задача, с помощью формализма термополевой динамики разработана техника приближенного проектирования по числу частиц при $T \neq 0$, обобщающая известный метод Липкина—Ногами. Получены уравнения для коэффициентов разложения произвольного оператора по степеням оператора числа частиц и найдены их решения в следующем после БКШ приближении. Метод относится к разряду так называемых методов проектирования после варьирования. В качестве примера в его рамках исследована модель одного вырожденного уровня.

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Approximate Particle Number Projection in Hot Nuclei

Heated finite systems like, e.g., hot atomic nuclei have to be described by the canonical partition function. But this is a quite difficult technical problem and, as a rule, the grand canonical partition function is used in the studies. As a result, some shortcomings of the theoretical description appear because of the thermal fluctuations of the number of particles. Moreover, in nuclei with pairing correlations the quantal number fluctuations are introduced by some approximate methods (e.g., by the standard BCS method). The exact particle number projection is very cumbersome and an approximate number projection method for $T \neq 0$ basing on the formalism of thermofield dynamics is proposed. The idea of the Lipkin—Nogami method to perform any operator as a series in the number operator powers is used. The system of equations for the coefficients of this expansion is written and the solution of the system in the next approximation after the BCS one is obtained. The method which is of the «projection after variation» type is applied to a degenerate single j-shell model.

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

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1 Introduction

For a finite hot system like an atomic nucleus the number of particles in the system is fixed and any statistical calculations of properties of the system should be performed in the canonical ensemble. Since it is often 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. All standard approaches treating heated nuclear systems — the thermal Hartree - Fock or thermal Hartree - Fock - Bogoliubov methods, the thermal Bardeen - Cooper - Schrieffer method, the thermal RPA suffer from this shortcoming [1]. Less popular approaches have this shortcoming as well. For example in the thermo field approach [2] thermal fluctuations appear through the thermal Bogoliubov transformation.

Moreover, some methods of treating pairing correlations (BCS or HFB methods) introduce quantal fluctuations of the particle number in the finite system . These fluctuations are especially dangerous if pairing is weak, e.g., near the point of the phase transition from superconducting to normal phase.

That is why so many attempts were made to construct exact or approximate projection methods [4, 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 [6-9]. Until now the Lipkin – Nogami approximation has widely been used for approximate number projection in superconducting cold nuclei. To extend this method to finite temperature, we use the formalism of the thermo field dynamics [2].

2 The thermo field dynamics formalism

Let us assume that a hot nuclear system in the thermal equilibrium is described by the partition function of a grand canonical ensemble. The main idea behind the TFD [2] is to define a thermal vacuum $|0(T)\rangle$ such that the thermal expectation value of any operator

$$\ll A \gg = \frac{1}{Tr(exp(-H/T))} Tr[A\, exp(-H/T)]$$

equals the expectation value with respect to the thermal vacuum state

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

For this aim the TFD requires a doubling of the field degrees of freedom. The new Hilbert space of states is defined through tilde congugation rules for linear operators and by means of the 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

$$(A\tilde{B}) = \tilde{A}\tilde{B}\ ;\ (c_1 A + c_2 B)\tilde{} = c_1^* \tilde{A} + c_2^* \tilde{B}\ ,$$

where A and B stand for any operators and c_1 and c_2 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:

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

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 the particle number projection

The wave function of the thermal ground state represents the mixture of the state with a different number of particles:

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

The expectation value over the thermal vacuum corresponds to the averaging within the grand canonical ensemble. Since in atomic nuclei the number of

particles is fixed, any statistical studies of their properties should be performed in the canonical ensemble. In the TFD this means that one has to work only with the eigenfunction of the particle number operator N characterizing a certain eigenvalue n instead of averaging over wave function in the whole Hilbert space.

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

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

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

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

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

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

The elaboration of an approximate particle number projection method seems natural since the exact projection is a very hard task already in cold nuclei [11]. This approximate particle number projection method should be simple enough for practical realization as well as noticeably suppress the influence of the particle number fluctuation on calculated variables. To formulate the method, we closely followed the idea of the Lipkin-Nogami approximation [6-9] well-known in the theory of cold superfluid nuclei.

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

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

Then we obtain that

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

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

$$\langle n\tilde{n}|Q|n\tilde{n}\rangle = \langle 0(T)|Q|0(T)\rangle - \langle 0(T)|\sum_{k=0}^{\infty} q_k N^k|0(T)\rangle + \sum_{k=0}^{\infty} q_k n^k = \qquad (2)$$

$$= \langle 0(T)|Q - \sum_{k=1}^{\infty} q_k N^k|0(T)\rangle + \sum_{k=1}^{\infty} q_k n^k$$

The important point is that the above manipulation yields the expectation value of the operator Q with respect to the projected states $|n\tilde{n}\rangle$ in terms of the thermal vacuum. The use of formula (2) allows one to obtain a canonical average value $\langle n\tilde{n}|Q|n\tilde{n}\rangle$ without explicit involving $|n\tilde{n}\rangle$. But the coefficients q_k are still unknown. To find them let us introduce the operator

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

The following relation takes place for the operator Q and any arbitrary function of the particle number operator $f(N)$:

$$\langle 0(T)|Qf(N)|0(T)\rangle = \langle 0(T)|Q|0(T)\rangle\langle 0(T)|f(N)|0(T)\rangle$$

The above-mentioned equation is satisfied for any arbitrary function $f(N)$ then and only then if the following set of equations is valid:

$$\langle 0(T)|QN|0(T)\rangle = \langle 0(T)|Q|0(T)\rangle\langle 0(T)|N|0(T)\rangle$$
$$\langle 0(T)|QN^2|0(T)\rangle = \langle 0(T)|Q|0(T)\rangle\langle 0(T)|N^2|0(T)\rangle$$
$$\ldots.$$
$$\langle 0(T)|QN^m|0(T)\rangle = \langle 0(T)|Q|0(T)\rangle\langle 0(T)|N^m|0(T)\rangle$$
$$\ldots.$$

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

$$\begin{pmatrix} \langle QN\rangle - \langle Q\rangle\langle N\rangle \\ \langle QN^2\rangle - \langle Q\rangle\langle N^2\rangle \\ .... \\ \langle QN^m\rangle - \langle Q\rangle\langle N^m\rangle \\ .... \end{pmatrix} = A \begin{pmatrix} q_1 \\ q_2 \\ .... \\ q_m \\ .... \end{pmatrix} \tag{3}$$

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 $\langle ...\rangle$ means averaging over the thermal vacuum $|0(T)\rangle$.

So far our considerations were exact. But for practical calculations one has to truncate expansion (1) by retaining the first 3 terms (the usual Lipkin-Nogami approximation [6-9]). In this case, one can derive for the coefficients q_1 and q_2 the following expressions:

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

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

where

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

Noteworthy that there is another method of determining the coefficients q_k, which is more proper to the project operator Q of complicated structure. The use of expansion (1) allows one to get for q_k the following relation:

$$q_k = \frac{1}{k!}\frac{d^k q(n)}{dn^k}\bigg|_{n=0} \tag{5}$$

4 The degenerate single j-shell model

Let us consider the case of n nucleons with the BCS Hamiltonian on the single $j-$ shell. There is no essential difference between this and more general case where there are several degenerate $j-$levels with different j's. Place the energy $E_j = 0$. In this case the Hamiltonian is

$$H = -\frac{G}{4}\sum_{mm'} a^+_m a^+_{\overline{m}} a_{\overline{m'}} a_{m'} \tag{6}$$

Following the prescriptions of TFD we introduce temperature. The Hamiltonian of a hot system is the thermal Hamiltonian $\mathcal{H} = H - \tilde{H}$. It is possible to diagonalize the thermal Hamiltonian by means of the so-called thermofield transformation [12, 13]. This transformation is constructed as two successive Bogoliubov transformations: the standard canonical $\{u, v\}$ transformation and the thermal $\{\sqrt{n}, \sqrt{1-n}\}$ one.

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

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

With the thermofield transformation one gets the temperature dependent ground state $|0(T)\rangle$ as a vacuum for thermal quasiparticles β and $\tilde{\beta}$:

$$\beta|0(T)\rangle = 0$$

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

The matrix element over thermal vacuum $|0(T)\rangle$ equals its grand canonical average.

To choose the coefficients u, v, n, we use the conditions for nuclei to be in the thermal equilibrium. It means that we have to find minimum of the grand thermodynamic potential $F = \langle 0(T)|H - \lambda N|0(T)\rangle - TS$. For u, v, n the following standard FT BCS relations are valid:

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

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

In its turn the correlation function Δ and chemical potential λ are found from FT BCS equations. In this case, we have both quantal and statistical fluctuations, the quantal one 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}. To this aim, we assume that the thermal ground state is a vacuum for the thermal quasiparticles $\beta, \tilde{\beta}$ and use formula (2), where we place Hamiltonian H instead of the operator Q

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

$$-2\lambda_2\Omega\left\{[uv(1-2n)]^2 + (u^2 n + v^2(1-n))(u^2(1-n) + v^2 n)\right\}$$

The coefficient $\lambda_2 = \frac{G}{4}$ at $T < T_{cr}$ (T_{cr} is the critical temperature when the phase transition from superfluid to normal nuclei takes place), and $\lambda_2 = -\frac{G}{2(2\Omega-1)}$ at $T > T_{cr}$. 2Ω is the degeneration of the $j-$ level.

In the table we display the projected energy E_{pr} and BCS energy E_{BCS} (in arbitrary units) as the functions of the temperature T (also in arbitrary units). The calculations have been performed for $j = 13/2$ and the constant G is adjusted in such a way, that $\Delta = 1$ at $T = 0$.

At $T \leq 0.5$ not only the thermal but also the quantal number fluctuations are suppressed by the projection. Both the functions $E_{pr}(T)$ and $E_{BCS}(T)$ increase rapidly with temperature because the correlation function Δ decreases with T. At $T \sim 0.5$ the correlation function vanishes (the system isn't any more superconducting) and both functions change their behaviour sharply. At this point the quantal fluctuations disappear and only the thermal ones exist.

5 Conclusion

The above formulated approximate number projection method for hot finite systems is of the "projection after variation" type. It means that at the first stage we solve a variational problem with a "nonperfect" trial function and only then the number projection of matrix elements of some operator is performed. One hopes that because of its relative simplicity the method can be widely applied in the studies of hot nuclear systems. Noteworthy that the method can be used in the framework of other approaches not only within the thermo field dynamics. One can calculate the ensemble average of the

operators N^k and Q by any convenient method and then use formulas (4) for the q^k coefficients.

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

But our method can not be explored to study the phase transitions in hot nuclei. To this end one has to use the "projection before variation" method like it has been done within the static path approximation [4] or to make directly a projection between statistical ensembles [14]. A method of this type can be formulated within the thermofield dynamics too but on this way one has to resolve a longstanding problem how to project the operator of entropy.

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Table 1

The total projected energy E_{pr} and the FTBCS ground state energy E_{BCS} as a function of the temperature. T, E_{pr}, E_{BCS} in arbitrary units.

T	E_{BCS}	E_{pr}
0	-3.840	-4.335
0.1	-3.839	-4.334
0.2	-3.744	-4.233
0.3	-3.241	-3.694
0.4	-2.151	-2.256
0.5	-0.419	-0.670
0.6	-0.371	-0.333
0.7	-0.371	-0.333
∞	-0.371	-0.333

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