ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E4-96-7

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SELF-CONSISTENT RPA IN HOT FINITE FERMION SYSTEMS

Submitted to «Physical Review E»

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1996

1 Introduction

Tools to deal with many-body fermionic systems at finite temperature were developed long ago for applications to large samples like solid crystals, magnetic materials, quantum liquids, etc. The thermal perturbation theory, thermal Green function method, random phase approximation (RPA), functional methods and many others are presented in the textbooks [1, 2]. The mathematical accuracy of all these approaches is based to a certain extend on the thermodynamic limit. Actually, these methods are widely applied to finite fermionic systems like hot nuclei [3] with temperatures of an order of several Mev's and also to the metal clusters [4, 5] produced by hot molecular beams of low-point-boiling metals. There are many differences between these two physical objects, but also some similarities could be shown like the shell structure, deformation, collective excitations (especially, giant resonances). However, for the finite systems the fluctuations around the most probable values of physical variables are significant. Thermodynamic limit does not exist. Therefore, well-known statistical methods as applied to the finite systems have to be treated with special care.

In this paper, we consider N fermions in statistical equilibrium ($T = const$) interacting via two-body forces. The RPA for a system of that sort is reexamined as a quasiboson approximation. In comparison with other works treating the same problem [6-8] the following aspects of the present approach have to been underlined:

- Self-consistent mean field depends on the temperature from the very beginning
- This mean field depends also on the parameters describing the collective vibrations
- The Pauli principle is included into the formalism in a more proper way than in the usual RPA approach. The commutation rules between operators take their fermionic structure into account [9].

All calculations are performed within the thermo field dynamics (TFD) [10] approach. These calculations are equivalent to the minimization of the grand canonical potential (the condition for a system to be in statistical equilibrium) but look more compact and convenient. In sect. 2, basic equations for thermal self-consistent RPA are derived. Sect. 3 provides a summary and discussion.

2 Derivation of basic equations

We assume only the two-body interaction and thus we write the N-body Hamiltonian as

$$H = \sum_{12} t_{12} a_1^+ a_2 + \frac{1}{4} \sum_{1234} V_{1234} a_1^+ a_2^+ a_4 a_3 \ , \tag{1}$$

where a^+, a are fermion creation and annihilation operators,

$$t_{12} = T_{12} - \lambda \delta_{12}$$

λ is the chemical potential, T_{12} is the kinetic energy matrix.

Using the Wick theorem one can expand the Hamiltonian (1) in normal order (: ... :) with respect to the temperature dependent ground state $|\Psi(T)\rangle$ and obtain for one- and two-body operators the following expressions:

$$a_1^+ a_2 = \langle a_1^+ a_2 \rangle + : a_1^+ a_2 :$$

$$a_1^+ a_2^+ a_4 a_3 = \langle a_1^+ a_3 \rangle \langle a_2^+ a_4 \rangle - \langle a_1^+ a_4 \rangle \langle a_2^+ a_3 \rangle - \langle a_1^+ a_4 \rangle : a_2^+ a_3 : +$$

$$\langle a_1^+ a_3 \rangle : a_2^+ a_4 : + \langle a_2^+ a_4 \rangle : a_1^+ a_3 : - \langle a_2^+ a_3 \rangle : a_1^+ a_4 : + : a_1^+ a_2^+ a_4 a_3 : \ .$$

We denote

$$\rho_{ij} = \langle a_j^+ a_i \rangle \ . \tag{2}$$

where $\langle ... \rangle$ is the statistical average. In the TFD the thermal expectation value corresponds to the expectation value with respect to the temperature dependent ground state $|\Psi(T)\rangle$.

We can write

$$a_i^+ a_j = \rho_{ji} + : a_i^+ a_j :$$

$$a_1^+ a_2^+ a_4 a_3 = \rho_{31} \rho_{42} - \rho_{41} \rho_{32} - \rho_{41} : a_2^+ a_3 : +$$

$$\rho_{31} : a_2^+ a_4 : + \rho_{42} : a_1^+ a_3 : - \rho_{32} : a_1^+ a_4 : + : a_1^+ a_2^+ a_4 a_3 : \ .$$

The Hamiltonian looks like

$$H = h_0 + h_{11} + h_{22} \ ,$$

where

$$h_0 = \sum_{12} t_{12} \rho_{21} + \frac{1}{2} \sum_{1234} V_{1234} \rho_{31} \rho_{42} \ ,$$

$$h_{11} =: \sum_{12} t_{12} a_1^+ a_2 + \sum_{1234} \rho_{42} a_1^+ a_3 : \ ,$$

$$h_{22} =: \frac{1}{4} \sum_{1234} V_{1234} a_1^+ a_2^+ a_4 a_3 : \ .$$

To diagonalize the h_{11}-part of Hamiltonian quadratic in a^+, a operators, one has to perform the unitary transformation:

$$a_l^+ = \sum_k D_{lk}^* \alpha_k^+ \ ,$$

$$a_l = \sum_k D_{lk} \alpha_k \ ,$$

where $DD^+ = D^+ D = I$, and α^+, α are new fermionic operators. The result of this transformation is the following:

$$h_{11} =: \sum_{kk'} \left[\sum_{12} t_{12} D_{1k}^* D_{2k'} \right] \alpha_k^+ \alpha_{k'} + \sum_{kk'} \left[\sum_{1234} V_{1234} \rho_{42} D_{1k}^* D_{2k'} \right] \alpha_k^+ \alpha_{k'} : \ . \tag{3}$$

If we require h_{11} (3) to be diagonal we obtain the following system of equations for the matrix D elements and for the single-particle energy ε_1:

$$\sum_2 \left(t_{12} + \sum_{34} V_{1324} \rho_{43} \right) D_{25} = \varepsilon_5 D_{15} \tag{4}$$

with the auxiliary condition (conservation of the average number of particles)

$$\sum_1 \rho_{11} = N \ . \tag{5}$$

At this stage of calculations, the structure of the matrix ρ cannot be given explicitly because $|\Psi(T)\rangle$ is still unknown. It is clear, that the omission of the residual interaction:

$$h_{22} = 0$$

leads to the standard temperature dependent Hartre-Fock (HF) theory. The term h_{22} transformed to the α^+, α quasiparticle basis has the form :

$$h_{22} =: \frac{1}{4} \sum_{1234} U_{1234} \alpha_1^+ \alpha_2^+ \alpha_4 \alpha_3 : ,$$

where

$$U_{ijkl} = \sum_{1234} V_{1234} D^*_{1i} D^*_{2j} D_{3k} D_{4l} \, . \tag{6}$$

It is simple to prove that the matrix U possesses the same symmetries as the interaction matrix V.

Following the TFD methods [10] we take into account the thermal degrees of freedom by doubling the dimension of the initial Hilbert space. In the whole space the operator (thermal Hamiltonian)

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

is considered. The properties of the system could be obtained by diagonalisation of this thermal Hamiltonian $\mathcal{H}$. Therefore,

$$\mathcal{H} =: \sum_1 \varepsilon_1 (\alpha_1^+ \alpha_1 - \tilde{\alpha}_1^+ \tilde{\alpha}_1) + \frac{1}{4} \sum_{1234} U_{1234} (\alpha_1^+ \alpha_2^+ \alpha_4 \alpha_3 - \tilde{\alpha}_1^+ \tilde{\alpha}_2^+ \tilde{\alpha}_4 \tilde{\alpha}_3) : \, . \tag{7}$$

To consider the collective excitation modes of the system, it is convenient to use a new temperature dependent Fock space. This space is produced by action of the thermal quasiparticle creation operators $\beta^+, \tilde{\beta}^+$ on the corresponding thermal vacuum $|O(T)\rangle$ [11, 12]

$$\alpha_i = x_i \beta_i + y_i \tilde{\beta}_i^+ \, ,$$
$$\alpha_i^+ = x_i \beta_i^+ + y_i \tilde{\beta}_i \, , \tag{8}$$

where

$$x_i = \sqrt{1 - n_i} \qquad y_i = \sqrt{n_i} \, ,$$
$$n_i = \frac{1}{1 + \exp(\frac{\varepsilon_i}{T})} \, ,$$

and ε_i are solutions of the system of equations (14),

$$\beta_i |O(T)\rangle = \tilde{\beta}_i |O(T)\rangle = 0 \, . \tag{9}$$

The thermal Hamiltonian (7) can be transformed to the thermal quasiparticle basis (8). The structure $\mathcal{H}$ as $\mathcal{H}(\beta^+, \beta, \tilde{\beta}^+, \tilde{\beta})$ (see App. A) prompts the structure of the collective excitations. Namely, the operators

$$A_{12}^+ = \beta_1^+ \tilde{\beta}_2^+ \quad , \quad A_{12} = \tilde{\beta}_2 \beta_1$$

can be exploited as the building blocks to construct the excitation wave functions of the system.

The main approximations of the present approach are:

1. To take, from the r.h.s. of the exact commutator
$$\left[A_{12}, A_{34}^+\right] == \delta_{13}\delta_{24} - \delta_{13}\tilde{\beta}_4^+ \tilde{\beta}_2^+ - \delta_{24}\beta_3^+ \beta_1 \, ,$$
only c-numbers [9, 13, 14]. Thus one assumes that
$$\left[A_{12}, A_{34}^+\right] = \delta_{13}\delta_{24} (1 - q_1 - q_2) \, ,$$
where
$$\langle \beta_1^+ \beta_2 \rangle = \langle \tilde{\beta}_1^+ \tilde{\beta}_2 \rangle = \delta_{12} q_1 \, ; \tag{10}$$
2. To choose a certain structure of the thermal ground state for the whole Hamiltonian (the intrinsic structure of this vector will be described below) by neglecting the anharmonic terms in $\mathcal{H}$.

The substitution [9, 13, 14]

$$b_{12} = \frac{A_{12}}{\sqrt{1 - q_{12}}} \quad , \quad b_{12}^+ = \frac{A_{12}^+}{\sqrt{1 - q_{12}}} \, , \tag{11}$$

where

$$q_{12} = q_1 + q_2$$

leads to the following commutation rule

$$\left[b_{12}, b_{34}^+\right] = \delta_{13}\delta_{24} \, ;$$

i.e. b_{ij}, b_{ij}^+ are pure boson operators.

The harmonic part of the thermal Hamiltonian $\mathcal{H}$ is a form quadratic in the b_{ik}^+, b_{ik} operators (see App. A), which can be exactly diagonalised by the bosonic Bogoliubov transformation:

$$b_{12}^+ = \sum_\nu \psi_{12}^\nu Q_\nu^+ + \phi_{12}^+ Q_\nu \, ,$$
$$b_{12} = \sum_\nu \psi_{12}^\nu Q_\nu + \phi_{12}^\nu Q_\nu^+ \, ,$$

with the unitary conditions

$$\sum_{12} \psi_{12}^\nu \psi_{12}^\mu - \phi_{12}^\nu \phi_{12}^\mu = \delta_{\nu\mu} \tag{12}$$

Now, the structure of the approximate thermal vacuum state can be required as the solution of the following equation:

$$Q_\nu |\Psi(T)\rangle = 0 \, .$$

The equation of motion for the Q_ν^+ operators

$$[\mathcal{H}, Q_\nu^+] = \omega_\nu Q_\nu^+ \qquad (13)$$

allows one to get the system of equations for the amplitudes $\psi_{12}^\nu, \phi_{12}^\nu$ and frequencies ω_ν (see App. B).

$$\varepsilon_{24}\frac{\phi_{42}^\nu}{y_2x_4} + \frac{1}{2}\sum_{13} U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}(n_1-n_2)\frac{\phi_{13}^\nu}{y_3x_1} = \omega_\nu\frac{\phi_{42}^\nu}{y_2x_4} \qquad (14)$$

where

$$\varepsilon_{12} = \varepsilon_1 - \varepsilon_2 \quad , \quad \psi_{24}^\nu = -\frac{x_2y_4}{x_4y_2}\phi_{42}^\nu$$

Difference between (14) and the standard thermal RPA [7, 8] is due to the existence of the $\sqrt{1-q_{13}}$, $\sqrt{1-q_{24}}$ — blocking factors connected with the Pauli repulsion.The matrix U depends on the HF transformation matrix D.

To couple equations (14) to the equations for the optimal mean field, one has to calculate the single particle density matrix ρ_{ij}, when the structure of the $|\Psi(T)\rangle$ state is known [9].

$$\rho_{12} = \langle\Psi(T)|a_2^+a_1|\Psi(T)\rangle = \sum_k D_{2k}^* D_{1k}(x_k^2 q_k + y_k^2(1-q_k)) \qquad (15)$$

where the thermal quasiparticle occupation numbers are given by (see App.C):

$$q_i = \sum_{\nu k} [\phi_{ik}^\nu]^2 \qquad (16)$$

The whole solution of the self-consistent thermal RPA problem may be gathered as the following coupled system of equations:

$$\sum_2 \left(t_{12} + \sum_{34} V_{1324}\rho_{42}\right) D_{25} = \varepsilon_5 D_{15} , \qquad (4')$$

$$\sum_1 \rho_{11} = N , \qquad (5')$$

$$\varepsilon_{24}\frac{\phi_{42}^\nu}{y_2x_4} + \frac{1}{2}\sum_{13} U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}(n_1-n_2)\frac{\phi_{13}^\nu}{y_3x_1} = \omega_\nu\frac{\phi_{42}^\nu}{y_2x_4} , \qquad (14')$$

$$q_i = \sum_{\nu k} [\phi_{ik}^\nu]^2 , \qquad (16')$$

where ρ_{12} is given by formula (15) and U_{1234} depends on the interaction matrix and the element of D-matrix (17)

3 Summary

The problem of unified description of the single-particle and collective excitations of a hot finite fermion system has been solved as general as possible within the harmonic approximation. The advantage of the present method consists in:

- the interplay between single-particle and collective (phonon) excitation branches of the system is seen;
- this method allows one to understand the role of the Pauli principle in hot finite fermionic systems;
- intrinsic structure of the thermal collective states is treated more accurately by taking the fermionic origin of the bosonic operators into account [9].

Under the standard thermal RPA assumption that the numbers of virtual thermal quasiparticles in the thermal ground state vanish (i.e. all $q_i = 0$), one can decouple the system of equation ($4', 5', 14', 16'$) as two independent systems: the first, describing thermal a mean field in the HF approximation and the second describing collective excitations in the usual thermal RPA.

The model calculations to illustrate the results of the present article are in preparation. The discussions with A.V. Avdeenkov and Prof. A.I. Vdovin are acknowledged. This work was partially supported by the Russian Foundation for Basic Research (grant 95-02-05701) (D.S.K) and by polish grant KBN No2 P302 01804 (W.N.)

Appendix A

The thermal Hamiltonian (7)

$$\mathcal{H}=:\sum_1 \varepsilon_1(\alpha_1^+\alpha_1-\tilde{\alpha}_1^+\tilde{\alpha}_1)+\frac{1}{4}\sum_{1234}U_{1234}(\alpha_1^+\alpha_2^+\alpha_4\alpha_3-\tilde{\alpha}_1^+\tilde{\alpha}_2^+\tilde{\alpha}_4\tilde{\alpha}_3):=$$

$$=:\sum_1 \varepsilon_1(\alpha_1^+\alpha_1-\tilde{\alpha}_1^+\tilde{\alpha}_1)+\frac{1}{4}\sum_{1234}U_{1234}(\alpha_1^+\alpha_3\alpha_2^+\alpha_4-\tilde{\alpha}_1^+\tilde{\alpha}_3\tilde{\alpha}_2^+\tilde{\alpha}_4):$$

can be expressed in thermal quasiparticles (8):

$$\alpha_i=x_i\beta_i+y_i\tilde{\beta}_i^+ ,$$

$$\alpha_i^+=x_i\beta_i^+ +y_i\tilde{\beta}_i .$$

The term bilinear in quasiparticles looks like:

$$\alpha_1^+\alpha_3=x_1x_3\beta_1^+\beta_3+x_1y_3\beta_1^+\tilde{\beta}_3^+y_1x_3\tilde{\beta}_1\beta_3+y_1y_3\tilde{\beta}_1\tilde{\beta}_3^+$$

By omiting the anharmonic terms in the thermal Hamiltonian one can obtain:

$$\mathcal{H}\simeq:\sum_1\varepsilon_i(\beta_1^+\beta_1-\tilde{\beta}_1^+\tilde{\beta}_1)+$$

$$+\frac{1}{4}\sum_{1234}U_{1234}\left((x_1y_3\beta_1^+\tilde{\beta}_3^+ +y_1x_3\tilde{\beta}_1\beta_3)(x_2y_4\beta_2^+\tilde{\beta}_4^+ +y_2x_4\tilde{\beta}_2\beta_4)-(t.c.)\right):$$

where $(t.c.)$ means the tilde conjugation operation [10]. Now the Bose operators b_{ik}^+ and b_{ik} are defined via eqs. (28). One can easily check that two-fermion terms $\beta^+\beta$ and $\tilde{\beta}^+\tilde{\beta}$ satisfy the same commutation rules as their boson images:

$$\beta_i^+\beta_i=\sum_k b_{ik}^+b_{ik} \qquad , \qquad \tilde{\beta}_i^+\tilde{\beta}_i=\sum_k b_{ki}^+b_{ki} . \qquad (A1)$$

Finally, the harmonic part of the thermal Hamiltonian has the form:

$$\mathcal{H}=\sum_{12}\varepsilon_{12}b_{12}^+b_{12}+$$

$$+\frac{1}{4}\sum_{1234}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}\left[(x_1y_3b_{13}^+ +y_1x_3b_{31})(x_2y_4b_{24}^+ +y_2x_4b_{42})-\right.$$

$$\left.-(x_1y_3b_{31}^+ +y_1x_3b_{13})(x_2y_4b_{42}^+ +y_2x_4b_{24})\right] .$$

where

$$\varepsilon_{12}=\varepsilon_1-\varepsilon_2$$

Appendix B

The system of equations for the collective amplitudes results from the equation of motion (13) for the Bose operators. The amplitudes ψ, ϕ and friequencies ω obey the equations

$$\varepsilon_{24}\psi_{24}^\nu+\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}x_2y_4(x_1y_3\phi_{13}^\nu+y_1x_3\psi_{31}^\nu)-$$

$$-\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}x_4y_2(x_3y_1\phi_{13}^\nu+y_3x_1\psi_{31}^\nu)=\omega_\nu\psi_{24}^\nu ,$$

$$\varepsilon_{42}\phi_{42}^\nu+\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}x_4y_2(x_1y_3\phi_{13}^\nu+y_1x_3\psi_{31}^\nu)-$$

$$-\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}x_2y_4(x_3y_1\phi_{13}^\nu+y_3x_1\psi_{31}^\nu)=-\omega_\nu\phi_{42}^\nu .$$

The linear transformations of this system give rise to the following system:

$$\varepsilon_{24}X_{24}^\nu+\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}(n_1-n_3)X_{31}^\nu=\omega_\nu X_{24}^\nu ,$$

$$\varepsilon_{24}Y_{24}^\nu+\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}(n_1-n_3)Y_{31}^\nu=\omega_\nu Y_{24}^\nu ,$$

where

$$X_{24}^\nu=\frac{1}{x_2y_4+y_2x_4}(\psi_{24}^\nu-\phi_{42}^\nu) \qquad , \qquad Y_{24}^\nu=\frac{1}{x_2y_4-y_2x_4}(\psi_{24}^\nu+\phi_{42}^\nu)$$

The last two equations are uncoupled. Therefore one can put that

$$X_{24}^\nu=Y_{24}^\nu ,$$

and finally, the phonon amplitudes and frequencies are the solution of the following equations:

$$\varepsilon_{24}\frac{\phi_{42}^\nu}{y_2x_4}+\frac{1}{2}\sum_{13}U_{1234}\sqrt{1-q_{13}}\sqrt{1-q_{24}}(n_1-n_2)\frac{\phi_{13}^\nu}{y_3x_1}=\omega_\nu\frac{\phi_{42}^\nu}{y_2x_4} ,$$

$$\psi_{24}^\nu=-\frac{x_2y_4}{x_4y_2}\phi_{42}^\nu .$$

Appendix C

The thermal quasiparticle occupation numbers (10):

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

can be expressed in termes of the bosonic termal averages by using (A1) formulae. It means that

$$\langle\Psi(T)|\tilde{\beta}_i^+\tilde{\beta}_i|\Psi(T)\rangle = \langle\Psi(T)|\sum_k b_{ik}^+ b_{ik}|\Psi(T)\rangle$$

Substituting b_{ik}, b_{ik}^+ by the Q_ν^+, Q_ν and using the conditions

$$Q_\nu|\Psi(T)\rangle = 0$$

one obtain simply [9] that

$$q_i = \sum_{\nu k}[\phi_{ik}^\nu]^2 \ .$$

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Received by Publishing Department
on January 11, 1995.