

Superoperator Approach to the Theory of Hot Nuclei and Astrophysical Applications: I—Spectral Properties of Hot Nuclei

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Abstract—The method of superoperators in Liouville space was applied to study spectral properties of hot nuclei. It is shown that properly defined fermionic superoperators allow us to generalize the equation-of-motion method to hot nuclei. Within the superoperator approach, for the nuclear model with separable particle–hole residual interaction of Landau–Migdal type, we derived the equations of thermal quasiparticle random phase approximation, which allow the spectral densities and strength functions of charge-exchange and charge-neutral excitations of hot nuclei to be calculated in a thermodynamically consistent way, i.e., without violating the principle of detailed balance. For the quasiparticle-phonon nuclear model, a thermodynamically consistent way is proposed for going beyond the random phase approximation by considering the interaction of thermal phonons. Using the Donnelly–Walecka method and the superoperator approach, expressions for cross sections of semileptonic weak reactions with hot nuclei are obtained.

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1. INTRODUCTION

Properties of hot nuclei, in which the excitation energy is uniformly redistributed over many degrees of freedom, have been the subject of active experimental and theoretical research for four decades now. Despite the fact that atomic nuclei are isolated systems with a relatively small number of nucleons, the concept of nuclear temperature has been used since the mid-1930s, when thermodynamic methods were applied to the statistical description of the formation and decay of compound nuclei [1–4]¹. However, it was not until the early 1980s that the improvement of heavy ion accelerators made it possible to obtain hot nuclei with a temperature of $T \lesssim 5$ MeV (0.862 MeV $\approx 10^{10}$ K or 1 MeV $\approx 11.6T_9$, where $T_9 = 10^9$ K) [6, 9]. Since then, the experimental and theoretical study of hot nuclei has been an important source of information about the properties of atomic nuclei and nuclear matter in extreme states [10].

The study of hot nuclei has become especially important for the physics of giant resonances (GRs). The discovery of an isovector giant dipole resonance (GDR) built on highly excited ($E \sim 100$ MeV) states [11] has set the stage for systematic studies of collective motion in hot nuclei. To date, the extensive material has been accumulated on the GDR properties in hot

nuclei (see references in [10, 12–15]). It was experimentally found that the energy of the GDR maximum, as well as the degree of depletion of the energy-weighted sum rule, weakly depend on the nucleus excitation energy, while the GDR width increases with temperature up to a certain limit. The latter circumstance indicates a violation of the Brink–Axel hypothesis (BAH) [16, 17] on the independence of the strength function of the resonance on the energy of the excited state.

The theoretical description of the strength function of multipole resonances in hot nuclei, as a rule, is based on the temperature generalization of the methods and approximations used for cold nuclei. To date, most calculations in this area are based either on the linear response theory or on the Green’s function method and are limited by the thermal random phase approximation (TRPA) [18, 19] and its various improvements, which allow considering the effect of pairing correlations [20, 21], the presence of a single-particle continuum [22], or simultaneously both [23, 24]. The use of Skyrme forces and relativistic forces makes it possible to perform self-consistent TRPA calculations [21, 19].

The possibility of using Feynman’s diagram technique for Matsubara Green’s functions [25] has made them the main tool for temperature generalization of methods that go beyond the random phase approximation. For hot nuclei, this generalization took place in the context of the nuclear field theory [26] and the Theory of Finite Fermi Systems [27, 28]. Another

¹ The problem of the limits of applicability of the thermodynamic approach to describing the properties of atomic nuclei and the methods for determining the nucleus temperature are considered in many works (see, e.g., [5–8]).

approach to the study of hot nuclei, using the formalism of Matsubara Green's functions and the so-called time-blocking approximation [29], has recently been intensively developed in [30–32]. The fundamental problem, which these studies seek to solve, is to elucidate how the damping of collective excitations in hot nuclei works, in particular, to learn how to calculate for $T \neq 0$ the interaction of simple and complex configurations, which is responsible for the fragmentation of the strength of resonances, i.e., their width, in cold nuclei. Despite progress in this area, the problem of describing the GDR width in hot nuclei has not been completely solved to date. So, a comparison of the theoretical and experimental GDR widths in $^{120,132}\text{Sn}$, given in [32], showed that, in a certain temperature range, in order to correctly describe the GDR width, in addition to the interaction of simple and complex configurations, it is necessary to consider other factors, such as nucleus deformation and a fluctuation in its shape.

In addition to the temperature Green's functions, there are other statistical approaches that can be used to study the properties of hot systems. One such approach is thermofield dynamics (TFD) [33], which has become widely used in condensed matter theory [34]. Compared with the method of Matsubara Green's functions, TFD has a number of advantages that make its formalism convenient in practical terms. In particular, time and temperature in TFD are independent variables, and therefore, for studying the time-dependent processes, there is no need to use the procedure of analytic continuation in the complex time plane. Due to this property, using TFD, it is quite easy to study the spectral characteristics of hot systems, i.e., the energy of excited states and a response to an external disturbance (strength functions and spectral densities). In addition, all those working tools that are used with $T = 0$ are available in TFD, namely: the method of canonical transformations, Wick's theorem, the concept of a vacuum state, etc., which is convenient for constructing various approximations. The listed advantages are a consequence of the special operator structure of the TFD, which arises because of doubling the degrees of freedom of the hot system due to the introduction of its fictitious copy.

Despite the above advantages and the fact that the TFD main provisions were formulated in the mid-1970s, this formalism has not gained wide acceptance in the theory of hot nuclei. With the exception of our works, the number of publications in which TFD was used to study the properties of hot nuclei is very limited (see references [6–19] in our work [35]). There are two reasons for this, in our opinion. The first reason is the meaning of the additional degrees of freedom (associated with a fictitious system), which was not completely understood. In the TFD original version [33], the fictitious system introduction was considered as a convenient formal technique that allows the statistical average of an arbitrary operator to be

expressed as an average over a specially constructed thermal vacuum. Later, the fictitious system began to be interpreted as hole states, which are present due to the interaction of the system with the thermal bath [34]. This explanation, however, does little to justify the correspondence rules between operators acting in the state space of the original physical system and operators acting in the state space of the fictitious system. In TFD, this correspondence is *postulated* in the form of tilde-conjugation rules.

A mathematically rigorous interpretation of the thermal vacuum and fictitious system was obtained within the method of superoperators, i.e., operators in the Liouville space [36]. Adequate correspondence was shown between the thermal vacuum and an operator of the hot system density matrix, while the doubling of the degrees of freedom was justified as a consequence of the use of two sets of operators in Liouville space: the first one acts on the density matrix on the left, and the second, on the right. Although the viewpoint of superoperator method on thermofield dynamics later became widespread along with the C^* -algebraic approach [37] (see also [38]), this, nevertheless, did not contribute to the wide application of the superoperator method to the study of the hot nuclei properties. An obstacle in this direction is the second of the above reasons, namely the complexity of the so-called thermal state condition, which relates the action of the left and right superoperators on the thermal vacuum and, in fact, determines the system temperature. Both in TFD [33] and in the version of the superoperator method in [36] for fermionic systems, this relation is nontrivial and in a complex way depends on the structure of superoperators. Therefore, in our opinion, the generalization of methods that are used to study properties of the ground and excited states of cold nuclei has not received the due development for the case of hot nuclei. In particular, within the method of superoperators, the temperature analog of the equation of motion method [39–41] was not formulated, using which in a thermodynamically consistent manner, i.e., without violating the principle of detailed balance², the response of a hot nucleus to an external disturbance could be calculated.

Thus, it is of great interest to generalize the superoperator method in such a way as to make the theoretical description of spectral characteristics of hot nuclei, on the one hand, not much different from the calculations for cold nuclei, and, on the other hand, to ensure it to be thermodynamically consistent in the above sense. It turned out that this generalization is possible if the fermionic superoperators are defined in the same way as was done in the works by one of the

² In the case of a self-adjoint operator $\mathcal{J} = \mathcal{J}^\dagger$, the principle of detailed balance relates the excitation and deexcitation rates of hot systems, $S_{\mathcal{J}}(-E, T) = e^{-E/T} S_{\mathcal{J}}(E, T)$.

authors on studying the electron transport through correlated quantum systems [42–46].

As already noted, the presence of a large amount of experimental data has made the GDR thermal properties the main object of study in the theory of hot nuclei. However, from the viewpoint of astrophysical applications, the temperature properties of other modes of nuclear excitations, in particular, charge-exchange and charge-neutral Gamow–Teller (GT) resonances, are of considerable interest. It is known that GT transitions dominate in many nuclear reactions caused by the weak interaction and playing an important role at the late stage of the evolution of massive stars and the explosion of supernovae [47–49]. Among these reactions are the capture of electrons and neutrinos by atomic nuclei, β decay, scattering of neutrinos, etc. The astrophysical manifestations of the listed weak reactions include the initiation of the gravitational collapse of the massive star core, the neutronization of matter during the collapse, the neutrino trapping at high densities, the energy transfer by neutrino radiation and the neutrino heating of the shock wave, as well as the synthesis of heavy elements at the final stage of the explosion. In addition, weak reactions with nuclei affect the neutrino spectrum, which reflects the processes occurring in the interior of a star and is therefore important for verification of various models of explosion. The rates and cross sections of various weak nuclear reactions are used as input data for computer simulations of supernovae [50].

The temperature of the medium in which weak reactions occur in stars varies from hundreds of keV to several MeV at the final stage of collapse. As was shown by Hoyle [51], under conditions of a dense matter of a star, a fairly rapid exchange of energy occurs between matter and γ quanta, as a result of which a thermodynamic equilibrium is established between atomic nuclei and electromagnetic radiation. Actually, it is in the hot matter of a star that atomic nuclei can be considered as hot quantum systems, since the electromagnetic radiation acts as an external macroscopic thermal bath, upon interaction with which the nuclei heat up, that is, their excited levels are thermally populated according to the Boltzmann distribution.

The thermal population of nuclear levels can significantly affect the behavior of weak nuclear reactions, as well as the spectrum of neutrinos produced. So, for charge-exchange reactions (capture of an electron or neutrino), the reaction threshold, associated with the mass difference between the parent and daughter nuclei, decreases or completely disappears. In addition, exothermic processes become possible, in which the energy of the excited nucleus is transferred to the outgoing lepton. All this leads to an increase in cross sections and reaction rates. The influence of temperature effects on the course of explosive nucleosynthesis of heavy and superheavy nuclei in supernovae is discussed [52]. It is important to emphasize that

the results of computer simulations of supernovae largely depend on the input data on weak nuclear reactions used [53–61]. Therefore, it would not be a big exaggeration to say that the sensitivity of the results of supernova simulations to data on weak nuclear reactions largely means the sensitivity to the properties of hot nuclei.

From a microscopic viewpoint, there are two approaches to calculating the contribution of GT transitions to the cross sections and rates of weak reactions with hot nuclei. The first one involves the Boltzmann averaging of the contributions from thermally excited nuclear states. This requires knowledge of the strength function of GT transitions for both the ground and excited nuclear states. To date, this approach has been most fully implemented in the context of large-scale shell model (LSSM) calculations for the nuclei of the beginning and middle of the pf -shell (nuclei of the iron group) [62–65]. It is these nuclei that dominate in the stellar core at the initial stage of collapse. However, for heavier neutron-rich nuclei, which dominate in the composition of the core at densities exceeding 10^{10} g/cm³, the LSSM calculations are impossible for today, since their implementation requires too large a configuration space and is beyond the capabilities of modern computers. For the same reason, and also because of the rapid increase in the number of thermally excited levels with temperature, the LSSM calculations use the Brink–Axel hypothesis (BAH) in order to consider the contribution of thermally excited nuclear states to the total cross section and reaction rate. However, since the experimentally observed temperature-induced increase in the width of GDR [14], as well as changes in its low-energy part [66], in the pygmy resonance, indicate a violation of the BAH, then there is no reason to believe that the BAH is valid for the strength function of GT transitions. The joint use of the BAH and the so-called inverse resonance method in LSSM calculations leads to an underestimation of the contribution of GT transitions from excited states, which, in particular, is expressed in violation of the detailed balance principle and the Ikeda sum rule.

The second method for calculating the rates and cross sections of weak reactions with hot nuclei is based on a statistical approach to the nuclear many-body problem. Within this approach, the temperature-dependent strength function of GT transitions is first calculated, and then the rates and cross sections of weak reactions are expressed in terms of it. This approach, based on thermal RPA (TRPA), was first used in [67] to study the effect of thermal unblocking of GT_+ transitions in neutron-rich nuclei. Further, various versions of the self-consistent TRPA were used to calculate the electron capture rates and cross sections [68–71]. These calculations, however, have the disadvantage that they consider only the part of GT transitions, which corresponds to the energy transfer

to a nucleus. Therefore, the strength function of GT transitions calculated in the TRPA method does not satisfy the principle of detailed balance, while the cross sections demonstrate the presence of a reaction threshold even at high temperatures (see, e.g., Fig. 1 in [70] or Fig. 3 in [69]).

The implementation of the statistical approach within the nuclear shell model became possible with the development of the shell-model Monte Carlo (SMMC) quantum algorithm [72]. Its application to the calculation of the strength function of GT_+ transitions in the iron-group nuclei clearly demonstrated the dependence of the strength function on temperature and, consequently, the BAH violation. However, the SMMC method has a number of limitations associated with the procedure of statistical modeling and numerical inverse Laplace transform.

Thus, the problem of reliable calculation of the rates and cross sections of weak nuclear reactions in stellar matter is still far from its final solution. Therefore, from the viewpoint of astrophysical applications of the theory of hot nuclei, today it is important to create an approach that allows calculating the rates and cross sections of reactions without involving the Brink–Axel hypothesis and without violating the principle of detailed balance. Since at various stages of the evolution of a star, a wide variety of atomic nuclei are formed in its matter, including those whose characteristics are currently unknown, then this approach should not be extremely expensive in terms of computing resources, should have no restrictions on the mass of nuclei and should have sufficient predictive power.

This work is the first of a series of three articles devoted to the superoperator method application to the study of the properties of hot nuclei and to the calculation of the cross sections and rates of weak nuclear reactions with them under conditions that occur during the explosion of collapsing supernovae. The aim of this work is to create on the basis of superoperator method a thermodynamically consistent approach to studying the spectral characteristics of hot nuclei. Specific calculations for cold nuclei and hot nuclei in the matter of a star will be given in the next two articles.

The article structure is as follows. Section 3 presents the formalism of the superoperator method in the Liouville space and shows its relationship with the thermofield dynamics. The advantages of the used definition of fermionic creation and annihilation superoperators are discussed. In Sections 4 and 5, based on the formalism of superoperators and the equation of motion method, the general procedure for calculating the spectral densities and strength functions in hot nuclei is described. Section 6 gives a general view of the nuclear Hamiltonian with a separable residual interaction in the Landau–Migdal form, which is used in calculations. The corresponding thermal Hamiltonian is constructed. In Sections 7 and 8, the probabilities of single-particle transitions are cal-

culated in the approximation of independent thermal quasiparticles and the problem of the temperature evolution of charge-neutral and charge-exchange strength functions is considered qualitatively. In Sections 9 and 11, for charge-neutral and charge-exchange excitations, equations of the thermal quasiparticle random phase approximation (TQRPA) are obtained for the nuclear Hamiltonian with a separable residual particle–hole interaction in the Landau–Migdal form. In Section 10, for the Hamiltonian of the quasiparticle-phonon nuclear model, a thermodynamically consistent way of going beyond the random-phase approximation is described, which considers the interaction of thermal phonons. In the last section 12, based on the Donnelly–Walecka method and the procedure for calculating the spectral densities of multipole operators that was developed using the superoperator method, general expressions are obtained for calculating the cross sections for weak reactions with hot nuclei in the context of the statistical approach. The expressions for cross sections were obtained both considering the nonzero momentum transferred to the nucleus and in the long-wavelength approximation, when the allowed Fermi and Gamow–Teller transitions dominate in the cross section for weak reactions. Appendix A provides the derivation of some relations from Section 3, while in Appendices B and C, the derivation and explicit form of the TQRPA secular equations used in calculations of the structure and energy of charge-neutral and charge-exchange single-phonon excitations in hot nuclei are given.

2. SPECTRUM OF HOT SYSTEMS

In quantum mechanics, the problem of finding the spectrum of a cold system ($T = 0$) can be solved in two ways. According to the first one, the ground and excited states of the system are determined by solution to the stationary Schrödinger equation

$$H|i\rangle = E_i|i\rangle, \quad i = 0, 1, 2, \dots, \quad (1)$$

i.e., they correspond to the eigenfunctions of the Hamiltonian H , whereas its eigenvalues determine the entire energy spectrum of excited states, starting from the ground state $|0\rangle$. If we are only interested in those states that are excited under the action of the external perturbation operator \mathcal{T} , then the problem of finding them can be reduced to calculating the distribution function of the transition strength (strength function)

$$S_{\mathcal{T}}(E) = \sum_f |\langle f|\mathcal{T}|0\rangle|^2 \delta(E - E_f + E_0), \quad (2)$$

whose poles (i.e., singularities) just determine the spectrum of excited states with respect to the ground state.

For a hot system, the role of the ground state is played by the equilibrium mixed state, which is

described by the density matrix $\rho(T)$, and whose structure includes all solutions to Schrödinger equation (1). To define the notion of an excited state of a hot system, consider the strength function at $T \neq 0$

$$S_{\mathcal{T}}(E, T) = \sum_{i,f} p_i(T) |\langle f | \mathcal{T} | i \rangle|^2 \delta(E - E_f + E_i). \quad (3)$$

The strength function includes statistical averaging over all possible initial thermally-excited states, the probability to be in which is determined by the Boltzmann distribution function $p_i(T) = e^{-E_i/T} / Z(T)$ ($Z(T) = \sum_i e^{-E_i/T}$). By analogy with the case $T = 0$, we will call the poles of strength function (3) as the spectrum of a hot system. We emphasize that at $T \neq 0$, the spectrum consists of both positive and negative energies. Therefore, the phrase “excited states” at $T \neq 0$ implies states that are different from the equilibrium one.

In the Green’s function method and the theory of linear response, the calculation of strength function (3) is reduced to finding the response function $R_{\mathcal{T}\mathcal{T}}(E, T)$, the imaginary part of which determines $S_{\mathcal{T}}(E, T)$

$$S_{\mathcal{T}}(E, T) = -\frac{1}{\pi} \frac{1}{1 - e^{-E/T}} \text{Im} R_{\mathcal{T}\mathcal{T}}(E, T). \quad (4)$$

Formally, $R_{\mathcal{T}\mathcal{T}}(E, T)$ is a solution to the Bethe–Salpeter equation

$$R = R^0 + R^0 U R, \quad (5)$$

which includes a free response function R^0 and a vertex part U that considers the interaction. In the simplest approximation, U contains only one interaction vertex, and in this case, solution (5) corresponds to the thermal random phase approximation [73].

Next, we will show that, using the method of superoperators, it is possible to construct a temperature generalization of the Schrödinger equation (1). The solutions to this equation determine the poles of strength function (3) and thus correspond to the excited states (spectrum) of the hot system. In other words, the superoperator method makes it possible to generalize to finite temperatures the nuclear models that are based on the use of nuclear wave functions.

3. FORMALISM OF SUPEROPERATORS

We begin the statement of the superoperator method with general definitions [36, 74–76]. Consider a Hilbert space \mathfrak{H} whose elements are the state vectors of a system under consideration. The Liouville space \mathfrak{L} is the set of linear operators acting in \mathfrak{H} with the scalar product and the norm defined according to

$$\langle\langle A \| B \rangle\rangle = \text{Tr}\{A^\dagger B\}, \quad |A| = \langle\langle A \| A \rangle\rangle^{1/2}. \quad (6)$$

Following [76], we use the Dirac notation $\|A\rangle\rangle$ and $\langle\langle A|$ to distinguish between elements of the spaces \mathfrak{H} and \mathfrak{L} . In this notation, the statistical average $\langle\langle A \rangle\rangle$ of the operator A can be written as a matrix element

$$\langle\langle A \rangle\rangle \equiv \text{Tr}\{A\rho\} = \langle\langle A^\dagger \| \rho \rangle\rangle = \langle\langle \rho \| A^\dagger \rangle\rangle. \quad (7)$$

Here we have considered that the density matrix ρ is a Hermitian operator and $\text{Tr}\{A\rho\} = \text{Tr}\{\rho A\}$.

In \mathfrak{L} -space, the von Neumann equation for the density matrix ($\hbar = 1$)

$$i \frac{\partial}{\partial t} \rho(t) = [H, \rho(t)] \quad (8)$$

takes the form

$$i \frac{\partial}{\partial t} \|\rho(t)\rangle\rangle = \|H\rho(t)\rangle\rangle - \|\rho(t)H\rangle\rangle. \quad (9)$$

In the following sections, we formulate the rules that allow the last relation to be rewritten as the Schrödinger equation

$$i \frac{\partial}{\partial t} \|\rho(t)\rangle\rangle = \mathcal{L} \|\rho(t)\rangle\rangle, \quad (10)$$

where \mathcal{L} is a specially constructed Liouville superoperator (Liouvillian), i.e., an operator acting on vectors in the Liouville space or, equivalently, on operators in the Hilbert space. We will show how to obtain the explicit form of the Liouvillian \mathcal{L} from the Hamiltonian of the system $H(a^\dagger, a)$, written in terms of creation and annihilation operators.

3.1. Basis in Liouville Space

Let the set of vectors $\{|n\rangle\rangle$ form a complete orthonormal basis in the original Hilbert space \mathfrak{H} :

$$\sum_n |n\rangle\rangle \langle\langle n| = I, \quad \langle\langle m|n\rangle\rangle = \delta_{nm}, \quad (11)$$

and, consequently, for an arbitrary linear operator in \mathfrak{H} , the following decomposition is valid:

$$A = \sum_{mn} A_{mn} |m\rangle\rangle \langle\langle n|, \quad A_{mn} = \langle\langle m|A|n\rangle\rangle. \quad (12)$$

Consider the set of ket–bra operators $|m\rangle\rangle \langle\langle n|$ ³. To each operator $|m\rangle\rangle \langle\langle n|$ we associate in the Liouville space a ket vector $\| |m\rangle\rangle \langle\langle n| \rangle\rangle$ and a bra vector

³ If the set $\{|n\rangle\rangle$ consists of the eigenstates of the Hamiltonian H , then $|m\rangle\rangle \langle\langle n|$ are the eigenstates of the Liouville superoperator

$$\mathcal{L}(|m\rangle\rangle \langle\langle n|) = E_{mn} |m\rangle\rangle \langle\langle n|, \quad (13)$$

where $E_{mn} = E_m - E_n$. Moreover $|m\rangle\rangle \langle\langle n|$ and the Hermitian-adjoint operator $|n\rangle\rangle \langle\langle m|$ are matched by eigenvalues equal in absolute value but having opposite sign.

$\langle\langle mn || \equiv || |m\rangle\langle n| \rangle\rangle$. With this definition, the vectors $||mn\rangle\rangle$ form a complete orthonormal basis in \mathfrak{L} :

$$\begin{aligned} \langle\langle mn || m' n' \rangle\rangle &= \text{Tr}\{(|m\rangle\langle n|)^\dagger |m'\rangle\langle n'|\} \\ &= \langle m|m'\rangle\langle n'|n\rangle = \delta_{mm'}\delta_{nn'}, \end{aligned} \quad (14)$$

$$\sum_{mn} ||mn\rangle\rangle\langle\langle mn || = \mathbf{I}, \quad (15)$$

where \mathbf{I} is the identity superoperator in the Liouville space. If N is the dimension of the space \mathfrak{H} , then the dimension of the space \mathfrak{L} is N^2 .

Consider the scalar products of a vector $||A\rangle\rangle$ and basis vectors $||mn\rangle\rangle$:

$$\begin{aligned} \langle\langle mn || A \rangle\rangle &= \text{Tr}\{|n\rangle\langle m|A\} = \langle m|A|n\rangle = A_{mn}, \\ \langle\langle A || mn \rangle\rangle &= \text{Tr}\{A^\dagger |m\rangle\langle n|\} = \langle n|A^\dagger |m\rangle = A_{mn}^*. \end{aligned} \quad (16)$$

Therefore, using completeness property (15), for an arbitrary A , considered as a vector in the \mathfrak{L} -space, we obtain an expansion in basis vectors $||mn\rangle\rangle$:

$$\begin{aligned} ||A\rangle\rangle &= \sum_{mn} ||mn\rangle\rangle\langle\langle mn || A \rangle\rangle = \sum_{mn} A_{mn} ||mn\rangle\rangle, \\ \langle\langle A || &= \sum_{mn} \langle\langle A || mn \rangle\rangle\langle\langle mn || = \sum_{mn} A_{mn}^* \langle\langle mn ||. \end{aligned} \quad (17)$$

The expansions are consistent with the definition of the scalar product (6):

$$\langle\langle A || B \rangle\rangle = \sum_{mn} A_{mn}^* B_{mn} = \text{Tr}\{A^\dagger B\}. \quad (18)$$

In addition, from (17) it follows that

$$||cA\rangle\rangle = c||A\rangle\rangle, \quad \langle\langle cA || = c^* \langle\langle A ||, \quad (19)$$

where c is the complex number.

Let us also define the bra- and ket-vectors corresponding to the unit operator I (11) in the \mathfrak{L} -space:

$$||I\rangle\rangle = \sum_n ||nn\rangle\rangle, \quad \langle\langle I || = \sum_n \langle\langle nn ||. \quad (20)$$

With their help, the operation $\text{Tr}\{\dots\}$ is written as the matrix element

$$\text{Tr}\{A\} = \langle\langle I || A \rangle\rangle = \langle\langle A^\dagger || I \rangle\rangle. \quad (21)$$

In particular, for statistical average (7) of the operator A , we obtain

$$\langle\langle A \rangle\rangle = \langle\langle I || A\rho \rangle\rangle = \langle\langle A^\dagger \rho || I \rangle\rangle, \quad (22)$$

as well as

$$\langle\langle A \rangle\rangle = \langle\langle I || \rho A \rangle\rangle = \langle\langle \rho A^\dagger || I \rangle\rangle. \quad (23)$$

The normalization condition for the density matrix can be written as

$$\text{Tr}\{\rho\} = \langle\langle I || \rho \rangle\rangle = \langle\langle \rho || I \rangle\rangle = 1. \quad (24)$$

3.2. Superoperators of Creation and Annihilation

Here, as basis vectors $\{|n\rangle\}$ in the Hilbert space \mathfrak{H} of a many-particle quantum system, we will consider the eigenfunctions of the particle number operator:

$$|n\rangle = a_{j_1}^\dagger \dots a_{j_n}^\dagger |0\rangle, \quad a_j^\dagger a_j |n\rangle = n_j |n\rangle, \quad n = \sum_j n_j, \quad (25)$$

where the creation and annihilation operators a_j^\dagger , a_j satisfy the commutation relations

$$[a_i, a_j^\dagger]_\sigma = \delta_{ij}, \quad [a_i, a_j]_\sigma = [a_i^\dagger, a_j^\dagger]_\sigma = 0. \quad (26)$$

For fermions $\sigma = +1$, while for bosons $\sigma = -1$.

In the Liouville space formed by the basis vectors $||mn\rangle\rangle$, we define the creation and annihilation superoperators that act on the Hilbert space operators \mathfrak{H} from the *left*⁴:

$$\bar{a}_j ||mn\rangle\rangle \equiv ||a_j |m\rangle\langle n\rangle\rangle, \quad \bar{a}_j^\dagger ||mn\rangle\rangle \equiv ||a_j^\dagger |m\rangle\langle n\rangle\rangle. \quad (27)$$

Since

$$\begin{aligned} \langle\langle kl || \bar{a}_j || mn \rangle\rangle &= \langle k | a_j | m \rangle \delta_{ln}, \\ \langle\langle kl || \bar{a}_j^\dagger || mn \rangle\rangle &= \langle k | a_j^\dagger | m \rangle \delta_{ln}, \end{aligned} \quad (28)$$

then the action of the superoperators \bar{a}_j^\dagger , \bar{a}_j on the bra vector $\langle\langle mn ||$ is determined according to the rule

$$\begin{aligned} \langle\langle mn || \bar{a}_j &= \langle\langle a_j^\dagger | m \rangle\langle n ||, \\ \langle\langle mn || \bar{a}_j^\dagger &= \langle\langle a_j | m \rangle\langle n ||. \end{aligned} \quad (29)$$

The superoperators \bar{a}_j^\dagger , \bar{a}_j are Hermitian conjugate of each other, since

$$\langle\langle kl || \bar{a}_j^\dagger || mn \rangle\rangle = \langle\langle mn || \bar{a}_j || kl \rangle\rangle^*, \quad (30)$$

and they *inherit* the original commutation relations (26), i.e.,

$$[\bar{a}_i, \bar{a}_j^\dagger]_\sigma = \delta_{ij}, \quad [\bar{a}_i, \bar{a}_j]_\sigma = [\bar{a}_i^\dagger, \bar{a}_j^\dagger]_\sigma = 0. \quad (31)$$

In addition, $\bar{a}_j^\dagger \bar{a}_j$ is the particle number superoperator

$$\begin{aligned} \bar{a}_j^\dagger \bar{a}_j ||mn\rangle\rangle &= m_j ||mn\rangle\rangle, \\ \langle\langle mn || \bar{a}_j^\dagger \bar{a}_j &= m_j \langle\langle mn ||. \end{aligned} \quad (32)$$

⁴ The definition of left superoperators \bar{a}^\dagger , \bar{a} that we use does not differ from the definition in the paper by Schmutz [36]. However, for right fermionic superoperators, as will be shown below, we use a more convenient definition. Also note that in [36] the left superoperators were denoted with the symbol “hat,” while the right ones, with the symbol “tilde.”

From (27), (29) and the property $a_j = a_j I = I a_j$ it immediately follows⁵

$$\begin{aligned} \bar{a}_j ||I\rangle\rangle &= ||a_j\rangle\rangle, & \bar{a}_j^\dagger ||I\rangle\rangle &= ||a_j^\dagger\rangle\rangle, \\ \langle\langle I || \bar{a}_j &= \langle\langle a_j^\dagger ||, & \langle\langle I || \bar{a}_j^\dagger &= \langle\langle a_j ||. \end{aligned} \quad (33)$$

In other words, the vectors of Liouville space corresponding to the creation and annihilation operators can be represented as the action of the superoperators $\bar{a}_j^\dagger, \bar{a}_j$, on the unit vector $||I\rangle\rangle$.

Let us show that this statement is true for an arbitrary operator A . Let $A = A(a^\dagger, a)$ be an operator in \mathfrak{S} -space written as a polynomial of creation and annihilation operators.

$$A(a^\dagger, a) = \sum_{mn, pq} c_{p_1 \dots p_m; q_1 \dots q_n} a_{p_1}^\dagger \dots a_{p_m}^\dagger a_{q_1} \dots a_{q_n}. \quad (34)$$

The convention is that an operator $A(a^\dagger, a)$ is called *fermion-like (boson-like)* if each term in expansion (34) contains an odd (even) number of fermionic operators. We will assume that expansion (34) does not contain simultaneously both fermion-like and boson-like terms. By successively applying (27) and (29) and taking property (19) into account, it is easy to verify that

$$\begin{aligned} \bar{A} ||mn\rangle\rangle &= ||A|m\rangle\rangle \langle\langle n|, \\ \langle\langle mn || \bar{A} &= \langle\langle A^\dagger |m\rangle\rangle \langle\langle n|, \end{aligned} \quad (35)$$

where the left superoperator is constructed from (34) by replacing operators a_j^\dagger, a_j with left superoperators $\bar{a}_j^\dagger, \bar{a}_j$, i.e., $\bar{A} = A(\bar{a}_j^\dagger, \bar{a}_j)$.

Using (35) and the definition of scalar product (6), we obtain an expression for matrix elements of \bar{A}

$$\langle\langle kl || \bar{A} || mn \rangle\rangle = \langle\langle k | A | m \rangle\rangle \delta_{ln}. \quad (36)$$

We also define the superoperator $(\bar{A})^\dagger$ that is Hermitian-conjugate of \bar{A} :

$$\langle\langle kl || (\bar{A})^\dagger || mn \rangle\rangle = \langle\langle mn || \bar{A} || kl \rangle\rangle^*. \quad (37)$$

Then it follows from the equality $\langle\langle mn || \bar{A} || kl \rangle\rangle^* = \langle\langle kl || \bar{A}^\dagger || mn \rangle\rangle$ that $(\bar{A})^\dagger = \bar{A}^\dagger$.

⁵ Another way to prove relations (33) is to consider the scalar products of the right and left sides with basis vectors. For example:

$$\begin{aligned} \langle\langle mn || \bar{a}_i || I \rangle\rangle &= \sum_k \langle\langle mn || a_i | k \rangle\rangle \langle\langle k | \rangle\rangle \\ &= \sum_k \langle\langle m | a_i | k \rangle\rangle \delta_{kn} = \langle\langle m | a_i | n \rangle\rangle = \langle\langle mn || a_i \rangle\rangle, \end{aligned}$$

from where follows $\bar{a}_i ||I\rangle\rangle = ||a_i\rangle\rangle$. The other relations are proved similarly.

Using the properties (35) corresponding to the operator (34), the ket and bra vectors in the \mathfrak{S} -space can be represented as

$$||A\rangle\rangle = \bar{A} ||I\rangle\rangle, \quad \langle\langle A || = \langle\langle I || \bar{A}^\dagger. \quad (38)$$

From here, considering property (21) of the vectors $||I\rangle\rangle$ and $\langle\langle I ||$, we obtain

$$\text{Tr}\{A\} = \langle\langle I || \bar{A} || I \rangle\rangle. \quad (39)$$

Therefore, as it should be, $\text{Tr}\{A\} = 0$ for a fermion-like A .

For the product of operators, we have $\overline{\bar{A}\bar{B}} = \bar{A}\bar{B}$ and $(\bar{A}\bar{B})^\dagger = \bar{B}^\dagger \bar{A}^\dagger$ ⁶. Therefore

$$\begin{aligned} ||AB\rangle\rangle &= \bar{A}\bar{B} ||I\rangle\rangle = \bar{A} ||B\rangle\rangle, \\ \langle\langle AB || &= \langle\langle I || \bar{B}^\dagger \bar{A}^\dagger = \langle\langle B || \bar{A}^\dagger. \end{aligned} \quad (40)$$

We emphasize that these rules are consistent with relation (19), as well as with the definition of the scalar product in the Liouville space (6)

$$\begin{aligned} \langle\langle A || B \rangle\rangle &= \langle\langle I || \bar{A}^\dagger \bar{B} || I \rangle\rangle \\ &= \langle\langle I || A^\dagger B \rangle\rangle = \langle\langle B^\dagger A || I \rangle\rangle, \end{aligned} \quad (41)$$

where we used (39). Using properties (40), the statistical mean (22) of the operator A can be represented as a matrix element of the corresponding left superoperator

$$\langle\langle A \rangle\rangle = \langle\langle I || \bar{A} || \rho \rangle\rangle = \langle\langle \rho || \bar{A} || I \rangle\rangle. \quad (42)$$

Using the left superoperators defined according to (27) and (29), the ket vector $||H\rho(t)\rangle\rangle$ in von Neumann equation (9) can be written as $\bar{H} ||\rho(t)\rangle\rangle$, where $\bar{H} = H(\bar{a}_j^\dagger, \bar{a}_j)$ is the left superoperator corresponding to the Hamiltonian $H = H(a^\dagger, a)$. However, in order to be able to write Eq. (9) in the form of Schrödinger equation (10), we need to define the superoperator \bar{H} acting on the density matrix from the *right*, i.e., such that $\bar{H} ||\rho(t)\rangle\rangle = ||\rho(t)H\rangle\rangle$. The idea arises to define the right superoperators of creation and annihilation in a manner similar to that considered above, i.e., put

$$\begin{aligned} \bar{a}_j ||mn\rangle\rangle &\equiv |||m\rangle\rangle \langle\langle n | a_j^\dagger \rangle\rangle, \\ \bar{a}_j^\dagger ||mn\rangle\rangle &\equiv |||m\rangle\rangle \langle\langle n | a_j \rangle\rangle, \\ \langle\langle mn || \bar{a}_j &\equiv \langle\langle |m\rangle\rangle \langle\langle n | a_j ||, \\ \langle\langle mn || \bar{a}_j^\dagger &\equiv \langle\langle |m\rangle\rangle \langle\langle n | a_j^\dagger ||. \end{aligned} \quad (43)$$

It is easy to show that, with this definition, \bar{a}_j and \bar{a}_j^\dagger are Hermitian conjugate of each other and satisfy

⁶ Really, $(\bar{A}\bar{B})^\dagger = (\overline{\bar{A}\bar{B}})^\dagger = \overline{(\overline{\bar{A}\bar{B}})^\dagger} = \overline{\bar{B}^\dagger \bar{A}^\dagger} = \bar{B}^\dagger \bar{A}^\dagger$.

the commutation rules (26). In addition, the following relations are valid for them:

$$\begin{aligned} \bar{a}_j ||I\rangle\rangle &= ||a_j^\dagger\rangle\rangle, \quad \bar{a}_j^\dagger ||I\rangle\rangle = ||a_j\rangle\rangle, \\ \langle\langle I ||\bar{a}_j &= \langle\langle a_j ||, \quad \langle\langle I ||\bar{a}_j^\dagger = \langle\langle a_j^\dagger ||, \end{aligned} \quad (44)$$

while $\bar{a}_j^\dagger \bar{a}_j$ is the superoperator for the number of particles

$$\bar{a}_j^\dagger \bar{a}_j ||mn\rangle\rangle = n_j ||mn\rangle\rangle, \quad \langle\langle mn ||\bar{a}_j^\dagger \bar{a}_j = n_j \langle\langle mn ||. \quad (45)$$

However, with this definition, the left and right superoperators commute with each other, regardless of whether they refer to fermions or bosons:

$$[\bar{a}_i, \bar{a}_j^\dagger]_{-1} = [\bar{a}_i, \bar{a}_j^\dagger]_{-1} = [\bar{a}_i, \bar{a}_j]_{-1} = [\bar{a}_i^\dagger, \bar{a}_j^\dagger]_{-1} = 0. \quad (46)$$

In other words, the above defined set of left and right superoperators of creation and annihilation inherits original commutation rules (26) only for a bosonic system. For fermionic systems, however, the permutation relations for superoperators differ from the original ones.

In order for the set of superoperators to inherit commutation relations (26), and also in order to be able to subsequently apply canonical transformations mixing left and right fermionic superoperators (the so-called Bogolyubov thermal transform), the latter must be defined so that they anticommute with left ones. To this end, we use the method from [76] and modify it. For generality, we will simultaneously consider fermionic and bosonic superoperators. We leave the definition of the left superoperators unchanged (see (27)), and for the right superoperators we set

$$\begin{aligned} \bar{a}_j ||mn\rangle\rangle &\equiv \alpha(m, n) ||m\rangle\langle n | a_j^\dagger\rangle\rangle, \\ \bar{a}_j^\dagger ||mn\rangle\rangle &\equiv \beta(m, n) ||m\rangle\langle n | a_j\rangle\rangle, \end{aligned} \quad (47)$$

where $\alpha(m, n)$, $\beta(m, n)$ are complex numbers depending on $m = \sum_j m_j$ and $n = \sum_j n_j$. We require the following conditions to be met:

(1) The right creation and annihilation operators obey the original permutation relations (26).

(2) Operators \bar{a}_j^\dagger and \bar{a}_j are Hermitian-conjugate of each other, e.g., $\langle\langle m_1 n_1 ||\bar{a}_j^\dagger ||m_2 n_2\rangle\rangle = \langle\langle m_2 n_2 ||\bar{a}_j ||m_1 n_1\rangle\rangle^*$.

(3) Bosonic (fermionic) left and right creation and annihilation operators commute (anticommute) with each other.

(4) $\bar{a}_i^\dagger ||I\rangle\rangle = c ||a_i\rangle\rangle$, where c is a complex number.

In Appendix A, we show that the mentioned conditions determine the functions $\alpha(m, n)$ and $\beta(m, n)$ to within a phase factor:

$$\begin{aligned} \beta(m, n) &= c(-\sigma)^{m+n}, \\ \alpha(m, n) &= c^*(-\sigma)^{m+n+1} \quad \text{and} \quad cc^* = 1. \end{aligned} \quad (48)$$

For bosonic ($\sigma = -1$) right superoperators, definition (43) corresponds to the choice of $c = +1$. Schmutz [36] chose the phase factor $c = +1$ also to determine the right fermionic superoperators. The disadvantages of such a definition are discussed below. We, however, following our papers [42–46], will use $c = i$ in the definition of right fermionic superoperators. The transition from the right fermionic superoperators of [36] to those that we use is carried out according to the rules:

Definition used by Schmutz		Our definition	
\bar{a}_j	\leftrightarrow	$i\bar{a}_j$. (49)
\bar{a}_j^\dagger	\leftrightarrow	$-i\bar{a}_j^\dagger$	

With this choice of the phase factor, the right fermionic superoperators act on the basis ket vectors of the Liouville space according to the rule

$$\begin{aligned} \bar{a}_j ||mn\rangle\rangle &= i(-1)^{m+n} ||m\rangle\langle n | a_j^\dagger\rangle\rangle, \\ \bar{a}_j^\dagger ||mn\rangle\rangle &= i(-1)^{m+n} ||m\rangle\langle n | a_j\rangle\rangle. \end{aligned} \quad (50)$$

Let us determine how the right fermionic superoperators act on the basis bra vectors. For this, we note that

$$\begin{aligned} \langle\langle kl ||\bar{a}_j ||mn\rangle\rangle &= i(-1)^{m+n} \delta_{km} \langle n | a_j^\dagger | l \rangle \\ &= -i(-1)^{k+l} \delta_{km} \langle n | a_j^\dagger | l \rangle, \\ \langle\langle kl ||\bar{a}_j^\dagger ||mn\rangle\rangle &= i(-1)^{m+n} \delta_{km} \langle n | a_j | l \rangle \\ &= -i(-1)^{k+l} \delta_{km} \langle n | a_j | l \rangle. \end{aligned} \quad (51)$$

Whence it follows

$$\begin{aligned} \langle\langle mn ||\bar{a}_j &= -i(-1)^{m+n} \langle\langle m | \langle n | a_j ||, \\ \langle\langle mn ||\bar{a}_j^\dagger &= -i(-1)^{m+n} \langle\langle m | \langle n | a_j^\dagger ||. \end{aligned} \quad (52)$$

In addition, $\bar{a}_j^\dagger \bar{a}_j$ satisfies property (45), i.e., it is the particle number superoperator.

Using the right and left fermionic creation superoperators, the basis vectors in the Liouville space can be represented as

$$||mn\rangle\rangle = \mathcal{D}_{mn} ||00\rangle\rangle, \quad \langle\langle mn || = \langle\langle 00 || \mathcal{D}_{mn}^\dagger, \quad (53)$$

where $\mathcal{D}_{mn} = \sigma_n \bar{a}_{p_1}^\dagger \dots \bar{a}_{p_m}^\dagger \bar{a}_{q_1}^\dagger \dots \bar{a}_{q_n}^\dagger$ and

$$\sigma_n = (-i)^{n^2} = \begin{cases} -i, & n = 2k + 1 \\ +1, & n = 2k. \end{cases} \quad (54)$$

The ket vector $||00\rangle\rangle$ is the vacuum for \bar{a}_j and \bar{a}_j^\dagger , while $\langle\langle 00 ||$, for \bar{a}_j^\dagger and \bar{a}_j . Since

$$||nn\rangle\rangle = (-i)^n \bar{a}_{j_1}^\dagger \bar{a}_{j_2}^\dagger \dots \bar{a}_{j_n}^\dagger \bar{a}_{j_n}^\dagger ||00\rangle\rangle, \quad (55)$$

then $||I\rangle\rangle$ can be presented as

$$||I\rangle\rangle = \exp(-i \sum_j \bar{a}_j^\dagger \bar{a}_j^\dagger) ||00\rangle\rangle. \quad (56)$$

By successively applying (50) and (52) and considering property (19), it is easy to verify that for fermion-like operator $A(a^\dagger, a)$ (34), the following equalities are valid

$$\begin{aligned}\bar{A}||mn\rangle\rangle &= i(-1)^{m+n} ||m\rangle\langle n|A^\dagger\rangle\rangle, \\ \langle\langle mn|\bar{A} &= -i(-1)^{m+n} \langle\langle m|\langle n|A||,\end{aligned}\quad (57)$$

where the right superoperator is constructed from $A(a^\dagger, a)$ by replacing a_j^\dagger, a_j with $\bar{a}_j^\dagger, \bar{a}_j$ and by the complex conjugation of all numerical coefficients, i.e., $\bar{A} = A^{(*)}(\bar{a}^\dagger, \bar{a})$, where the complex conjugation $(*)$ acts only on c -numbers. For a boson-like operator, we have

$$\begin{aligned}\bar{A}||mn\rangle\rangle &= ||m\rangle\langle n|A^\dagger\rangle\rangle, \\ \langle\langle mn|\bar{A} &= \langle\langle m|\langle n|A||.\end{aligned}\quad (58)$$

Regardless of whether A is fermion-like or boson-like, the matrix elements of the right superoperator \bar{A} can be written in the following form (cf. (36)):

$$\langle\langle kl|\bar{A}||mn\rangle\rangle = \sigma_{k+l}^* \sigma_{m+n} \langle n|A^\dagger|l\rangle \delta_{km}. \quad (59)$$

This expression for matrix elements also directly follows from the relation (78) obtained below. As in the case of left superoperators, from the equality $\langle\langle mn|\bar{A}||kl\rangle\rangle^* = \langle\langle kl|\bar{A}^\dagger||mn\rangle\rangle$, it follows that $(\bar{A})^\dagger = \bar{A}^\dagger$.

Based on properties (57) and equality (38), we obtain

$$\begin{aligned}||A\rangle\rangle &= \bar{A}||I\rangle\rangle = \sigma_A \bar{A}^\dagger ||I\rangle\rangle, \\ \langle\langle A|| &= \langle\langle I|\bar{A}^\dagger = \sigma_A^* \langle\langle I|\bar{A},\end{aligned}\quad (60)$$

where $\sigma_A = -i(+1)$ for the fermion-like (boson-like) operator $A(a^\dagger, a)$. Thus, an arbitrary vector in the Liouville space can be represented either as the action of the left superoperator on the unit vector $||I\rangle\rangle$ or as the action of the right superoperator. From (60) it also follows

$$(\bar{A} - \sigma_A \bar{A}^\dagger) ||I\rangle\rangle = 0, \quad \langle\langle I|(\bar{A}^\dagger - \sigma_A^* \bar{A}) = 0 \quad (61)$$

and

$$\text{Tr}\{A\} = \langle\langle I|\bar{A}||I\rangle\rangle = \langle\langle I|\bar{A}^\dagger||I\rangle\rangle, \quad (62)$$

where we considered that $\text{Tr}\{A\} = 0$ for a fermion-like A .

For a product of right superoperators, we have $\bar{A}\bar{B} = \overline{AB}$ and $(\bar{A}\bar{B})^\dagger = \bar{B}^\dagger \bar{A}^\dagger$. Therefore, based on (60) and (40), it can be written

$$\begin{aligned}\bar{A}||B\rangle\rangle &= ||AB\rangle\rangle \\ &= \sigma_{AB} \bar{B}^\dagger \bar{A}^\dagger ||I\rangle\rangle = \sigma_{AB} \sigma_A^* \bar{B}^\dagger ||A\rangle\rangle, \\ \langle\langle B|\bar{A}^\dagger &= \langle\langle AB|| \\ &= \sigma_{AB}^* \langle\langle I|\bar{A}\bar{B} = \sigma_{AB}^* \sigma_A \langle\langle A|\bar{B}.\end{aligned}\quad (63)$$

Note that $\sigma_{AB} \sigma_A^* = i$ if both A and B are fermion-like operators, and $\sigma_{AB} \sigma_A^* = \sigma_B$ if one of the operators is boson-like. With the use of (40) and (63), the product of operators can be represented as an action of a right or left superoperator on a vector in the Liouville space. It is important that due to the introduction of right and left superoperators, any of the factors can be represented as a vector.

Equalities (63) are consistent with definition (6) of scalar product in the Liouville space:

$$\begin{aligned}\langle\langle A||B\rangle\rangle &= \sigma_A^* \sigma_B \langle\langle I|\bar{A}\bar{B}^\dagger||I\rangle\rangle \\ &= \sigma_A^* \sigma_B \sigma_{AB} \langle\langle I|BA^\dagger\rangle\rangle \\ &= \langle\langle I|A^\dagger B\rangle\rangle = \sigma_A^* \sigma_B \sigma_{AB}^* \langle\langle AB^\dagger||I\rangle\rangle \\ &= \langle\langle B^\dagger A||I\rangle\rangle.\end{aligned}\quad (64)$$

Here we have considered that the matrix elements are equal to zero if AB is a fermion-like operator.

Since the density matrix is a boson-like operator, then the statistical average $\langle\langle A\rangle\rangle = \text{Tr}\{A\rho\}$ is nonzero only for a boson-like operator A . Therefore, from (23) and (63), it follows that

$$\langle\langle A\rangle\rangle = \langle\langle I|\bar{A}^\dagger|\rho\rangle\rangle = \langle\langle \rho|\bar{A}^\dagger||I\rangle\rangle. \quad (65)$$

Thus, the statistical average of an operator A can be represented either as a matrix element of the right superoperator or as a matrix element of the left superoperator (see (42)).

It should be particularly emphasized that relations (60) and (63) for fermionic superoperators are satisfied only if the right superoperators of creation and annihilation are defined according to (50). If the right fermionic superoperators are defined “according to Schmutz” [36] (i.e., in (48) we put $c = 1$), then relations of the form of (60) can be obtained only for an operator $A(a^\dagger, a)$ such that the value $(-1)^{(m-n+1)(m-n)/2}$ is the same for all terms of expansion (34). In this case,

$$\bar{A}||I\rangle\rangle = (-1)^{(\eta+1)\eta/2} \bar{A}^\dagger ||I\rangle\rangle, \quad (66)$$

where $\eta = m - n$ (see Eq. 2.31 in [36]). In addition, when determining the right fermionic superoperators according to Schmutz, the relations similar to (63) hold only for A and B such that the value

$(-1)^{(m_B-n_B+1)(m_B-n_B)/2}(-1)^{(m_B+n_B)(m_A+n_A)}$ is the same for all terms of the expansion of the operators A and B . So, e.g., if B preserves the number of particles (i.e., $m_B = n_B$), then $\|AB\rangle\rangle = \bar{B}^\dagger\|A\rangle\rangle$. However, if the right superoperators of creation and annihilation are defined according to (50), then the equality $\|AB\rangle\rangle = \bar{B}^\dagger\|A\rangle\rangle$ holds for *all* boson-like B . Therefore, definition (50) of right fermionic superoperators, which we use, expands the range of applicability of relations like (60) and (63). In addition, it will be shown below that the definition of right fermionic superoperators according to (50) greatly facilitates the application of the equation of motion method to the study of the spectral characteristics of a hot system.

Using the above relations for the product of operators, we can write $\|\rho(t)H\rangle\rangle = \bar{H}\|\rho(t)\rangle\rangle$, where we consider that the Hamiltonian $H(a^\dagger, a)$ is a boson-like Hermitian operator, and, consequently, $\bar{H}^\dagger = \bar{H} = H(\bar{a}^\dagger, \bar{a})$. Now we can write the explicit form of the Liouville superoperator \mathcal{L} in Schrödinger equation (10) for the vector $\|\rho(t)\rangle\rangle$ as follows:

$$\mathcal{L} = \bar{H} - \bar{H} \quad (67)$$

and $\mathcal{L} = \mathcal{L}^\dagger$, i.e., is a Hermitian superoperator.

Let us point out some properties of \mathcal{L} . First of all, we show that \mathcal{L} is the time-translation operator in the Liouville space. Indeed, if $A(t)$ is the Heisenberg representation of the operator A , then the corresponding Heisenberg representation of the left superoperator can be written as

$$\bar{A}(t) = e^{i\bar{H}t} \bar{A} e^{-i\bar{H}t} = e^{i\mathcal{L}t} \bar{A} e^{-i\mathcal{L}t}, \quad (68)$$

where we considered that $[\bar{H}, \bar{A}] = 0$ because the Hamiltonian H is a boson-like operator. The Heisenberg representation of the right superoperator is obtained similarly:

$$\bar{A}(t) = e^{i\mathcal{L}t} \bar{A} e^{-i\mathcal{L}t}. \quad (69)$$

Therefore, the Heisenberg representation of the operator \mathcal{C} , which is an arbitrary linear combination of the product of left and right superoperators, is

$$\mathcal{C}(t) = e^{i\mathcal{L}t} \mathcal{C} e^{-i\mathcal{L}t}, \quad (70)$$

which proves the original statement.

It follows from (60) that $\|I\rangle\rangle$ and $\langle\langle I|$ are, respectively, the right and left eigenstates of the Liouvillian \mathcal{L} with zero eigenvalue:

$$\mathcal{L}\|I\rangle\rangle = 0, \quad \langle\langle I|\mathcal{L} = 0. \quad (71)$$

Whence it follows that Eq. (10) preserves the density matrix norm:

$$\frac{\partial}{\partial t} \text{Tr}\{\rho(t)\} = \left\langle\left\langle I \left| \frac{\partial}{\partial t} \right| \rho(t) \right\rangle\right\rangle = -i \langle\langle I | \mathcal{L} | \rho(t) \rangle\rangle = 0. \quad (72)$$

If we consider the density matrix as a bra vector in Liouville space, then the corresponding Schrödinger equation has the form

$$-i\hbar \frac{\partial}{\partial t} \langle\langle \rho(t) | = \langle\langle \rho(t) | \mathcal{L}, \quad (73)$$

where we considered property (19). It follows from (10) and (73) that the vectors $\|\rho\rangle\rangle$ and $\langle\langle \rho|$ corresponding to the stationary (i.e., time-independent) density matrix are also eigenstates \mathcal{L} with zero eigenvalue

$$\mathcal{L}\|\rho\rangle\rangle = 0, \quad \langle\langle \rho | \mathcal{L} = 0. \quad (74)$$

So, we have shown that, in the context of the superoperator formalism, finding statistical averages reduces to solving Schrödinger equation (10) (or (73)) for a given initial condition⁷ and then calculating the matrix elements from left superoperator (42) or right superoperator (65). When passing from the von Neumann equation to the Schrödinger equation, the number of creation and annihilation operators doubles. Due to this doubling, the mixed state of the system, described by the density matrix ρ , is described by a pure state $\|\rho\rangle\rangle$ in the Liouville space.

In our works [42–46], the superoperator formalism was applied to the study of electron transport through correlated quantum systems. It was shown that the equation for the density matrix in the form of the Schrödinger equation can be obtained also in the case when the evolution of an open quantum system is described using the Lindblad equation⁸. However, in this case, the corresponding evolution superoperator is not Hermitian, i.e., $\mathcal{L}^\dagger \neq \mathcal{L}$.

⁷ For a time-independent Liouvillian, the formal solution of Eq. (10) has the form

$$\|\rho(t)\rangle\rangle = e^{-i\mathcal{L}(t-t_0)} \|\rho(t_0)\rangle\rangle.$$

⁸ In [42–46], in order to obtain the superoperator representation of the Lindblad equation for the density matrix of an open quantum system, relations (63) were used in the following way

$$\|A\rho B\rangle\rangle = \sigma_B \bar{A} \bar{B}^\dagger \|\rho\rangle\rangle. \quad (75)$$

Products of the form $A\rho B$ are contained in the part of Lindblad equation that describes the processes of dissipation in the system [77].

3.3. Tilde Conjugation Operation

By direct verification, it can be found that the right and left fermionic annihilation superoperators defined above satisfy the property⁹

$$\langle\langle kl \|\bar{a}_j \|\ mn \rangle\rangle = \sigma_{k+l}^* \sigma_{m+n} \langle\langle lk \|\bar{a}_j \|\ nm \rangle\rangle^*, \quad (76)$$

where σ_{m+n} is defined according to (54). The same relation holds for right and left fermionic creation superoperators. Moreover, relation (76) remains valid if the right and left superoperators in it are interchanged.

Consider an arbitrary superoperator \mathcal{C} , which is a polynomial in the right and left superoperators of creation and annihilation:

$$\mathcal{C} = \mathcal{C}(\bar{a}^\dagger, \bar{a}, \bar{a}^\dagger, \bar{a}). \quad (77)$$

Using relation (76) and property (15) of completeness of basis vectors $\|\ mn \rangle\rangle$, it is easy to obtain that

$$\begin{aligned} \langle\langle kl \|\mathcal{C} \|\ mn \rangle\rangle &= \sigma_{k+l}^* \sigma_{m+n} \langle\langle lk \|\tilde{\mathcal{C}} \|\ nm \rangle\rangle^* \\ &= \sigma_{k+l}^* \sigma_{m+n} \langle\langle nm \|\tilde{\mathcal{C}}^\dagger \|\ lk \rangle\rangle, \end{aligned} \quad (78)$$

where $\tilde{\mathcal{C}} \equiv \mathcal{C}^\sim$ is the so-called superoperator tilde-conjugate of \mathcal{C} . The tilde conjugation operation changes all right (left) superoperators to left (right) ones, while c -numbers are converted by it to complex conjugates. It has obvious properties¹⁰

$$\begin{aligned} (\alpha_1 \mathcal{C}_1 + \alpha_2 \mathcal{C}_2)^\sim &= \alpha_1^* \tilde{\mathcal{C}}_1 + \alpha_2^* \tilde{\mathcal{C}}_2, \\ (\mathcal{C}_1 \mathcal{C}_2)^\sim &= \tilde{\mathcal{C}}_1 \tilde{\mathcal{C}}_2, \quad (\mathcal{C}^\dagger)^\sim = (\tilde{\mathcal{C}})^\dagger, \\ (\tilde{\mathcal{C}})^\sim &= \mathcal{C}. \end{aligned} \quad (79)$$

With the use of the above rules, each superoperator $\mathcal{C} = \mathcal{C}(\bar{a}^\dagger, \bar{a}, \bar{a}^\dagger, \bar{a})$ is assigned a tilde conjugate superoperator $\tilde{\mathcal{C}}$, such that for arbitrary $\|\ mn \rangle\rangle$ and $\|\ kl \rangle\rangle$, equality (78) is true. Since $\bar{A} = (\bar{A})^\sim$ and $\bar{A} = (\bar{A})^\sim$,

⁹ From (50) it follows that

$$\langle\langle k \|\bar{a}_j \|\ mn \rangle\rangle = i(-1)^{(m+n)} \langle\langle lk \|\bar{a}_j \|\ nm \rangle\rangle^*.$$

However, since only matrix elements with $k+l = m+n-1$ differ from zero, then

$$\begin{aligned} \sigma_{k+l}^* \sigma_{m+n} &= (+i)^{(k+l)^2} (-i)^{(m+n)^2} \\ &= (+i)^{(k+l+m+n)(k+l-m-n)} = (+i)^{-2(m+n)+1} = i(-1)^{(m+n)}. \end{aligned}$$

¹⁰ The latter rule, the double tilde rule, is consistent with (78), since

$$\begin{aligned} \langle\langle kl \|\tilde{\mathcal{C}}^\sim \|\ mn \rangle\rangle &= \sigma_{k+l}^* \sigma_{m+n} \langle\langle kl \|\tilde{\mathcal{C}} \|\ mn \rangle\rangle^* \\ &= \langle\langle kl \|\mathcal{C} \|\ mn \rangle\rangle. \end{aligned}$$

then, applying the tilde conjugation operation to Liouvillian (67), we obtain an important property

$$\tilde{\mathcal{L}} = -\mathcal{L}. \quad (80)$$

Relation (78) establishes a relation between the matrix elements of the left $\bar{A} = A(\bar{a}^\dagger, \bar{a})$ and right $\bar{A} = A^{(*)}(\bar{a}^\dagger, \bar{a})$ superoperators. From it, in particular, expression (59) for $\langle\langle kl \|\bar{A} \|\ mn \rangle\rangle$ follows.

The tilde conjugation operation is closely related to the Liouville conjugation operation \mathbb{C}_L [78].

$$\mathbb{C}_L \|\ mn \rangle\rangle = \|\ nm \rangle\rangle, \quad \mathbb{C}_L = \mathbb{C}_L^{-1}. \quad (81)$$

Indeed, if we represent the basis ket vector $\|\ mn \rangle\rangle$ as $\|\ mn \rangle\rangle = \mathcal{D}_{mn} \|\ 00 \rangle\rangle$, where the superoperator \mathcal{D}_{mn} is defined according to (53), then the tilde conjugate ket vector can be written as

$$\|\widetilde{mn}\rangle\rangle \equiv \tilde{\mathcal{D}}_{mn} \|\ 00 \rangle\rangle = \sigma_{m+n}^* \|\ nm \rangle\rangle. \quad (82)$$

Similarly for the basis bra vector

$$\langle\langle\widetilde{mn}\|\equiv \langle\langle 00 \|\tilde{\mathcal{D}}_{mn}^\dagger = \sigma_{m+n} \langle\langle nm \|\rangle. \quad (83)$$

Thus, for even $m+n$, the Liouville conjugation operation coincides with the tilde conjugation of the basis vector. For odd $m+n$, an additional phase factor $+i$ appears.

Using (82) and (83), relations (78) can be written in a more compact form

$$\langle\langle kl \|\mathcal{C} \|\ mn \rangle\rangle = \langle\langle\widetilde{kl} \|\tilde{\mathcal{C}} \|\widetilde{mn}\rangle\rangle^* = \langle\langle\widetilde{mn} \|\tilde{\mathcal{C}}^\dagger \|\widetilde{kl}\rangle\rangle. \quad (84)$$

These equalities can be generalized to the case of arbitrary vectors. Indeed, let $\|\ O \rangle\rangle$ be a vector in the Liouville space:

$$\|\ O \rangle\rangle = \sum_{mn} O_{mn} \|\ mn \rangle\rangle, \quad O_{mn} = \langle\langle mn \|\ O \rangle\rangle. \quad (85)$$

We define the tilde conjugate vector $\|\ \tilde{O} \rangle\rangle$ as

$$\|\ \tilde{O} \rangle\rangle = \sum_{mn} O_{mn}^* \|\widetilde{mn}\rangle\rangle = \sum_{mn} O_{nm}^* \sigma_{m+n}^* \|\ mn \rangle\rangle, \quad (86)$$

i.e., $\langle\langle mn \|\ \tilde{O} \rangle\rangle = O_{nm}^* \sigma_{m+n}^*$. It follows directly from this definition that the double tilde conjugation does not change the vector

$$\|\ \tilde{\tilde{O}} \rangle\rangle = \sum_{mn} O_{nm} \sigma_{m+n} \|\widetilde{mn}\rangle\rangle = \|\ O \rangle\rangle. \quad (87)$$

In addition, from (84) it follows

$$\langle\langle O_1 \|\mathcal{C} \|\ O_2 \rangle\rangle = \langle\langle\tilde{O}_1 \|\tilde{\mathcal{C}} \|\ \tilde{O}_2 \rangle\rangle^* = \langle\langle\tilde{O}_2 \|\tilde{\mathcal{C}}^\dagger \|\ \tilde{O}_1 \rangle\rangle. \quad (88)$$

Let us consider as \mathcal{C} the unit superoperator $\mathbf{I} = \tilde{\mathbf{I}}$ (15). Then from (88) it follows that

$$\langle\langle O_1 \|\ O_2 \rangle\rangle = \langle\langle\tilde{O}_1 \|\ \tilde{O}_2 \rangle\rangle^* = \langle\langle\tilde{O}_2 \|\ \tilde{O}_1 \rangle\rangle. \quad (89)$$

We will call a vector $|\theta\rangle$ as tilde-invariant if $|\theta\rangle = |\tilde{\theta}\rangle$, i.e., $\langle mn|\theta\rangle = \langle mn|\tilde{\theta}\rangle$ for any $|mn\rangle$. If A is a Hermitian boson-like operator, then $|A\rangle$ is tilde-invariant, since $\langle mn|A\rangle = \langle mn|\tilde{A}\rangle = A_{mn}$. The vacuum $|00\rangle$ is tilde-invariant by definition. Other examples of tilde-invariant vectors are $|I\rangle$ and $|\rho\rangle$.¹¹ For tilde-invariant vectors, relations (88) take the form

$$\langle\langle\theta_1|\mathcal{C}|\theta_2\rangle\rangle = \langle\langle\theta_1|\tilde{\mathcal{C}}|\theta_2\rangle\rangle^* = \langle\langle\theta_2|\tilde{\mathcal{C}}^\dagger|\theta_1\rangle\rangle. \quad (90)$$

Consider a ket vector $|O\rangle \equiv \mathcal{C}|\theta\rangle$, where $|\theta\rangle$ is the tilde-invariant vector and \mathcal{C} is the superoperator of the form of (77). Let us show that $|\tilde{O}\rangle = \tilde{\mathcal{C}}|\theta\rangle$, where $\tilde{\mathcal{C}}$ is the superoperator tilde-conjugate of \mathcal{C} . For arbitrary $|mn\rangle$, we have

$$\begin{aligned} \langle\langle mn|\tilde{\mathcal{C}}|\theta\rangle\rangle &= \langle\langle \widetilde{mn}|\mathcal{C}|\theta\rangle\rangle^* = \langle\langle \widetilde{mn}|O\rangle\rangle^* \\ &= \sigma_{m+n}^* \langle\langle nm|O\rangle\rangle^* = \sigma_{m+n}^* O_{nm}^* = \langle\langle mn|\tilde{O}\rangle\rangle, \end{aligned} \quad (91)$$

which just proves the required equality. The resulting equality admits a double interpretation: (i) the action of the superoperator $\tilde{\mathcal{C}}$, tilde-conjugate of \mathcal{C} , on $|\theta\rangle$ gives a vector $|\tilde{O}\rangle$, tilde-conjugate of $|O\rangle$; (ii) a vector $|\tilde{O}\rangle$ can be represented as the result of the action of the superoperator $\tilde{\mathcal{C}}$, tilde-conjugate of \mathcal{C} , on $|\theta\rangle$.

We especially emphasize that equalities (90) are valid for an arbitrary \mathcal{C} and its tilde-conjugate partner $\tilde{\mathcal{C}}$ only if the right superoperators of creation and annihilation are defined according to (50). If the right superoperators of creation and annihilation are defined according to Schmutz, then relations (90) do not hold in the general case. This is easy to verify if \mathcal{C} is presented in the form

$$\mathcal{C} = \sum_i c_i \bar{A}_i \bar{B}_i, \quad (92)$$

where \bar{A}_i (\bar{B}_i) are monomials of the left (right) creation and annihilation superoperators, and $|\theta\rangle$ are taken as $|I\rangle$. Denote $\eta_{A_i} = m_{A_i} - n_{A_i}$, $N_{A_i} = m_{A_i} + n_{A_i}$, $\eta_{B_i} = m_{B_i} - n_{B_i}$, $N_{B_i} = m_{B_i} + n_{B_i}$ (see (34)). Then from (66) it follows that

$$\begin{aligned} \langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle &= (-1)^{(\eta_{A_i}+1)\eta_{A_i}/2} (-1)^{(\eta_{B_i}+1)\eta_{B_i}/2} \\ &\times (-1)^{N_{A_i}N_{B_i}} \langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle^* \\ &= (-1)^{N_{A_i}N_{B_i}} \langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle^*, \end{aligned} \quad (93)$$

¹¹From the tilde invariance of the density matrix, it follows that $\tilde{\mathcal{L}} = -\mathcal{L}$ even in the case when $\mathcal{L} \neq \mathcal{L}^\dagger$ [42–46].

where we used the fact that the matrix elements on the left and right are nonzero only for $\eta_{A_i} = \eta_{B_i}$.¹² The value of multiplier in front of the right matrix element depends on the specific form of A_i and B_i . Consequently, when defining right superoperators according to Schmutz, relation (90) between \mathcal{C} and $\tilde{\mathcal{C}}$ is not satisfied¹³.

3.4. Relationship of the Superoperator Method with the Thermofield Dynamics

Until now, we have not used in any way the fact that the density matrix of the equilibrium state at temperature T has a well-defined form

$$\rho(T) = Z(T)^{-1} e^{-H/T}, \quad (95)$$

where $Z(T) = \text{Tr}\{e^{-H/T}\}$ is the statistical sum. We define an exponential function of the equilibrium density matrix:

$$\rho(T)^\alpha = Z(T)^{-\alpha} e^{-\alpha H/T}. \quad (96)$$

Obviously, $\rho(T)^\alpha$ is also a boson-like Hermitian operator and $\rho(T)^\alpha \rho(T)^{1-\alpha} = \rho(T)$. Moreover, $\rho(T)^\alpha$ commutes with the Hamiltonian. Using the cyclic property of the trace $\text{Tr}\{ABC\} = \text{Tr}\{CAB\}$ and relations (42) and (65), the statistical average of the operator A can be written as the matrix element

$$\langle\langle A\rangle\rangle = \langle\langle \sqrt{\rho(T)} \| A \| \sqrt{\rho(T)} \rangle\rangle = \langle\langle \sqrt{\rho(T)} \| \bar{A}^\dagger \| \sqrt{\rho(T)} \rangle\rangle. \quad (97)$$

In this sense, the vector $|\sqrt{\rho(T)}\rangle = \bar{\rho}(T)^{1/2} |I\rangle$ in Liouville space describes the equilibrium state of the system at temperature T . The relation (97), i.e., the possibility to represent the equilibrium average value of an operator A as a matrix element with respect to some state lies at the basis of thermofield dynamics [33, 34].

We list the properties of the equilibrium state $|\sqrt{\rho(T)}\rangle$:

- Let the vectors $|n\rangle$ form a complete set of eigenstates of the Hamiltonian H , and let E_n be the corre-

¹²If

$$\langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle = (-1)^{(\eta_{B_i}+1)\eta_{B_i}/2} \text{Tr}(A_i B_i^\dagger) \neq 0, \quad (94)$$

then $N_{A_i} + N_{B_i}$ is even, while $m_{A_i} + n_{B_i} = n_{A_i} + m_{B_i}$.

¹³If right superoperators of creation and annihilation are defined according to (50), then

$$\langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle = \sigma_{A_i}^* \sigma_{B_i}^* (-1)^{N_{A_i}N_{B_i}} \langle\langle I|\bar{A}_i \bar{B}_i|I\rangle\rangle^*.$$

For a fermion-like $A_i B_i$, the left and right matrix elements are zero. Otherwise, $\sigma_{A_i}^* \sigma_{B_i}^* (-1)^{N_{A_i}N_{B_i}} = 1$.

sponding eigenvalues. Then $|\langle\sqrt{\rho(T)}\rangle\rangle$ can be written in the following form

$$|\langle\sqrt{\rho(T)}\rangle\rangle = \frac{1}{\sqrt{Z(T)}} \sum_n e^{-E_n/2T} |nn\rangle. \quad (98)$$

• The vector $|\langle\sqrt{\rho(T)}\rangle\rangle$ is tilde invariant. Therefore, for an arbitrary superoperator $\mathcal{C} = \mathcal{C}(\bar{a}^\dagger, \bar{a}, \bar{a}^\dagger, \bar{a})$, the equality (see (90)) holds:

$$\begin{aligned} & \langle\langle\sqrt{\rho(T)}\|\mathcal{C}\|\sqrt{\rho(T)}\rangle\rangle \\ &= \langle\langle\sqrt{\rho(T)}\|\tilde{\mathcal{C}}\|\sqrt{\rho(T)}\rangle\rangle^* = \langle\langle\sqrt{\rho(T)}\|\tilde{\mathcal{C}}^\dagger\|\sqrt{\rho(T)}\rangle\rangle. \end{aligned} \quad (99)$$

If \mathcal{C} is a fermion-like superoperator, then matrix elements (99) are equal to zero.

• Since $|\langle H\sqrt{\rho(T)}\rangle\rangle = |\langle\sqrt{\rho(T)}H\rangle\rangle$, then (see (63))

$$\mathcal{L}|\langle\sqrt{\rho(T)}\rangle\rangle = 0, \quad \langle\langle\sqrt{\rho(T)}\|\mathcal{L} = 0. \quad (100)$$

• Given that \tilde{H} is a boson-like superoperator and therefore commutes with any right superoperator, using (63) it can be shown that the following equalities hold for an arbitrary A^{14} :

$$\begin{aligned} \tilde{A}|\langle\sqrt{\rho(T)}\rangle\rangle &= \sigma_A e^{\mathcal{L}/2T} \tilde{A}^\dagger |\langle\sqrt{\rho(T)}\rangle\rangle, \\ \langle\langle\sqrt{\rho(T)}\|\tilde{A} &= \sigma_A^* \langle\langle\sqrt{\rho(T)}\|\tilde{A}^\dagger e^{\mathcal{L}/2T}. \end{aligned} \quad (101)$$

Whence, for Heisenberg superoperators (68) and (69) it follows

$$\begin{aligned} \tilde{A}(t)|\langle\sqrt{\rho(T)}\rangle\rangle &= \sigma_A \tilde{A}^\dagger(t - i/2T)|\langle\sqrt{\rho(T)}\rangle\rangle, \\ \langle\langle\sqrt{\rho(T)}\|\tilde{A}(t) &= \sigma_A^* \langle\langle\sqrt{\rho(T)}\|\tilde{A}^\dagger(t + i/2T). \end{aligned} \quad (102)$$

• Using the previous properties, for the equilibrium correlation function of two Heisenberg operators $\langle\langle A(t)B(t')\rangle\rangle$ we obtain the following relation¹⁵:

¹⁴Let us prove the first equality:

$$\begin{aligned} \tilde{A}|\langle\sqrt{\rho(T)}\rangle\rangle &= \tilde{A}\bar{\rho}^{1/2}|I\rangle\rangle = \sigma_A \bar{\rho}^{1/2} \tilde{A}^\dagger |I\rangle\rangle \\ &= \sigma_A \bar{\rho}^{1/2} \tilde{A}^\dagger \bar{\rho}^{-1/2} \bar{\rho}^{1/2} |I\rangle\rangle = \sigma_A e^{\mathcal{L}/2T} \tilde{A}^\dagger |\langle\sqrt{\rho(T)}\rangle\rangle. \end{aligned}$$

We have taken into account that \tilde{A} commutes with $\bar{\rho}^{1/2}$ and that in the equilibrium case the operator inverse to $\bar{\rho}^{1/2}$ is equal to $\bar{\rho}^{-1/2}$ (see (96)).

¹⁵Consider the following chain of equalities

$$\begin{aligned} & \langle\langle\sqrt{\rho(T)}\|\tilde{A}(t)\tilde{B}(t')\|\sqrt{\rho(T)}\rangle\rangle \\ &= \sigma_{AB} \langle\langle\sqrt{\rho(T)}\|\tilde{B}^\dagger(t')\tilde{A}^\dagger(t)\|\sqrt{\rho(T)}\rangle\rangle = \sigma_{AB}\sigma_A^*\sigma_B \\ & \quad \times \langle\langle\sqrt{\rho(T)}\|\tilde{B}^\dagger(t' - i/2T)\tilde{A}^\dagger(t + i/2T)\|\sqrt{\rho(T)}\rangle\rangle \\ &= \sigma_{AB}\sigma_A^*\sigma_B \langle\langle\sqrt{\rho(T)}\|\tilde{B}(t')\tilde{A}(t + i/T)\|\sqrt{\rho(T)}\rangle\rangle. \end{aligned}$$

If AB is the fermion-like operator, then matrix elements are zero. Otherwise $\sigma_{AB}\sigma_A^*\sigma_B = 1$, which proves (103).

$$\begin{aligned} \langle\langle A(t)B(t')\rangle\rangle &= \langle\langle\sqrt{\rho(T)}\|\tilde{A}(t)\tilde{B}(t')\|\sqrt{\rho(T)}\rangle\rangle \\ &= \langle\langle\sqrt{\rho(T)}\|\tilde{B}(t')\tilde{A}(t + i/T)\|\sqrt{\rho(T)}\rangle\rangle \\ &= \langle\langle B(t')A(t + i/T)\rangle\rangle, \end{aligned} \quad (103)$$

which is usually called the Kubo–Martin–Schwinger (KMS) condition [79, 80]. The KMS condition uniquely determines the state of system, which is described by equilibrium density matrix (95) [81, 2.2.5]. In the equilibrium case, the correlation functions in (103) depend only on the difference $t - t'$, i.e., $\langle\langle A(t)B(t')\rangle\rangle = \langle\langle A(t - t')B(0)\rangle\rangle$. Therefore, in what follows, we set $t' = 0$.

The correspondence between the superoperator method and thermofield dynamics (TFD) was first noted by Schmutz [36]. In its original formulation [33, 34], thermofield dynamics is based on the observation that the statistical average of an operator A can be represented as a matrix element $\langle 0(T)|A|0(T)\rangle$, where $|0(T)\rangle$ is a vector in the extended Hilbert space $\tilde{\mathfrak{H}} \otimes \tilde{\mathfrak{H}}$, which is defined as the tensor product of the original Hilbert space \mathfrak{H} of the quantum system under consideration and the Hilbert space $\tilde{\mathfrak{H}}$ of the fictitious system identical to the original one. All quantities related to the fictitious system are marked with a tilde. The identity of two quantum systems, the original physical and fictitious ones, implies that they have the same spectrum. In other words, if the physical system is described by the Hamiltonian H and $H|n\rangle = E_n|n\rangle$, then the fictitious system is characterized by the Hamiltonian \tilde{H} , such that $\tilde{H}|\tilde{n}\rangle = E_n|\tilde{n}\rangle$. The basis in $\mathfrak{H} \otimes \tilde{\mathfrak{H}}$ is the tensor product $|m\rangle \otimes |\tilde{n}\rangle \equiv |m\tilde{n}\rangle$. Representing $|0(T)\rangle$ in the form of a decomposition

$$|0(T)\rangle = \frac{1}{\sqrt{Z(T)}} \sum_n e^{-E_n/2T} |n\tilde{n}\rangle, \quad (104)$$

we obtain

$$\langle 0(T)|A|0(T)\rangle = \frac{1}{Z(T)} \sum_n e^{-E_n/T} \langle n|A|n\rangle = \langle\langle A\rangle\rangle, \quad (105)$$

where we used the fact that $\langle \tilde{m}|\tilde{n}\rangle = \delta_{mn}$, while the physical operator A acts only on vectors in the space \mathfrak{H} . The presence of a tensor product $|n\rangle \otimes |\tilde{n}\rangle$ in the definition of a vector $|0(T)\rangle$ allows pick up diagonal matrix elements during the calculation of $\langle 0(T)|A|0(T)\rangle$.

In the original paper by Takahashi and Umezawa [33], the vector $|0(T)\rangle$ was called the thermal vacuum, while the operator $\mathcal{H} = H - \tilde{H}$ was called the thermal Hamiltonian. Note that, by construction, the thermal vacuum is an eigenstate of the thermal Hamiltonian with a zero eigenvalue

$$\mathcal{H}|0(T)\rangle = 0. \quad (106)$$

In thermofield dynamics, the correspondence between operators in the original and fictitious Hilbert spaces is given by the tilde operation

$$(AB)^\sim = \tilde{A}\tilde{B}, \quad (aA + bB)^\sim = a^*\tilde{A} + b^*\tilde{B}, \quad (107)$$

$$(\tilde{A})^\sim = \rho_A A,$$

where a, b are the c -numbers, and $\rho_A = +1(-1)$ for a boson-like (fermion-like) operator. In addition to the mentioned rules, the so-called thermal state condition appears in the thermofield dynamics, which determines the structure of the thermal vacuum at a temperature T (cf. (101))

$$A|0(T)\rangle = (-1)^{(F+1)F/2} e^{\mathcal{H}/2T} \tilde{A}^\dagger |0(T)\rangle, \quad (108)$$

where F is the operator of the number of fermions [34, Eq. 4.2.31]. In TFD, the Kubo–Martin–Schwinger relation for the correlation functions follows from the thermal state condition.

In [33, 34], the appearance of a fictitious tilde-system was regarded as a consequence of the interaction of a physical system under consideration with a thermal bath. The presence of a thermal bath leads to the existence of a certain number of excited quanta in the system. Therefore, the energy absorption can occur in two ways: either due to the excitation of additional quanta, or due to the destruction of holes that exist due to the thermal bath. The second process is described as the destruction of the tilde quantum with negative energy. In other words, the particles (holes) of the tilde system were interpreted as holes (particles) of the physical system.

Schmutz [36] has shown that the doubling of degrees of freedom arises naturally in the transition from the description of system dynamics in Hilbert space to the description of dynamics in Liouville space. The correspondence between the Schmutz superoperator notation and the notation used in thermofield dynamics is as follows: $\vec{A} \leftrightarrow A$ and $\vec{\tilde{A}} \leftrightarrow \tilde{A}$ and $||mn\rangle\rangle \leftrightarrow |m\tilde{n}\rangle$. We recall, however, that Schmutz put $c = +1$ in (48) when defining the right fermionic creation and annihilation superoperators. With this definition, the vector $||\sqrt{\rho(T)}\rangle\rangle$ satisfies the thermal state condition in the form (108).

An alternative interpretation of thermofield dynamics was proposed by Ojima [37], who established the equivalence of the axiomatic approach in quantum field theory, associated with the use of C^* -algebra, and thermofield dynamics. In particular, he showed the relation between the tilde operation and the modular involution operation J , $JAJ = \tilde{A}$. However, to do this, he needed to redefine the fermionic creation and annihilation operators associated with the fictitious system, according to the rule $\tilde{a}_j \rightarrow i\tilde{a}_j$ and $\tilde{a}_j^\dagger \rightarrow -i\tilde{a}_j^\dagger$. Note that this redefinition completely coincides with the redefinition of the right fermionic

Schmutz superoperators, which we previously obtained (see (49)). As was shown in [37], owing to this redefinition, the relation $(\tilde{\tilde{A}})^\sim = A$ holds for both boson-like and fermion-like operators, while the thermal state condition takes a simpler form (cf. (108))

$$A|0(T)\rangle = \sigma_A e^{\mathcal{H}/2T} \tilde{A}^\dagger |0(T)\rangle, \quad (109)$$

where $\sigma_A = +1(-i)$ for a boson-like (fermion-like) operator. As can be seen, when defining tilde fermionic operators according to Ojima’s work, the double tilde conjugation rule and the thermal state condition take exactly the same form that we obtained using the superoperator formalism (see (79) and (101)).

Despite the convenience of definition of tilde operators “in the sense of Ojima,” for a long time the application of TFD to the study of the properties of hot nuclei was limited to the original version of the theory (see, e.g., [82–84]). The advantage of using the redefined tilde fermionic operators was first demonstrated in our work [35]. It was shown that by using them it is possible to obtain the correct asymptotic limit for phonon amplitudes when the strength of the residual interaction tends to zero. Later, in our papers [42–46], the redefinition of tilde (i.e., right) fermion operators was substantiated in the context of the superoperator method and demonstrated its merits in studying the properties of nonequilibrium open quantum systems.

For the sake of convenience and using the fact that the first work on thermofield dynamics [33] was published earlier than the work by Schmutz [36], we will henceforth use the TFD notation and terminology. In order to avoid misunderstandings, we give a “dictionary” of correspondences between the two notation options:

$$\begin{aligned} \vec{A} &\leftrightarrow A \\ \vec{\tilde{A}} &\leftrightarrow \tilde{A} \\ ||\sqrt{\rho(T)}\rangle\rangle &\leftrightarrow |0(T)\rangle \\ \mathcal{L} &\leftrightarrow \mathcal{H}. \end{aligned} \quad (110)$$

In other words, instead of the phrase “left (right) superoperator” we will use the term “physical (tilde) operator”; instead of “equilibrium state” we will use “thermal vacuum,” while instead of “Liouville superoperator” we will use “thermal Hamiltonian.” In this case, all the properties of the equilibrium state $||\sqrt{\rho(T)}\rangle\rangle$, mentioned at the beginning of this paragraph, become the properties of thermal vacuum $|0(T)\rangle$. In addition, rules (79) of tilde conjugation also remain valid.

We emphasize once again that we consider the thermofield dynamics as one of the options for implementing the superoperator method. Initially, the TFD was not based on the formalism of superoperators, and the introduction of an additional Hilbert space associated with a fictitious system was an artificial technique

in order to ensure the fulfillment of condition (105). The relation between TFD and the superoperator method was established by Schmutz, who showed that TFD is consistent with the choice $c = +1$ in defining right fermionic superoperators (48). The choice $c = i$ as the phase factor was substantiated in our papers [42–46]. It turned out that a simple change in the phase factor leads to a number of useful relations (see, e.g., (63) and (90)), which do not exist in TFD, and the use of which allows the thermal state condition to be written in a simpler form (cf. (108) and (109)), and also makes it possible to use the equation-of-motion method in the study of the spectral characteristics of hot systems.

4. CALCULATION OF SPECTRAL DENSITIES AND STRENGTH FUNCTIONS

Let us apply the above formalism to the calculation of the spectral characteristics of hot nuclei. We will assume that the distribution function $p_i(T)$ in (3) corresponds to the grand canonical ensemble. For highly excited nuclear compound-states, the transition from the microcanonical distribution to the grand canonical distribution is based on the use of the saddle point method when calculating the integrals characterizing the statistical averages [85, v. 1, p. 275] (see also [73, 86, 87]). For hot nuclei in the stellar matter, the argument in favor of using the distribution function of the grand canonical ensemble is the presence of a thermal bath (photon gas) and a reservoir of particles, a role of which is played by the nucleon gas surrounding the nuclei.

Let H be the nuclear Hamiltonian while $\mathcal{E}_i = \mathcal{E}_i(Z, N)$ be its eigenvalues, which depend on the number of nucleons in a nucleus. The total energy of the nucleus, $E_i = \mathcal{E}_i + M_p Z + M_n N$, includes a mass of free nucleons. We define the transition energy from state i to state f as $\Delta E_{if} = E_f - E_i$. For charge-neutral transitions, when the number of nucleons of each type does not change, this energy is equal to

$$\Delta E_{if} = \mathcal{E}_f - \mathcal{E}_i. \quad (111)$$

In the charge-exchange $n \rightarrow p$ or $p \rightarrow n$ transitions, the number of nucleons of each type changes by one and, consequently,

$$\Delta E_{if} = \mathcal{E}_f - \mathcal{E}_i \pm \Delta M_{np}. \quad (112)$$

Here, $\Delta M_{np} = M_n - M_p = 1.29$ MeV is the difference between the neutron and proton masses, and the upper (lower) sign corresponds to the $p \rightarrow n$ ($n \rightarrow p$) transition. The transition energy from excited nuclear states can be either positive or negative. In what follows, we will agree to designate transitions with positive energy as \uparrow -transitions (upward transitions), and transitions with negative energy as \downarrow -transitions (downward transitions).

For a statistical ensemble of nuclei that are in a thermal equilibrium with a bath of energy and particles at a temperature T , the probability of finding a nucleus ${}^Z_N A$ in the i th excited state is given by the distribution function of the grand canonical ensemble

$$p(\mathcal{E}_i, Z, N) = \exp\left\{-\frac{\mathcal{E}_i - \mu_n N - \mu_p Z}{T}\right\} / Z(T), \quad (113)$$

where $Z(T)$ is the partition function while $\mu_{n,p}$ are the chemical potentials of neutrons and protons. For arbitrary operators A and B , we define the spectral density of the corresponding correlation function

$$S_{AB}(E, T) = \sum_{Z, N} \sum_{i, f} p(\mathcal{E}_i, Z, N) \langle f | B | i \rangle \langle f | A | i \rangle^* \delta(E - \Delta E_{if}). \quad (114)$$

For charge-neutral operators, matrix elements are calculated between states with the same number of nucleons of each type. In the case of charge-exchange operators, the number of nucleons of each type in the initial and final states differs by one¹⁶. For $A = B$, expression (114) passes into the definition of a strength function.

$$S_A(E, T) = \sum_{Z, N} \sum_{i, f} p(\mathcal{E}_i, Z, N) B_{if}(A) \delta(E - \Delta E_{if}), \quad (115)$$

where $B_{if}(A) = |\langle f | A | i \rangle|^2$ is the probability (strength) of the transition $i \rightarrow f$. For $T \neq 0$ due to \downarrow -transitions from thermally excited states, the spectral density and the strength function have poles (singularities) in the negative energy region, i.e., at $E < 0$. Thermal effects also lead to the appearance of low-energy poles associated with transitions between closely spaced excited states of a nucleus.

Using the integral representation of the delta function $\delta(\epsilon) = \frac{1}{2\pi} \int e^{i\epsilon t} dt$, we express spectral density (114) in terms of the correlation function. For charge-neutral operators, we get

$$S_{AB}(E, T) = \int \frac{dt}{2\pi} e^{iEt} \langle\langle A^\dagger(t) B(0) \rangle\rangle. \quad (116)$$

In the case of charge-exchange operators, the relationship between the spectral density and the correla-

¹⁶We assume that the proton has an isospin projection $-1/2$, while neutron, $+1/2$. Then charge-exchange operators of $n \rightarrow p$ transitions contain the operator lowering the isospin t_- ($t_- | n \rangle = | p \rangle$), while operators of $p \rightarrow n$ transitions contain the isospin-raising operator t_+ ($t_+ | p \rangle = | n \rangle$). Note also that if A corresponds to transition $n \rightarrow p$, then A^\dagger is the $p \rightarrow n$ transition operator and vice versa.

tion function in the grand canonical ensemble takes the form

$$S_{AB}(E, T) = \int \frac{dt}{2\pi} e^{i(E \mp \Delta_{np})t} \langle\langle A^\dagger(t)B(0) \rangle\rangle, \quad (117)$$

where the upper (lower) sign corresponds to $p \rightarrow n$ ($n \rightarrow p$) transitions. The value $\Delta_{np} = \Delta\mu_{np} + \Delta M_{np}$ ($\Delta\mu_{np} = \mu_n - \mu_p$) in the exponent arises as a result of using a grand canonical ensemble and changing the number of protons and neutrons in charge-exchange transitions. Note that when using the distribution function of the grand canonical ensemble, the Heisenberg representation of operators contains chemical potentials, i.e.,

$$A(t) = e^{i(H - \mu_n N - \mu_p Z)t} A e^{-i(H - \mu_n N - \mu_p Z)t}, \quad (118)$$

where N (Z) is the operator of the number of neutrons (protons).

From the KMS condition (103) for the correlation functions, it follows that the spectral densities satisfy the property

$$S_{B^\dagger A^\dagger}(-E, T) = e^{-E/T} S_{AB}(E, T) \quad (119)$$

for charge-neutral operators, and

$$S_{B^\dagger A^\dagger}(-E, T) = e^{-(E \mp \Delta_{np})/T} S_{AB}(E, T) \quad (120)$$

for charge-exchange operators. As before, the upper (lower) sign corresponds to the case when $S_{AB}(E, T)$ is the spectral density of the $p \rightarrow n$ ($n \rightarrow p$) transition operators, and, therefore, $S_{B^\dagger A^\dagger}(E, T)$ is the spectral density of the ‘‘inverse’’ $n \rightarrow p$ ($p \rightarrow n$) transition operators (see footnote 16 on page 899). Relations (119) and (120) will be referred to below as the principle of detailed balance for spectral densities. We emphasize that the latter equation, which relates the spectral densities and charge-exchange operators, is valid only in the grand canonical ensemble. In contrast, relation (119) is also valid in the canonical ensemble.

Let us use (97) and write the spectral densities (116) and (117) in the form of the Fourier transform of the thermal vacuum average

$$S_{AB}(E, T) = \int \frac{dt}{2\pi} e^{iEt} \langle 0(T) | A^\dagger(t) B(0) | 0(T) \rangle \quad (121)$$

for charge-neutral operators, and

$$S_{AB}(E, T) = \int \frac{dt}{2\pi} e^{i(E \mp \Delta_{np})t} \langle 0(T) | A^\dagger(t) B(0) | 0(T) \rangle \quad (122)$$

in the case of charge-exchange operators. Recall that, in the original superoperator notation, A and B are left superoperators, while the thermal vacuum is a vector in the Liouville space (see (110)).

Let us derive an energy representation for the spectral densities (121) and (122), based on the fact that the time translation operator in the extended Hilbert

space (i.e., in the Liouville space) is the thermal Hamiltonian \mathcal{H} (see (70))¹⁷. Since $\mathcal{H} = \mathcal{H}^\dagger$, then all eigenvalues of the thermal Hamiltonian are real. In addition, to each eigenstate of the thermal Hamiltonian \mathcal{H} with positive energy

$$\mathcal{H} | \mathbb{O}_k \rangle = \mathcal{E}_k | \mathbb{O}_k \rangle, \quad (124)$$

a tilde conjugate eigenstate with negative energy corresponds:

$$\mathcal{H} | \tilde{\mathbb{O}}_k \rangle = -\mathcal{E}_k | \tilde{\mathbb{O}}_k \rangle. \quad (125)$$

Indeed, since $\tilde{\mathcal{H}} = -\mathcal{H}$ (see (80)), then considering (88) and (89), for an arbitrary vector $|mn\rangle$ we have

$$\begin{aligned} \langle mn | \mathcal{H} | \tilde{\mathbb{O}}_k \rangle &= \langle \widetilde{mn} | \tilde{\mathcal{H}} | \mathbb{O}_k \rangle^* = -\langle \widetilde{mn} | \mathcal{H} | \mathbb{O}_k \rangle^* \\ &= -\mathcal{E}_k \langle \widetilde{mn} | \mathbb{O}_k \rangle^* = -\mathcal{E}_k \langle mn | \tilde{\mathbb{O}}_k \rangle, \end{aligned} \quad (126)$$

which proves (125). In what follows, the eigenstates of the thermal Hamiltonian with positive (negative) energy will be called the nontilde (tilde) states.

The completeness property of the eigenstates of the thermal Hamiltonian allows the spectral density of charge-neutral operators to be written in the form of the following expansion

$$\begin{aligned} S_{AB}(E, T) &= \sum_k \{ \langle \mathbb{O}_k | B | 0(T) \rangle \langle \mathbb{O}_k | A | 0(T) \rangle^* \delta(E - \mathcal{E}_k) \\ &+ \langle \tilde{\mathbb{O}}_k | B | 0(T) \rangle \langle \tilde{\mathbb{O}}_k | A | 0(T) \rangle^* \delta(E + \mathcal{E}_k) \}. \end{aligned} \quad (127)$$

A similar expansion for charge-exchange operators has the form

$$\begin{aligned} S_{AB}(E, T) &= \sum_k \{ \langle \mathbb{O}_k | B | 0(T) \rangle \langle \mathbb{O}_k | A | 0(T) \rangle^* \delta(E - \mathcal{E}_k \mp \Delta_{np}) \\ &+ \langle \tilde{\mathbb{O}}_k | B | 0(T) \rangle \langle \tilde{\mathbb{O}}_k | A | 0(T) \rangle^* \delta(E + \mathcal{E}_k \mp \Delta_{np}) \}, \end{aligned} \quad (128)$$

where, as before, the upper (lower) sign corresponds to $p \rightarrow n$ ($n \rightarrow p$) transitions. We especially note the fact that poles of the charge-exchange spectral densities are shifted with respect to the eigenvalues of the thermal Hamiltonian by Δ_{np} .

Formally, the Eqs. (127) and (128) have the same form as the spectral densities at zero temperature: they contain a single summation over the eigenstates of the (thermal) Hamiltonian, and the thermal vacuum plays the role of the ground state. The position of poles of the spectral density is determined by the eigenvalues of the thermal Hamiltonian, and its intensity depends on the amplitude of transitions from the thermal vacuum to the eigenstates of thermal Hamiltonian. The difference from the case $T = 0$ is that the spectrum of ther-

¹⁷Since the calculations are carried out in the grand canonical ensemble, the thermal Hamiltonian contains the chemical potentials

$$\mathcal{H} = (H - \mu_p Z - \mu_n N) - (\tilde{H} - \mu_p \tilde{Z} - \mu_n \tilde{N}). \quad (123)$$

mal Hamiltonian consists of both positive and negative eigenvalues and, in principle, depends on temperature. The transition amplitudes also depend on the temperature.

Acting on both sides of equality (109) on the eigenfunctions of thermal Hamiltonian and using the fact that $\langle \tilde{\mathcal{O}}_k | \tilde{A}^\dagger | 0(T) \rangle = \langle \tilde{\mathcal{O}}_k | A^\dagger | 0(T) \rangle^*$ (see (88)), we obtain the following formulation of the thermal state condition

$$\langle \tilde{\mathcal{O}}_k | A | 0(T) \rangle = \sigma_A e^{-\mathcal{E}_k/2T} \langle \tilde{\mathcal{O}}_k | A^\dagger | 0(T) \rangle^*, \quad (129)$$

from which the validity of the principle of detailed balance for spectral densities (127) and (128) follows. As it should be, for $T = 0$, the amplitudes of transitions to tilde states are equal to zero. Therefore, in cold nuclei, the spectral densities of charge-neutral operators vanish for $E < 0$. For $T = 0$, the spectral density of operators of $p \rightarrow n$ ($n \rightarrow p$) transitions vanishes at $E < \Delta_{np}$ ($E < -\Delta_{np}$), i.e., the quantity Δ_{np} ($-\Delta_{np}$) plays a role of an effective threshold for charge-exchange reactions on the ground state.

Using (127) and (128), we write the energy representation of strength functions (115) in the form

$$S_A(E, T) = \sum_k \{ B_k(A) \delta(E - \mathcal{E}_k) + \tilde{B}_k(A) \delta(E + \mathcal{E}_k) \} \quad (130)$$

for a charge-neutral operator, and

$$S_A(E, T) = \sum_k \{ B_k(A) \delta(E - \mathcal{E}_k \mp \Delta_{np}) + \tilde{B}_k(A) \delta(E + \mathcal{E}_k \mp \Delta_{np}) \} \quad (131)$$

for the charge-exchange operator. Quantities

$$B_k(A) = |\langle \tilde{\mathcal{O}}_k | A | 0(T) \rangle|^2, \quad \tilde{B}_k(A) = |\langle \tilde{\mathcal{O}}_k | A | 0(T) \rangle|^2 \quad (132)$$

denote the strength (probability) of the transition from the thermal vacuum to the eigenstates of thermal Hamiltonian. The poles (singularities) E_k , \tilde{E}_k of the strength functions will be called the transition energy.

In charge-neutral processes, the transition energy coincides with the state energy

$$E_k = \mathcal{E}_k, \quad \tilde{E}_k = -\mathcal{E}_k. \quad (133)$$

Therefore, the excitation of a hot nucleus in a charge-neutral process corresponds to the \uparrow -transition to a nontilde state of the thermal Hamiltonian, while deexcitation corresponds to the \downarrow -transition to a tilde state. According to (129), the excitation and deexcitation probabilities are related by the detailed balance principle

$$\tilde{B}_k(A) = e^{-E_k/T} B_k(A^\dagger). \quad (134)$$

For charge-exchange processes, the transition energy differs from the state energy by the value of effective threshold

$$E_k^{(\pm)} = \mathcal{E}_k \pm \Delta_{np}, \quad \tilde{E}_k^{(\pm)} = -\mathcal{E}_k \pm \Delta_{np}, \quad (135)$$

where the sign + (−) corresponds to the $p \rightarrow n$ ($n \rightarrow p$) transition. Therefore, a part of the nontilde (tilde) states may appear at a negative (positive) transition energy. In this case, each $p \rightarrow n$ transition is matched by an inverse $n \rightarrow p$ transition to the tilde-conjugated state. The energies of these transitions differ in sign, $\tilde{E}_k^{(\pm)} = -E_k^{(\mp)}$, while the probabilities are related by the principle of detailed balance

$$\tilde{B}_k(A) = e^{-(E_k^{(\pm)} \mp \Delta_{np})/T} B_k(A^\dagger). \quad (136)$$

We recall once again that relation (136) between the probabilities of excitation and deexcitation of a hot nucleus in charge-exchange transitions is valid only in the grand canonical ensemble. In the canonical ensemble, a similar relationship has a more complex form and includes the ratio of the partition functions of the parent and daughter nuclei [88, Eq. 8]¹⁸.

So, we have shown that, within the formalism of superoperators, the problem of calculating the spectral densities and strength functions in a hot nucleus is reduced to finding the eigenstates (i.e., diagonalization) of the thermal Hamiltonian. As in the case of $T = 0$, this problem for most systems with interaction can only be solved approximately. The advantage of the formalism is that to find the eigenstates of the thermal Hamiltonian, we can apply the methods used at zero temperature: the approximation of independent quasiparticles, the random phase approximation, etc. At the same time, as will be shown in the next section, the procedure for diagonalizing the thermal Hamiltonian has its own peculiarities related to the requirement that the thermal state condition (129) be satisfied.

At the end of this section, we present the well-known relations for spectral densities, which directly follow from the expansions of (127) and (128) considering that $[A, \tilde{H}] = 0$. Namely:

$$S_{|A, H|B}(E, T) = E S_{AB}(E, T) \quad (137)$$

for charge-neutral operators, and

$$S_{|A, H|B}(E, T) = (E \mp \Delta_{np}) S_{AB}(E, T) \quad (138)$$

for charge-exchange operators. In the latter equality, the upper (lower) sign corresponds to $p \rightarrow n$ ($n \rightarrow p$) transitions. As is known, the indicated relation of spectral densities, containing the operator A and its

¹⁸The expression for the detailed balance obtained in [88] transforms into (136) if the ratio of the partition functions of the parent and daughter nuclei is set equal to unity, while a difference in the masses of the nuclei is considered equal to the effective threshold.

commutator with the Hamiltonian as an argument, is the basis for constructing a chain of equations for the two-time temperature Green's functions [89]. Here, this relation is given only to show its validity within the superoperator method.

5. EQUATION-OF-MOTION METHOD WITH $T \neq 0$

To emphasize the features inherent in the diagonalization of the thermal Hamiltonian, we use the equation-of-motion method [39–41]. Let the vectors $|\mathbb{O}_k\rangle$ in the extended Hilbert space (i.e., in the Liouville space) be eigenstates of the thermal Hamiltonian:

$$\mathcal{H}|\mathbb{O}_k\rangle = \mathcal{E}_k|\mathbb{O}_k\rangle.$$

Let us define (super)operators \mathbb{O}_k^\dagger and \mathbb{O}_k such that

$$|\mathbb{O}_k\rangle = \mathbb{O}_k^\dagger|0(T)\rangle$$

and

$$\mathbb{O}_k|0(T)\rangle = 0 \text{ for all } k,$$

where $|0(T)\rangle$ is the thermal vacuum, i.e., $\mathcal{H}|0(T)\rangle = 0$.

In particular, we can put $\mathbb{O}_k^\dagger = |\mathbb{O}_k\rangle\langle 0(T)|$ and $\mathbb{O}_k = |0(T)\rangle\langle \mathbb{O}_k|$. Since

$$[\mathcal{H}, \mathbb{O}_k^\dagger]|0(T)\rangle = \mathcal{E}_k\mathbb{O}_k^\dagger|0(T)\rangle,$$

then, multiplying this equality from the left by an arbitrary vector $\langle 0(T)|\delta\mathcal{O}$, we arrive at an equation for \mathbb{O}_k^\dagger

$$\begin{aligned} \langle 0(T)|[\delta\mathcal{O}, [\mathcal{H}, \mathbb{O}_k^\dagger]]|0(T)\rangle \\ = \mathcal{E}_k\langle 0(T)|[\delta\mathcal{O}, \mathbb{O}_k^\dagger]|0(T)\rangle. \end{aligned} \quad (139)$$

According to the properties proved earlier (see pages 896 and 900) $\mathcal{H}|\tilde{\mathbb{O}}_k\rangle = -\mathcal{E}_k|\tilde{\mathbb{O}}_k\rangle$, where $|\tilde{\mathbb{O}}_k\rangle = \tilde{\mathbb{O}}_k^\dagger|0(T)\rangle$. Besides, $\tilde{\mathbb{O}}_k|0(T)\rangle = 0$.

The fact that $\tilde{\mathbb{O}}_k^\dagger$ also satisfies equation of motion (139) is easy to verify if we consider that $\delta\mathcal{O}$ is an arbitrary operator. Using in (139) instead of $\delta\mathcal{O}$ the tilde-conjugate operator $\delta\tilde{\mathcal{O}}$ and applying the complex conjugation operation to both parts of the equality, with the help of (88) we obtain

$$\begin{aligned} \langle 0(T)|[\delta\mathcal{O}, [\mathcal{H}, \tilde{\mathbb{O}}_k^\dagger]]|0(T)\rangle \\ = -\mathcal{E}_k\langle 0(T)|[\delta\mathcal{O}, \tilde{\mathbb{O}}_k^\dagger]|0(T)\rangle. \end{aligned} \quad (140)$$

Recall that in order to distinguish between the positive and negative energy eigenstates of the thermal Hamiltonian, the latter are marked with a tilde (see (125)).

Until now, the consideration has not differed from the standard presentation of the application of the equation-of-motion method to finding the eigenstates of the cold nucleus Hamiltonian [39–41]. Note, however, that in the case of a thermal Hamiltonian, equa-

tion of motion (139) does not in itself lead to a unique definition of the structure of the diagonalizing operators. Indeed, using in (139) instead of $\delta\mathcal{O}$ the operator $\delta\tilde{\mathcal{O}}^\dagger$ and applying property (88), we get

$$\begin{aligned} \langle 0(T)|[\delta\mathcal{O}, [\mathcal{H}, \tilde{\mathbb{O}}_k]]|0(T)\rangle \\ = \mathcal{E}_k\langle 0(T)|[\delta\mathcal{Q}, \tilde{\mathbb{O}}_k]|0(T)\rangle. \end{aligned} \quad (141)$$

Therefore, the solution to the equation of motion for a given \mathcal{E}_k is an arbitrary linear combination $\mathcal{Q}_k^\dagger = x\mathbb{O}_k^\dagger + y\tilde{\mathbb{O}}_k$. However, the thermal vacuum cannot simultaneously be a vacuum state both for the operators \mathbb{O}_k and for the operators \mathcal{Q}_k . Therefore, from all the set of solutions (139), it is necessary to single out those whose vacuum state satisfies the thermal state condition at a given temperature. To this end, we require the fulfillment of the thermal state condition in the form (129), from which it follows that

$$\begin{aligned} e^{-\mathcal{E}_k/2T}\langle 0(T)|[\mathbb{O}_k, A]_\pm|0(T)\rangle \\ = \sigma_A\langle 0(T)|[A, \tilde{\mathbb{O}}_k^\dagger]_\pm|0(T)\rangle \end{aligned} \quad (142)$$

for an arbitrary physical operator A . The anticommutator $[\dots]_\pm$ corresponds to the case when \mathbb{O}_k and A are both fermion-like operators.

Formally, the equation of motion (139) together with the thermal state condition in the form (142) makes it possible to find the exact eigenstates of the thermal Hamiltonian. In practical calculations, however, we are looking for a solution to the equation of motion in the form of an expansion in a limited set of some basic operators $\delta\mathcal{O}$. However, even in this case, solution (139) requires knowledge of the vacuum state of the operators \mathbb{O}_k . This condition can be satisfied by solving the equation of motion using iterations. However, since the presence of a double commutator on the left-hand side of (139) reduces the sensitivity of the equation of motion solution to the choice of $|0(T)\rangle$, then its approximation $|\psi_0(T)\rangle$ ¹⁹ can be used as a thermal vacuum. The mandatory requirement for $|\psi_0(T)\rangle$ is its tilde invariance.

To guarantee the orthogonality of the thermal Hamiltonian eigenfunctions in the approximate solution to the equation of motion, the double commutator on the right-hand side of (139) should be replaced by a symmetric double commutator [39–41]. As a

¹⁹Recall that it is precisely this situation is realized in the derivation of the RPA equations, when the Hartree–Fock vacuum is used as the ground state in the equation of motion instead of the phonon vacuum [41].

result, we arrive at the equation of motion in the following form

$$\begin{aligned} & \langle \Psi_0(T) | [\delta O, \mathcal{H}, \mathbb{O}_k^\dagger] | \Psi_0(T) \rangle \\ & = \mathcal{E}_k \langle \Psi_0(T) | [\delta O, \mathbb{O}_k^\dagger] | \Psi_0(T) \rangle, \end{aligned} \quad (143)$$

where

$$[A, B, C] = \frac{1}{2} \{ [A, [B, C]] + [[A, B], C] \}. \quad (144)$$

If \mathbb{O}_k^\dagger is a fermion-like operator, then in (143) instead of commutators, anticommutators are used.

The approximate nature of the solution to the equation of motion leads to the fact that the thermal state condition (142) can be satisfied only for a certain class of operators A . Let us pay attention to the fact that if (142) is valid for some set of operators A_n , then it is also valid for their linear combination. Therefore, in order for the spectral densities of one-particle operators describing the external action on a hot nucleus to satisfy the detailed balance principle (119), (120), we will consider the one- and two-fermion operators of the form a^\dagger , a , $a_1^\dagger a_2^\dagger$, $a_1^\dagger a_2$, $a_1 a_2$, as a set. It should be emphasized that, regardless of which vacuum state is used in (143), it is precisely the vacuum of the operators \mathbb{O}_k that appears in the thermal state condition (142).

Before proceeding to the consideration of various approximate methods for finding the eigenstates of a thermal Hamiltonian, we note once again that the requirement that the thermal state condition (142) be satisfied at each stage of diagonalization of the thermal Hamiltonian is a distinctive feature of the presented approach, which makes it thermodynamically consistent, since it guarantees the fulfillment of the principle of detailed balance (119), (120) for spectral densities and strength functions of one-particle operators.

6. MODELING THE NUCLEAR HAMILTONIAN

We apply the above formalism for calculating spectral densities and strength functions to the nuclear Hamiltonian, which consists of the mean field for protons and neutrons H_{mf} , pairing interaction and residual nucleon–nucleon interaction H_{res} :

$$H = H_{mf} + H_{pair} + H_{res}. \quad (145)$$

In all further theoretical calculations and numerical calculations, we will assume the spherical symmetry of the mean field potential. In this case, $(2j+1)$ -fold degenerate single-particle levels of the mean field are characterized by quantum numbers $nljm$, where m is the projection of the total moment j . For the sake of brevity of the notation, the indices nl will be omitted (i.e., $j \equiv nlj$), while the nucleon creation and annihilation operators will be denoted as a_{jm}^\dagger and a_{jm} . Using

these notations, we write the one-particle part of the Hamiltonian as

$$H_{mf} = \sum_{\tau=p,n} \sum_{jm}^\tau (E_{jm} - \mu_\tau) a_{jm}^\dagger a_{jm}, \quad (146)$$

where \sum^τ means that the summation is performed either over proton ($\tau = p$) or neutron ($\tau = n$) single-particle states. If there is no special notation, then the summation over j means, in addition, the summation over the isotopic index τ .

Since all calculations are carried out in the grand canonical ensemble, then the inclusion of a term containing the chemical potential μ_τ in the Hamiltonian makes it possible to ensure that the number of particles is conserved on average. Single-particle energies E_{jm} either correspond to a phenomenological potential (e.g., the Woods–Saxon potential) or are obtained as a result of solving the Hartree–Fock equations using the effective nucleon–nucleon interaction. Strictly speaking, the energies of single-particle levels depend on temperature. However, Hartree–Fock calculations performed using the Skyrme interaction demonstrate the mean field stability with respect to temperature increase up to $T \lesssim 5$ MeV [90, 91] (see also [12, p. 166]). Since the temperatures at which the reactions of interest to us proceed during a supernova explosion do not exceed this value, we further assume that the energies and wave functions of nuclear single-particle states are the same as at zero temperature.

As a pairing interaction, we use monopole forces that act only between identical nucleons

$$H_{pair} = -\frac{1}{4} \sum_{\tau=n,p} G_\tau \sum_{j_1 m_1, j_2 m_2}^\tau a_{j_1 m_1}^\dagger a_{j_1 m_1}^\dagger a_{j_2 m_2} a_{j_2 m_2}, \quad (147)$$

where the bar above quantum numbers means the time reversal operation $a_{j\bar{m}} = (-1)^{j-m} a_{j-m}$. The choice of constants $G_{n,p}$ is based on the reproduction of an even–odd mass difference.

As a residual interaction H_{res} , we use the central particle–hole interaction of two types: (i) a schematic separable interaction, which is used in the Hamiltonian of the quasiparticle–phonon nuclear model [92]; (ii) interaction in the form of Landau–Migdal forces [93], the parameters of which are expressed in terms of the parameters of Skyrme forces [94]. The separabilization procedure proposed in [95, 96] makes it possible to write the Landau–Migdal interaction as a sum of a finite number N of separabilization terms.

Let us briefly describe the separabilization procedure for the Landau–Migdal forces and, along the way, introduce the notation used in what follows. Fol-

lowing [94, 95], we write the Landau–Migdal forces in the coordinate representation as follows

$$H_{\text{res}}(r_1, r_2) = N_0^{-1} [F_0(r_1) + G_0(r_1) \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 + (F_0'(r_1) + G_0'(r_1) \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2) \boldsymbol{\tau}_1 \boldsymbol{\tau}_2] \delta(r_{12}). \quad (148)$$

Here $N_0 = 2k_F m^* / \pi^2 \hbar^2$, where k_F is the Fermi momentum and m^* is the effective nucleon mass. Traditionally, residual forces in the Landau–Migdal form are used in the study of charge-neutral and charge-exchange excitations of the nucleus in the context of the theory of finite Fermi systems [93, 97–99]. Matrix elements of the interaction (148) can be represented in the form of N separable terms using the Gaussian integration formula for N points [100, Eq. 25.4.30]

$$\int_0^R f(r) dr \approx \frac{R}{2} \sum_{k=1}^N w_k f(r_k). \quad (149)$$

The values of abscissas r_k and weights w_k depend on the number N of points in the Gauss formula. In numerical calculations, we always assumed $N = 40$. Although formally, when calculating matrix elements of $H_{\text{res}}(\mathbf{r}_1, \mathbf{r}_2)$, integration extends up to $r = \infty$, a choice of the sufficiently large truncation radius $R = 3R_{\text{nuc}}$ allows the radial integral to be calculated with good accuracy. This choice of R and the number N of Gauss integration points makes it possible to almost completely eliminate the errors associated with the calculation of the matrix elements of the residual interaction. As shown in [95], the use of the separable form of residual interaction (148) makes it possible to reduce solving the RPA equations to the secular equation of the order of $\sim N$, which greatly simplifies calculations in a large configuration space and makes it possible to perform global microscopic calculations for a large number of nuclei.

In the second quantization representation, the residual interaction (148) after the separabilization procedure is written as the sum of multipole and spin-multipole components

$$H_{\text{res}} = H_{\text{ph}}^m + H_{\text{ph}}^s. \quad (150)$$

In turn, each of the components is written as the sum of N separable terms:

$$H_{\text{ph}}^m = -\frac{1}{2} \sum_{k=1}^N [\chi_0^{(m;k)} + \boldsymbol{\tau}_1 \boldsymbol{\tau}_2 \chi_1^{(m;k)}] \sum_{JM} \mathcal{M}_{JM}^{(k)\dagger} \mathcal{M}_{JM}^{(k)}, \quad (151)$$

$$H_{\text{ph}}^s = -\frac{1}{2} \sum_{k=1}^N [\chi_0^{(s;k)} + \boldsymbol{\tau}_1 \boldsymbol{\tau}_2 \chi_1^{(s;k)}] \times \sum_{JM} \sum_{L=J, J \pm 1} \mathcal{S}_{LJM}^{(k)\dagger} \mathcal{S}_{LJM}^{(k)}. \quad (152)$$

We use the following definition of multipole and spin-multipole operators²⁰

$$\begin{aligned} \mathcal{M}_{JM}^{(k)\dagger} &= -\hat{J}^{-1} \sum_{j_1 j_2} f_{j_1 j_2}^{(J;k)} [a_{j_1}^\dagger a_{j_2}^\dagger]_{JM} = \mathcal{M}_{JM}^{(k)}, \\ \mathcal{S}_{LJM}^{(k)\dagger} &= -\hat{J}^{-1} \sum_{j_1 j_2} f_{j_1 j_2}^{(LJ;k)} [a_{j_1}^\dagger a_{j_2}^\dagger]_{JM} = -\mathcal{S}_{LJM}^{(k)}, \end{aligned} \quad (157)$$

where $f_{j_1 j_2}^{(J;k)}$ and $f_{j_1 j_2}^{(LJ;k)}$ are the corresponding reduced matrix elements

$$\begin{aligned} f_{j_1 j_2}^{(J;k)} &= i^J u_{j_1}(r_k) u_{j_2}(r_k) \langle j_1 \| Y_J \| j_2 \rangle, \\ f_{j_1 j_2}^{(LJ;k)} &= i^L u_{j_1}(r_k) u_{j_2}(r_k) \langle j_1 \| [Y_L \boldsymbol{\sigma}]_J \| j_2 \rangle, \end{aligned} \quad (158)$$

which have the properties $f_{j_1 j_2}^{(J;k)} = (-1)^{j_1 - j_2 + J} f_{j_2 j_1}^{(J;k)}$ and $f_{j_1 j_2}^{(LJ;k)} = (-1)^{j_1 + j_2 + J} f_{j_2 j_1}^{(LJ;k)}$. The value $u_j(r_k)$ denotes the radial part of the wave function of the nucleon $\phi_j(r) = u_j(r)/r$ at the point with the abscissa r_k used in the Gauss integration formula (149). The isoscalar $\chi_0^{(m;k)}, \chi_0^{(s;k)}$ and isovector $\chi_1^{(m;k)}, \chi_1^{(s;k)}$ constants of the multipole and spin-multipole interactions are expressed in terms of the parameters of the Landau–Migdal forces (148). For example, $\chi_0^{(m;k)} = -F_0(r_k) R w_k / (2N_0 r_k^2)$. Expressions for $\chi_0^{(s;k)}, \chi_1^{(m;k)}$ and $\chi_1^{(s;k)}$ are obtained, respectively, by replacing F_0 with F_0', G_0 and G_0' .

At $N = 1$, the multipole and spin-multipole residual interaction in the form (151), (152) becomes iden-

²⁰ Following [85, v. 1, p. 86], we use the following definition of a reduced matrix element $t_{j_1 j_2}^{(J)} = \langle j_1 \| T_J \| j_2 \rangle$

$$\langle j_1 m_1 | T_{JM} | j_2 m_2 \rangle = \hat{J}^{-1} \langle j_2 m_2 J M | j_1 m_1 \rangle t_{j_1 j_2}^{(J)}. \quad (153)$$

Then for the M th component of an arbitrary one-particle tensor operator T_J , we can write

$$\begin{aligned} T_{JM} &= \sum_{j_1 m_1} \langle j_1 m_1 | T_{JM} | j_2 m_2 \rangle a_{j_1 m_1}^\dagger a_{j_2 m_2} \\ &= -\hat{J}^{-1} \sum_{j_1 j_2} t_{j_1 j_2}^{(J)} [a_{j_1}^\dagger a_{j_2}^\dagger]_{JM}, \end{aligned} \quad (154)$$

where $\hat{J} = \sqrt{2J+1}$, and with the use of square brackets $[\dots]_{JM}$, the coupling of two angular momenta into the total angular momentum J with the projection M is denoted:

$$[a_{j_1}^\dagger a_{j_2}^\dagger]_{JM} = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | J M \rangle a_{j_1 m_1}^\dagger a_{j_2 m_2}^\dagger. \quad (155)$$

The notation $[a_{j_1}^\dagger a_{j_2}^\dagger]_{JM}$ in (154) and (157) means

$$[a_{j_1}^\dagger a_{j_2}^\dagger]_{JM} = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | J M \rangle a_{j_1 m_1}^\dagger a_{j_2 m_2}^\dagger. \quad (156)$$

We also introduce the notation used in what follows $A_{JM} = (-1)^{J-M} A_{J-M}$.

tical to the residual interaction used in the quasiparticle–phonon nuclear model (QPM) Hamiltonian

$$H_{\text{ph}}^m = -\frac{1}{2} \sum_J [\chi_0^{(J)} + \tau_1 \tau_2 \chi_1^{(J)}] \sum_M \mathcal{M}_{JM}^\dagger \mathcal{M}_{JM},$$

$$H_{\text{ph}}^s = -\frac{1}{2} \sum_J \sum_{L=J, J \pm 1} [\chi_0^{(LJ)} + \tau_1 \tau_2 \chi_1^{(LJ)}] \sum_M \mathcal{S}_{LJM}^\dagger \mathcal{S}_{LJM}, \quad (159)$$

while the expressions for multipole and spin-multipole operators are the same as (157) up to the replacement of reduced matrix elements by

$$f_{j_1 j_2}^{(J)} = \langle j_1 \| i^J R_J(r) Y_J M \| j_2 \rangle,$$

$$f_{j_1 j_2}^{(LJ)} = \langle j_1 \| i^L R_J(r) [Y_L \sigma]_J \| j_2 \rangle, \quad (160)$$

where $R(r)$ is the radial dependence of the separable forces used in the QPM.

The equations obtained below for calculating the structure and energy of thermal phonons are also used in our calculations with the QPM Hamiltonian. There is, however, a fundamental difference. In (151) and (152) all coupling constants are related to the parameters of the Landau–Migdal forces, which, in turn, are expressed in terms of the parameters of the Skyrme forces [94]. In QPM, there is no unambiguous procedure for choosing the radial dependence of separable forces and coupling constants. Traditionally, QPM uses the forces $R(r) = r^\lambda$, where λ is the rank of spherical harmonic $Y_{\lambda\mu}$ in the definition of multipole and spin-multipole operators (159), or the forces $R(r) = dV(r)/dr$, where $V(r)$ is the central part of the one-particle potential. The values of the constants of the multipole $\chi_{0,1}^{(J)}$ and spin-multipole $\chi_{0,1}^{(LJ)}$ forces depend on the type of $R(r)$, and their choice is based on experimental data and qualitative estimates [101].

The residual interaction (151), (152) contains the scalar product of the Pauli matrices τ_1 and τ_2 , acting on the isotopic wave functions of the nucleon. Expanding the scalar product $\tau_1 \tau_2$ as

$$\tau_1 \tau_2 = \tau_0^{(1)} \tau_0^{(2)} + 2(t_+^{(1)} t_-^{(2)} + t_-^{(1)} t_+^{(2)}), \quad (161)$$

where $\tau_0 |n\rangle = +|n\rangle$, $\tau_0 |p\rangle = -|p\rangle$ and $t_- |n\rangle = |p\rangle$, $t_+ |p\rangle = |n\rangle$, we divide the residual interaction into the charge-neutral part

$$H_{\text{ch.n}} = -\frac{1}{2} \sum_{JM} \sum_{\tau, \rho = \pm 1} \sum_k \chi_\rho^{(m;k)} \mathcal{M}_{JM}^{(k)\dagger}(\tau) \mathcal{M}_{JM}^{(k)}(\rho\tau)$$

$$- \frac{1}{2} \sum_{JM} \sum_{L=J, J \pm 1} \sum_{\tau, \rho = \pm 1} \sum_k \chi_\rho^{(s;k)} \mathcal{S}_{LJM}^{(k)\dagger}(\tau) \mathcal{S}_{LJM}^{(k)}(\rho\tau) \quad (162)$$

and the charge-exchange part

$$H_{\text{ch.ex}} = -2 \sum_{JM} \sum_k \chi_1^{(m;k)} \mathcal{M}_{JM}^{(k)\dagger} \mathcal{M}_{JM}^{(k)}$$

$$- 2 \sum_{JM} \sum_{L=J, J \pm 1} \sum_k \chi_1^{(s;k)} \mathcal{S}_{LJM}^{(k)\dagger} \mathcal{S}_{LJM}^{(k)}. \quad (163)$$

In the charge-neutral part (162) the notations $\chi_\rho^{(m;k)} = \chi_0^{(m;k)} + \rho \chi_1^{(m;k)}$, $\chi_\rho^{(s;k)} = \chi_0^{(s;k)} + \rho \chi_1^{(s;k)}$ ($\rho = \pm 1$) are introduced, and the multipole and spin-multipole operators contain summation over either neutron ($\tau = n$) or proton ($\tau = p$) single-particle states. The replacement $\tau \leftrightarrow -\tau$ means the substitution $n \leftrightarrow p$. In the charge-exchange part of the residual interaction

(163) the single-particle operators \mathcal{M}^\dagger , \mathcal{S}^\dagger contain summation over proton-neutron states, i.e., $\sum_{j_1 j_2} \equiv \sum_{j_p j_n}$ in expressions (157).

As was shown in the previous section, in order to calculate the spectral densities and strength functions of a hot nucleus in the context of the superoperator method, it is necessary to diagonalize the thermal Hamiltonian

$$\mathcal{H} = H - \tilde{H} = \mathcal{H}_{\text{mf}} + \mathcal{H}_{\text{pair}} + \mathcal{H}_{\text{res}}, \quad (164)$$

where \tilde{H} is obtained from original Hamiltonian (145) by replacing the creation and annihilation operators a_{jm}^\dagger, a_{jm} , with tilde partners $\tilde{a}_{jm}^\dagger, \tilde{a}_{jm}$, i.e., if $H \equiv H(a^\dagger, a)$, then $\tilde{H} \equiv H(\tilde{a}^\dagger, \tilde{a})$. The thermal Hamiltonian \mathcal{H} inherits the structure of original Hamiltonian H . Therefore, to find its eigenstates, the same methods can be applied which are used in studying the properties of excited states of cold nuclei. These methods are the BCS approximation for considering pairing correlations, treatment of the residual interaction within the random phase approximation, bosonic expansions²¹, etc. An essential difference, as already noted, is the requirement that the thermal state condition (142) be satisfied. It is this condition that determines the temperature of the system and allows the thermodynamically consistent (i.e., without violating the principle of detailed balance) calculation of the spectral densities and strength functions. In first works on the application of thermofield dynamics methods to the study of the hot nuclei properties, this fact was ignored, and a temperature, as a parameter characterizing the thermodynamic properties of a hot system, was introduced into consideration by determining and subsequent minimization of the free energy for a system of noninteracting quasiparticles [83, 84]. As a consequence of this approach, the thermal vacuum satisfies the thermal state condition only in the BCS approximation, but when the correlations caused by the residual interaction are considered, i.e., when constructing the phonon thermal vacuum, the thermal state condition is no longer satisfied. As a result, the principle of detailed balance for spectral densities (119), (120) and for strength functions (134), (136) is violated. As will be shown below, within the superoperator method, it is possible to generalize the BCS, RPA, and

²¹The bosonic expansion method was used to diagonalize the thermal Hamiltonian of the Lipkin model in our works [102, 103].

other methods in such a way that at each stage of diagonalization of the thermal Hamiltonian, the thermal vacuum satisfies the thermal state condition.

Before proceeding to the discussion of methods for diagonalization of the thermal Hamiltonian, we use the fact that for spherical nuclei the spectral densities of spherical tensor operators are expressed in terms of the reduced matrix elements

$$S_{A_j B_j}(E, T) = \sum_{Z, N} \sum_{i, f} p(\mathcal{E}_i, Z, N) \times \frac{\langle J_f \| B_J \| J_i \rangle \langle J_f \| A_J \| J_i \rangle^*}{2J_i + 1} \delta(E - \Delta E_{if}), \quad (165)$$

while the strength function has the form

$$S_{A_j}(E, T) = \sum_{Z, N} \sum_{i, f} p(\mathcal{E}_i, Z, N) B_{if}(A_j) \delta(E - \Delta E_{if}), \quad (166)$$

where $B_{if}(A_j) = \langle J_f \| A_J \| J_i \rangle^2 / (2J_i + 1)$ is the reduced transition probability (strength). The eigenstates of the thermal Hamiltonian $|JMk\rangle$ also have spherical symmetry, i.e., are degenerate with respect to the angular momentum projection. Therefore, in the expressions for spectral densities (127), (128) and for strength functions (130), (131) the summation over the projection M can be considered by determining the reduced matrix element

$$\begin{aligned} \langle \mathbb{O}_{Jk} \| A_J \| 0(T) \rangle &\equiv \hat{J} \langle \mathbb{O}_{JMk} | A_{JM} | 0(T) \rangle, \\ \langle \tilde{\mathbb{O}}_{Jk} \| A_J \| 0(T) \rangle &\equiv \hat{J} \langle \tilde{\mathbb{O}}_{JMk} | A_{JM} | 0(T) \rangle, \end{aligned} \quad (167)$$

where $\hat{J} = \sqrt{2J + 1}$. This definition agrees with (153), given above, if we assign zero angular momentum to the thermal vacuum. Let us also introduce the reduced transition probability from thermal vacuum to the state $|Jk\rangle$

$$\begin{aligned} B_{Jk}(A_j) &= |\langle \mathbb{O}_{Jk} \| A_J \| 0(T) \rangle|^2, \\ \tilde{B}_{Jk}(A_j) &= |\langle \tilde{\mathbb{O}}_{Jk} \| A_J \| 0(T) \rangle|^2. \end{aligned} \quad (168)$$

Obviously, with such a definition of the reduced matrix element, all relations for the amplitudes and transition probabilities, obtained in the previous section (in particular, the principle of detailed balance (134) and (136)), remain valid.

7. THERMAL QUASIPARTICLES

As in the case of zero temperature, we begin the diagonalization of the thermal Hamiltonian (164) by taking into account pairing correlations. To this end, we introduce the operators of creation β^\dagger , $\tilde{\beta}^\dagger$ and annihilation β , $\tilde{\beta}$ of thermal quasiparticles, which reduce

the pairing part of the thermal Hamiltonian to the diagonal form:

$$\begin{aligned} \mathcal{H}_{\text{BCS}} &= \mathcal{H}_{\text{mf}} + \mathcal{H}_{\text{pair}} \\ &\approx \sum_{\tau} \sum_{jm} \varepsilon_j(T) (\beta_{jm}^\dagger \beta_{jm} - \tilde{\beta}_{jm}^\dagger \tilde{\beta}_{jm}). \end{aligned} \quad (169)$$

The sign of approximate equality in (169) means that the terms describing the monopole interaction between thermal quasiparticles are not indicated in the expression for \mathcal{H}_{BCS} . The vacuum of thermal quasiparticles $|\varphi_0(T)\rangle$ under the additional condition (142) is the thermal vacuum in the BCS approximation, while the quantity $\pm \varepsilon_j(T)$ corresponds to the energy of thermal quasiparticles.

The creation and annihilation operators of thermal quasiparticles are related to the operators a^\dagger , a , \tilde{a}^\dagger , and \tilde{a} , which are included in the definition of the initial thermal Hamiltonian, through two unitary transformations. The first transformation is the standard Bogolyubov (u, v)-transformation from particle operators to quasiparticle operators ($u_j^2 + v_j^2 = 1$)

$$\begin{aligned} a_{jm}^\dagger &= u_j \alpha_{jm}^\dagger + v_j \alpha_{\bar{j}m}, \\ a_{jm} &= u_j \alpha_{jm} + v_j \alpha_{\bar{j}m}^\dagger. \end{aligned} \quad (170)$$

A similar transformation is performed on the creation and annihilation operators of tilde particles, thereby introducing into consideration the tilde operators of quasiparticles $\tilde{\alpha}_{jm}^\dagger$ and $\tilde{\alpha}_{\bar{j}m}$. The second one, the so-called Bogolyubov thermal (x, y)-transformation, mixes nontilde and tilde operators

$$\begin{aligned} \alpha_{jm}^\dagger &= x_j \beta_{jm}^\dagger + iy_j \tilde{\beta}_{jm}, \\ \tilde{\alpha}_{jm}^\dagger &= x_j \tilde{\beta}_{jm}^\dagger - iy_j \beta_{jm}. \end{aligned} \quad (171)$$

The requirement

$$x_j^2 + y_j^2 = 1 \quad (172)$$

leads to the preservation of fermionic anticommutation relations between the creation and annihilation operators of thermal quasiparticles. We note that, in contrast to earlier works on the application of thermofield dynamics to the study of the properties of hot nuclei (see, e.g., [82, 83, 104]), we use a complex thermal transformation. The complex thermal transformation arises as a consequence of our definition of the tilde (i.e., right) creation superoperators (50), due to which the thermal state condition (101) for fermion-like operators contains the phase factor $\sigma_A = -i$. In the complex form, thermal transformation (171) was first used in our work [35].

Since the fermionic quadratic form (169) is invariant under the transformation

$$\beta^\dagger \rightarrow x\beta^\dagger + iy\tilde{\beta}, \quad (x^2 + y^2 = 1), \quad (173)$$

then the requirement that the one-particle part \mathcal{H}_{BCS} be diagonal does not in itself lead to an unambiguous definition of the structure of thermal quasiparticles. Let us obtain an additional relation between the thermal transformation coefficients by requiring the fulfillment of the thermal state condition in the form (142). To do this, we consider the Bogolyubov quasiparticle creation operator α_{jm}^\dagger as an operator A . From the equality

$$\begin{aligned} e^{-\varepsilon_j/2T} \langle \varphi_0(T) | [\beta_{jm}, \alpha_{jm}^\dagger] | \varphi_0(T) \rangle \\ = -i \langle \varphi_0(T) | [\alpha_{jm}^\dagger, \tilde{\beta}_{jm}^\dagger] | \varphi_0(T) \rangle, \end{aligned} \quad (174)$$

it follows that

$$y_j = \exp\left(-\frac{\varepsilon_j}{2T}\right) x_j. \quad (175)$$

We obtain the same relation by using for A the annihilation operator α_{jm} . Thus, with normalization (172), the thermal state condition unambiguously relates the thermal transformation coefficients (171) to the energy of thermal quasiparticles

$$y_j = [1 + e^{\varepsilon_j/T}]^{-1/2}, \quad x_j = (1 - y_j^2)^{1/2}. \quad (176)$$

The vacuum of thermal quasiparticles can be represented as follows [37]

$$\begin{aligned} | \varphi_0(T) \rangle \\ = \exp\left[-i \sum_{\tau} \sum_{jm} \vartheta_j(T) (\alpha_{jm}^\dagger \tilde{\alpha}_{jm}^\dagger + \tilde{\alpha}_{jm} \alpha_{jm})\right] | 00 \rangle, \end{aligned} \quad (177)$$

where $\cos \vartheta_j(T) = x_j^2$, while $|00\rangle$ is the vacuum of Bogolyubov quasiparticles α_{jm} and $\tilde{\alpha}_{jm}$. As defined on page 896, the vector $| \varphi_0(T) \rangle$ is tilde-invariant.

To determine the energy of thermal quasiparticles, as well as to find the coefficients of (u, v) -transformation (170), we use equation of motion (143), in which we use the vacuum of thermal quasiparticles $| \varphi_0(T) \rangle$ as the thermal vacuum. For this purpose, we write the single-particle part of the thermal BCS Hamiltonian in terms of thermal quasiparticles:

$$\begin{aligned} \mathcal{H}_{\text{BCS}} \approx \sum_{\tau} \sum_{jm} \varepsilon_j (\beta_{jm}^\dagger \beta_{jm} - \text{t.c.}) \\ + \sum_{\tau} \sum_{jm} \{ (E_j' - \mu_{\tau}) u_j v_j - (u_j^2 - v_j^2) \Delta_{\tau} \} \\ \times \left\{ \frac{1}{2} (1 - 2y_j^2) (\beta_{jm}^\dagger \beta_{jm}^\dagger + \beta_{jm} \beta_{jm} - \text{t.c.}) \right. \\ \left. + 2ix_j y_j (\beta_{jm}^\dagger \tilde{\beta}_{jm} + \tilde{\beta}_{jm} \beta_{jm}^\dagger) \right\}, \end{aligned} \quad (178)$$

where to abbreviate the notation, the terms that are tilde conjugate of the specified ones are denoted by symbols "t.c.". The energy of thermal quasiparticles and

the correlation function, or pairing gap Δ_{τ} , are expressed by transformation coefficients (170) and (171):

$$\begin{aligned} \varepsilon_j &= (E_j' - \mu_{\tau})(u_j^2 - v_j^2) + 2u_j v_j \Delta_{\tau}, \\ \Delta_{\tau} &= \frac{G_{\tau}}{2} \sum_j (2j+1) u_j v_j (1 - 2y_j^2), \end{aligned} \quad (179)$$

while the quantity $E_j' = E_j - G_{\tau}(u_j^2 y^2 + v_j^2 x_j^2)$ determines the renormalized single-particle energy. With allowance for the normalization $u_j^2 + v_j^2 = 1$, solving equation of motion (143) at $\delta \mathcal{O} = a_{jm}^\dagger, a_{jm}$ leads to the following expressions for coefficients of the (u, v) -transformation:

$$\begin{aligned} u_j &= \frac{1}{\sqrt{2}} \left(1 + \frac{E_j' - \mu_{\tau}}{\varepsilon_j} \right)^{1/2}, \\ v_j &= \frac{1}{\sqrt{2}} \left(1 - \frac{E_j' - \mu_{\tau}}{\varepsilon_j} \right)^{1/2}. \end{aligned} \quad (180)$$

If the resulting expressions for the coefficients of the Bogolyubov transformation are substituted into the thermal Hamiltonian (178), then it takes diagonal form (169).

Using (179) we obtain an expression for the energy of thermal quasiparticles

$$\varepsilon_j = \sqrt{(E_j' - \mu_{\tau})^2 + \Delta_{\tau}^2} \quad (181)$$

and the equation for the pairing gap Δ_{τ}

$$\frac{G_{\tau}}{4} \sum_j \tau \frac{(2j+1)(1-2y_j^2)}{\sqrt{(E_j' - \mu_{\tau})^2 + \Delta_{\tau}^2}} = 1. \quad (182)$$

The equation for Δ_{τ} should be supplemented with the equation for the chemical potential μ_{τ} , which follows from the condition of conservation of the number of particles on average

$$\begin{aligned} N_{\tau} &= \sum_{jm} \tau \langle \varphi_0(T) | a_{jm}^\dagger a_{jm} | \varphi_0(T) \rangle \\ &= \sum_j \tau (2j+1) (v_j^2 x_j^2 + u_j^2 y_j^2) \\ &= \frac{1}{2} \sum_j \tau (2j+1) \left\{ 1 - \frac{(E_j' - \mu_{\tau})(1 - 2y_j^2)}{\sqrt{(E_j' - \mu_{\tau})^2 + \Delta_{\tau}^2}} \right\}. \end{aligned} \quad (183)$$

The resulting Eqs. (176), (182), and (183) are the well-known BCS equations at nonzero temperature [105, 106]. In the context of thermofield dynamics, these equations were obtained in [83, 84] using a method similar to that described above, i.e., diagonalizing the single-particle part of \mathcal{H}_{BCS} . However, in contrast to our consideration, the authors of [83, 84] did not use the thermal state condition to determine

the explicit form of the coefficients of the thermal (x, y) -transformation, but found them by minimizing a large thermodynamic potential. The diagonalization method based on the thermal state condition was first proposed in our paper [107]. In what follows, the method of diagonalization of \mathcal{H}_{BCS} on the basis of thermal quasiparticles using the thermal state condition will be called thermal quasiparticle BCS (TQBCS).

The solution of Eqs. (176), (182), and (183) determines the dependence of the pairing gap $\Delta_\tau(T)$ and chemical potential $\mu_\tau(T)$ on temperature. It is known that the solution of the BCS equations demonstrates the disappearance of pairing correlations ($\Delta_\tau = 0$) at temperatures exceeding T_{cr} , which is of the order of $T_{\text{cr}} \approx 0.5\Delta_\tau(T=0)$ (see Fig. 1 in [105]). The disappearance of pairing correlations and the phase transition from the superfluid state to the normal one is a consequence of the use of the grand canonical ensemble and the simplifications applied during the derivation of the TQBCS equations, i.e., the replacement of the original thermal Hamiltonian by the Hamiltonian of noninteracting quasiparticles. When studying the statistical properties of highly excited compound states of isolated nuclei, the use of the grand canonical ensemble is usually just the first step towards the more consistent calculations. Calculations using the particle-number projection demonstrate that the phase transition in nuclei is smooth; i.e., pairing correlations, though are weakened, but are preserved at $T \geq T_{\text{cr}}$ [108, 109]. Note, however, that the study of collective nuclear excitations in such calculations is a laborious task. To simplify the calculations, the approximate particle-number projection method using the TFD formalism was proposed in [110].

For hot nuclei in stellar matter, it is the use of approximate methods when considering pairing correlations that causes a sharp phase transition, since the use of the grand canonical ensemble is justified due to the presence of a bath of nucleons. As noted in [86, p. 68], the approximations used in the derivation of the BCS equations for $T \neq 0$ lead to the fact that, at a temperature above the critical one, multi-quasiparticle states without pairing correlation are most likely excited in the system. For macroscopic superconductors, it is the most probable configurations that determine the state of the system. In the case of microscopic systems, such as atomic nuclei, configurations with pairing correlations different from the most probable ones may significantly contribute to the average characteristics of the system, which leads to the absence of a sharp phase transition (see Fig. 28 in [86] and its discussion). However, since the average value of the pairing gap is small above the phase transition temperature, ($\Delta < 0.1$ MeV), then the preserved pairing correlations have little effect on the properties of the hot nucleus [86].

After diagonalization, the one-particle part \mathcal{H}_{BCS} of the thermal Hamiltonian given by expression (169) describes a system of noninteracting thermal quasiparticles with energy $\pm\varepsilon_j(T)$ depending on temperature. The vacuum of thermal quasiparticles determines the equilibrium state of the hot nucleus in the TQBCS approximation. To find the average value of any physical quantity (energy, occupation numbers, etc.), it is necessary to express the corresponding operator in terms of thermal quasiparticles, and then to calculate the vacuum average. In particular, for the average number of Bogolyubov quasiparticles in the state jm , we obtain²²

$$\langle \varphi_0(T) | \alpha_{jm}^\dagger \alpha_{jm} | \varphi_0(T) \rangle = y_j^2 = [1 + e^{\varepsilon_j/T}]^{-1}, \quad (184)$$

i.e., thermal transformation coefficients y_j are thermal occupation numbers for quasiparticle states in Fermi–Dirac statistics. The average number of nucleons in the state jm is

$$n_j = \langle \varphi_0(T) | a_{jm}^\dagger a_{jm} | \varphi_0(T) \rangle = u_j^2 y_j^2 + v_j^2 x_j^2. \quad (185)$$

The value on the right-hand side of this relation determines the smearing of the proton or neutron Fermi surface in the nucleus, which is due to both pairing correlations and thermal effects.

Excited nonequilibrium states that arise in a hot system under the influence of an external perturbation are described in the TQBCS approximation as thermal quasiparticle excitations over a thermal vacuum. States with one excited thermal quasiparticle have the form²³

$$|\beta_{jm}\rangle \equiv \beta_{jm}^\dagger | \varphi_0(T) \rangle, \quad |\tilde{\beta}_{jm}\rangle \equiv \tilde{\beta}_{jm}^\dagger | \varphi_0(T) \rangle. \quad (186)$$

To clarify the physical meaning of thermal quasiparticle excitations, we consider the following relations

$$\begin{aligned} \langle \beta_{jm} | \alpha_{jm}^\dagger | \varphi_0(T) \rangle^2 &= x_j^2, \\ \langle \tilde{\beta}_{jm} | \alpha_{\bar{j}\bar{m}} | \varphi_0(T) \rangle^2 &= y_j^2. \end{aligned} \quad (187)$$

Thus, as a result of adding one Bogolyubov quasiparticle to the thermal vacuum, a thermal quasiparticle with positive energy is produced with the probability x_j^2 , and as a result of the annihilation of a Bogolyubov quasiparticle, a thermal quasiparticle with negative energy is produced with the probability y_j^2 . The

²²In the absence of pairing correlations, we consider particles and holes as quasiparticles.

²³The second relation uses the fact that it is $\tilde{\beta}_{jm}^\dagger$ that is transformed as a spherical tensor operator of rank j during the rotation of the coordinate system. To verify this, it suffices to express the nucleon creation operator in terms of thermal quasiparticles $a_{jm}^\dagger = x_j(u_j\beta_{jm}^\dagger + v_j\tilde{\beta}_{\bar{j}\bar{m}}^\dagger) - iy_j(v_j\tilde{\beta}_{jm}^\dagger - u_j\beta_{jm}^\dagger)$.

factors y_j^2 and x_j^2 appear as a consequence of the Pauli principle: the factor y_j^2 corresponds to the probability of the process in which the Bogolyubov quasiparticle is annihilated from the state containing y_j^2 quasiparticles, and the factor $x_j^2 = 1 - y_j^2$ corresponds to the probability of the process in which a quasiparticle is added to the state already containing y_j^2 quasiparticles.

Let us now consider the eigenstates of the thermal Hamiltonian \mathcal{H}_{BCS} , consisting of two thermal quasiparticles coupled to the total angular momentum J with the projection M . As will be shown in the next section, these states are excited in a hot system under the influence of an external perturbation caused by a single-particle multipole operator. For fixed quantum numbers j_1 and j_2 , the following four types of two thermal quasiparticle states are possible:

$$|\beta_{j_1}\beta_{j_2}; JM\rangle \equiv [\beta_{j_1}^\dagger\beta_{j_2}^\dagger]_{JM}|\Phi_0(T)\rangle, \quad (188a)$$

$$\omega = \varepsilon_{j_1} + \varepsilon_{j_2} \equiv \varepsilon_{j_1j_2}^{(+)},$$

$$|\tilde{\beta}_{j_1}\tilde{\beta}_{j_2}; JM\rangle \equiv [\tilde{\beta}_{j_1}^\dagger\tilde{\beta}_{j_2}^\dagger]_{JM}|\Phi_0(T)\rangle, \quad \omega = -\varepsilon_{j_1j_2}^{(+)}, \quad (188b)$$

$$|\beta_{j_1}\tilde{\beta}_{j_2}; JM\rangle \equiv [\beta_{j_1}^\dagger\tilde{\beta}_{j_2}^\dagger]_{JM}|\Phi_0(T)\rangle, \quad (188c)$$

$$\omega = \varepsilon_{j_1} - \varepsilon_{j_2} \equiv \varepsilon_{j_1j_2}^{(-)},$$

$$|\tilde{\beta}_{j_1}\beta_{j_2}; JM\rangle \equiv [\tilde{\beta}_{j_1}^\dagger\beta_{j_2}^\dagger]_{JM}|\Phi_0(T)\rangle, \quad \omega = -\varepsilon_{j_1j_2}^{(-)}. \quad (188d)$$

On the right, the energy of the state relative to the thermal vacuum is indicated. In what follows, we will distinguish between the charge-neutral and charge-exchange two thermal quasiparticle states. In the first case, the states j_1 and j_2 have the same isospin projection, i.e., $\tau_{j_1} = \tau_{j_2}$. In the second case, the states j_1 and j_2 have opposite isospin projections, $\tau_{j_1} = -\tau_{j_2}$. Note that in the presence of pairing correlations, the charge-exchange two thermal quasiparticle states are a superposition of excitations in nuclei ${}^{Z-1}_{N+1}A$ and ${}^{Z+1}_{N-1}A$.

An analysis of the structure of states (188) shows that each two thermal quasiparticle state corresponds to a tilde-conjugate state with the energy opposite in sign. As follows from the correspondence between the thermal and Bogolyubov quasiparticles presented above, the excitation of two non-tilde thermal quasiparticles describes a process in which two Bogolyubov quasiparticles are added to the thermal vacuum, while the creation of two tilde thermal quasiparticles corresponds to the inverse process of annihilation of two thermally excited Bogolyubov quasiparticles. The addition of one non-tilde and one tilde thermal quasiparticle corresponds to the scattering of the Bogolyubov quasiparticle from one state to another. From here, in particular, it follows that if the component

associated with the nucleus ${}^{Z-1}_{N+1}A$ dominates in the charge-exchange two thermal quasiparticle state, then the component associated with the nucleus ${}^{Z+1}_{N-1}A$ dominates in the tilde-conjugate state.

We also give expressions for \mathcal{H}_{BCS} in terms of the creation and annihilation operators of two thermal quasiparticle states. To do this, we calculate the commutators of \mathcal{H}_{BCS} with the creation operators of a pair of thermal quasiparticles:

$$[\mathcal{H}_{\text{BCS}}, [\beta_{j_1}^\dagger\beta_{j_2}^\dagger]_{JM}] = \varepsilon_{j_1j_2}^{(+)}[\beta_{j_1}^\dagger\beta_{j_2}^\dagger]_{JM}, \quad (189)$$

$$[\mathcal{H}_{\text{BCS}}, [\beta_{j_1}^\dagger\tilde{\beta}_{j_2}^\dagger]_{JM}] = \varepsilon_{j_1j_2}^{(-)}[\beta_{j_1}^\dagger\tilde{\beta}_{j_2}^\dagger]_{JM} \quad (190)$$

and so on. Based on these relations, \mathcal{H}_{BCS} can be represented in a diagonal form with respect to the creation and annihilation operators of a pair of thermal quasiparticles:

$$\begin{aligned} \mathcal{H}_{\text{BCS}} \approx & \frac{1}{2} \sum_{JM} \sum_{\tau} \sum_{j_1j_2}^{\tau} \{ \varepsilon_{j_1j_2}^{(+)} [\beta_{j_1}^\dagger\beta_{j_2}^\dagger]_{JM} [\beta_{j_1}\beta_{j_2}]_{JM}^\dagger \\ & + \varepsilon_{j_1j_2}^{(-)} [\beta_{j_1}^\dagger\tilde{\beta}_{j_2}^\dagger]_{JM} [\beta_{j_1}\tilde{\beta}_{j_2}]_{JM}^\dagger \} \\ & + \sum_{JM} \sum_{j_\rho j_n} \{ \varepsilon_{j_\rho j_n}^{(+)} [\beta_{j_\rho}^\dagger\beta_{j_n}^\dagger]_{JM} [\beta_{j_\rho}\beta_{j_n}]_{JM}^\dagger \\ & + \varepsilon_{j_\rho j_n}^{(-)} [\beta_{j_\rho}^\dagger\tilde{\beta}_{j_n}^\dagger]_{JM} [\beta_{j_\rho}\tilde{\beta}_{j_n}]_{JM}^\dagger \} - (\text{t.c.}). \end{aligned} \quad (191)$$

Recall that symbol (t.c.) denotes the terms tilde conjugate of all presented.

8. REDUCED PROBABILITIES AND STRENGTH FUNCTION OF SINGLE-PARTICLE TRANSITIONS IN THE APPROXIMATION OF INDEPENDENT THERMAL QUASIPARTICLES

Let us obtain expressions for the reduced transition probability (strength) from thermal vacuum to two thermal quasiparticle states (188) for the single-particle tensor operator \mathcal{T}_{JM}

$$\begin{aligned} \mathcal{T}_{JM} &= \sum_{j_1m_1} \langle j_1m_1 | \mathcal{T}_{JM} | j_2m_2 \rangle a_{j_1m_1}^\dagger a_{j_2m_2} \\ &= -\hat{J}^{-1} \sum_{j_1j_2}^{(J)} [a_{j_1}^\dagger a_{j_2}^-]_{JM}, \end{aligned} \quad (192)$$

where $t_{j_1j_2}^{(J)}$ is the reduced matrix element (153). In the case of a charge-neutral operator, the summation occurs over states with the same isotopic index ($\tau_{j_1} = \tau_{j_2}$), and in the case of a charge-exchange operator, over states with opposite isotopic index ($\tau_{j_1} = -\tau_{j_2}$). Using transformations (170) and (171), we

express \mathcal{T}_{JM} through operators of thermal quasiparticles:

$$\begin{aligned} \mathcal{T}_{JM} = & \hat{J}^{-1} \sum_{j_1 j_2} t_{j_1 j_2}^{(J)} \{ A_{JM}(j_1 j_2) \\ & + A_{JM}^*(j_1 j_2) + B_{JM}(j_1 j_2) + B_{JM}^*(j_1 j_2) \}. \end{aligned} \quad (193)$$

Here the following notation is introduced for linear combinations of two thermal quasiparticle operators:

$$\begin{aligned} A_{JM}(j_1 j_2) = & u_{j_1} v_{j_2} x_{j_1} x_{j_2} [\beta_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM} \\ & + v_{j_1} u_{j_2} y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} \\ + i u_{j_1} u_{j_2} x_{j_1} y_{j_2} [\beta_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} - & i v_{j_1} v_{j_2} y_{j_1} x_{j_2} [\tilde{\beta}_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM}, \\ A_{JM}^*(j_1 j_2) = & v_{j_1} u_{j_2} x_{j_1} x_{j_2} [\beta_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM}^\dagger \\ & + u_{j_1} v_{j_2} y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM}^\dagger \\ + i v_{j_1} v_{j_2} x_{j_1} y_{j_2} [\beta_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM}^\dagger - & i u_{j_1} u_{j_2} y_{j_1} x_{j_2} [\tilde{\beta}_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM}^\dagger, \\ B_{JM}(j_1 j_2) = & -u_{j_1} u_{j_2} x_{j_1} x_{j_2} [\beta_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM} \\ & + v_{j_1} v_{j_2} y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} + \\ + i u_{j_1} v_{j_2} x_{j_1} y_{j_2} [\beta_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} + & i v_{j_1} u_{j_2} y_{j_1} x_{j_2} [\tilde{\beta}_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM}, \\ B_{JM}^*(j_1 j_2) = & v_{j_1} v_{j_2} x_{j_1} x_{j_2} [\beta_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM} \\ & - u_{j_1} u_{j_2} y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} \\ + i v_{j_1} u_{j_2} x_{j_1} y_{j_2} [\beta_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger]_{JM} + & i u_{j_1} v_{j_2} y_{j_1} x_{j_2} [\tilde{\beta}_{j_1}^\dagger \beta_{j_2}^\dagger]_{JM}. \end{aligned} \quad (194)$$

The operators A_{JM} and A_{JM}^* describe transitions between states in which the number of thermal quasiparticles differs by two, while the operators B_{JM} and B_{JM}^* describe transitions between states with the same number of thermal quasiparticles. Since in the TQBCS approximation the equilibrium state of the system (thermal vacuum) does not contain thermal quasiparticles, then transitions from thermal vacuum under the \mathcal{T}_{JM} action are possible only to two thermal quasiparticle states (188). The reduced transition probability (strength) to these states is expressed in terms of the reduced matrix element (168) of the transition operator. For example, for the strength of a charge-neutral transition to a state $|\beta_{j_1} \beta_{j_2}; J\rangle$, we obtain the expression:

$$\begin{aligned} B_{j_1 j_2}(\mathcal{T}_J) \equiv & \left| \langle \beta_{j_1} \beta_{j_2}; J | \mathcal{T}_J | 0(T) \rangle \right|^2 \\ = & \left| t_{j_1 j_2}^{(J)} u_{j_1} v_{j_2} + \bar{t}_{j_2 j_1}^{(J)} v_{j_1} u_{j_2} \right|^2 x_{j_1}^2 x_{j_2}^2, \end{aligned} \quad (195)$$

where $\bar{t}_{j_2 j_1}^{(J)} = (-1)^{j_1 - j_2 + J} t_{j_2 j_1}^{(J)}$. Let us show that the reduced probabilities of transitions to tilde-conjugate two thermal quasiparticle states satisfy the detailed balance principle. To this end, we express a product of two Fermi–Dirac distribution functions in terms of the Bose–Einstein distribution function

$$y_{j_1}^2 y_{j_2}^2 = (1 - y_{j_1}^2 - y_{j_2}^2) Y^2(\epsilon_{j_1 j_2}^{(+)}) , \quad (196)$$

$$y_{j_1}^2 x_{j_2}^2 = (y_{j_2}^2 - y_{j_1}^2) Y^2(\epsilon_{j_1 j_2}^{(-)}) , \quad (197)$$

where $Y(\omega) = \left[\exp\left(\frac{\omega}{T}\right) - 1 \right]^{-1/2}$ and it is assumed that $\epsilon_{j_1} > \epsilon_{j_2}$. Let us use these equalities and write the strength of charge-neutral transitions to states (188) in the following form

$$\begin{aligned} B_{j_1 j_2}(\mathcal{T}_J) = & \left| t_{j_1 j_2}^{(J)} u_{j_1} v_{j_2} + \bar{t}_{j_2 j_1}^{(J)} v_{j_1} u_{j_2} \right|^2 \\ & \times (1 - y_{j_1}^2 - y_{j_2}^2) X^2(\epsilon_{j_1 j_2}^{(+)}) , \end{aligned} \quad (198a)$$

$$\begin{aligned} B_{\tilde{j}_1 \tilde{j}_2}(\mathcal{T}_J) = & \left| t_{j_1 j_2}^{(J)} v_{j_1} u_{j_2} + \bar{t}_{j_2 j_1}^{(J)} u_{j_1} v_{j_2} \right|^2 \\ & \times (1 - y_{j_1}^2 - y_{j_2}^2) Y^2(\epsilon_{j_1 j_2}^{(+)}) , \end{aligned} \quad (198b)$$

$$\begin{aligned} B_{j_1 \tilde{j}_2}(\mathcal{T}_J) = & \left| t_{j_1 j_2}^{(J)} u_{j_1} u_{j_2} - \bar{t}_{j_2 j_1}^{(J)} v_{j_1} v_{j_2} \right|^2 \\ & \times (y_{j_2}^2 - y_{j_1}^2) X^2(\epsilon_{j_1 j_2}^{(-)}) , \end{aligned} \quad (198c)$$

$$\begin{aligned} B_{\tilde{j}_1 j_2}(\mathcal{T}_J) = & \left| t_{j_1 j_2}^{(J)} v_{j_1} v_{j_2} - \bar{t}_{j_2 j_1}^{(J)} u_{j_1} u_{j_2} \right|^2 (y_{j_2}^2 - y_{j_1}^2) Y^2(\epsilon_{j_1 j_2}^{(-)}) , \end{aligned} \quad (198d)$$

where $X^2(\omega) = 1 + Y^2(\omega)$. From here it follows that the strengths of transitions to two thermal quasiparticle states, which are tilde-conjugate of each other and, therefore, have energies opposite in sign, are linked by the relations

$$B_{j_1 \tilde{j}_2}(\mathcal{T}_J^\dagger) = \exp\left(-\frac{\epsilon_{j_1 j_2}^{(+)}}{T}\right) B_{j_1 j_2}(\mathcal{T}_J) , \quad (199)$$

$$B_{\tilde{j}_1 j_2}(\mathcal{T}_J^\dagger) = \exp\left(-\frac{\epsilon_{j_1 j_2}^{(-)}}{T}\right) B_{\tilde{j}_1 \tilde{j}_2}(\mathcal{T}_J) ,$$

which proves the fulfillment of the detailed balance principle for charge-neutral transitions. As it should be, at $T = 0$, the transition strength to states containing a tilde thermal quasiparticle is equal to zero.

We will also obtain expressions for the reduced probability of charge-exchange transitions from thermal vacuum to two thermal quasiparticle states (188). To be specific, we set $j_1 = j_p$ and $j_2 = j_n$. Then for the operator $\mathcal{T}_J^{(-)}$ of $n \rightarrow p$ transition we get

$$B_{j_p j_n}(\mathcal{T}_J^{(-)}) = \left| t_{j_p j_n}^{(J)} u_{j_p} v_{j_n} \right|^2 (1 - y_{j_p}^2 - y_{j_n}^2) X^2(\epsilon_{j_p j_n}^{(+)}) , \quad (200a)$$

$$B_{\tilde{j}_p \tilde{j}_n}(\mathcal{T}_J^{(-)}) = \left| t_{j_p j_n}^{(J)} v_{j_p} u_{j_n} \right|^2 (1 - y_{j_p}^2 - y_{j_n}^2) Y^2(\epsilon_{j_p j_n}^{(+)}) , \quad (200b)$$

$$\begin{aligned} B_{j_p \tilde{j}_n}(\mathcal{T}_J^{(-)}) = & \left| t_{j_p j_n}^{(J)} u_{j_p} u_{j_n} \right|^2 \\ & \times \begin{cases} (y_{j_n}^2 - y_{j_p}^2) X^2(\epsilon_{j_p j_n}^{(-)}) , & (\epsilon_{j_p} > \epsilon_{j_n}) , \\ (y_{j_p}^2 - y_{j_n}^2) Y^2(\epsilon_{j_p j_n}^{(-)}) , & (\epsilon_{j_p} < \epsilon_{j_n}) , \end{cases} \end{aligned} \quad (200c)$$

$$B_{j_p j_n}(\mathcal{T}_J^{(-)}) = \left| t_{j_p j_n}^{(J)} v_{j_p} v_{j_n} \right|^2 \times \begin{cases} (y_{j_n}^2 - y_{j_p}^2) Y^2(\epsilon_{j_p j_n}^{(-)}), & (\epsilon_{j_p} > \epsilon_{j_n}), \\ (y_{j_n}^2 - y_{j_p}^2) X^2(\epsilon_{j_p j_n}^{(-)}), & (\epsilon_{j_p} < \epsilon_{j_n}). \end{cases} \quad (200d)$$

The reduced probabilities of the operator of $p \rightarrow n$ “inverse” transition are equal to

$$B_{j_p j_n}(\mathcal{T}_J^{(+)}) = \left| \bar{t}_{j_n j_p}^{(J)} u_{j_n} v_{j_p} \right|^2 (1 - y_{j_p}^2 - y_{j_n}^2) X^2(\epsilon_{j_p j_n}^{(+)}), \quad (201a)$$

$$B_{j_p \tilde{j}_n}(\mathcal{T}_J^{(+)}) = \left| \bar{t}_{j_n j_p}^{(J)} v_{j_n} u_{j_p} \right|^2 (1 - y_{j_p}^2 - y_{j_n}^2) Y^2(\epsilon_{j_p j_n}^{(+)}), \quad (201b)$$

$$B_{j_p \tilde{j}_n}(\mathcal{T}_J^{(-)}) = \left| \bar{t}_{j_n j_p}^{(J)} v_{j_n} v_{j_p} \right|^2 \times \begin{cases} (y_{j_n}^2 - y_{j_p}^2) X^2(\epsilon_{j_p j_n}^{(-)}), & (\epsilon_{j_p} > \epsilon_{j_n}), \\ (y_{j_p}^2 - y_{j_n}^2) Y^2(\epsilon_{j_p j_n}^{(-)}), & (\epsilon_{j_p} < \epsilon_{j_n}), \end{cases} \quad (201c)$$

$$B_{j_p j_n}(\mathcal{T}_J^{(+)}) = \left| \bar{t}_{j_n j_p}^{(J)} u_{j_p} u_{j_n} \right|^2 \times \begin{cases} (y_{j_n}^2 - y_{j_p}^2) Y^2(\epsilon_{j_p j_n}^{(+)}), & (\epsilon_{j_p} > \epsilon_{j_n}), \\ (y_{j_n}^2 - y_{j_p}^2) X^2(\epsilon_{j_p j_n}^{(+)}), & (\epsilon_{j_p} < \epsilon_{j_n}), \end{cases} \quad (201d)$$

where $\bar{t}_{j_n j_p}^{(J)} = (-1)^{j_p - j_n + J} t_{j_n j_p}^{(J)}$. For operators $\mathcal{T}_J^{(-)}$ and $\mathcal{T}_J^{(+)}$, such that $\mathcal{T}_J^{(-)} = [\mathcal{T}_J^{(+)}]^\dagger$, the reduced probabilities (200) and (201) are related by the principle of detailed balance

$$B_{j_1 \tilde{j}_2}(\mathcal{T}_J^{(\pm)}) = \exp\left(-\frac{\epsilon_{j_1 j_2}^{(\pm)}}{T}\right) B_{j_1 j_2}(\mathcal{T}_J^{(\mp)}), \quad (202)$$

$$B_{j_1 j_2}(\mathcal{T}_J^{(\pm)}) = \exp\left(-\frac{\epsilon_{j_1 j_2}^{(\pm)}}{T}\right) B_{j_1 \tilde{j}_2}(\mathcal{T}_J^{(\mp)}).$$

Let's point out some features of the expressions obtained for the strength of transitions. If a single-particle transition between levels j_1 and j_2 is allowed by the selection rules (i.e., $t_{j_1 j_2}^{(J)} \neq 0$), then for $T \neq 0$ and in the presence of pairing correlations, transitions to all four two thermal quasiparticle states (188) are possible. By the possibility of a transition is meant a non-zero reduced probability. For $T > T_{\text{cr}}$, only two of the four given probabilities are nonzero. For particle–hole states²⁴, this is $B_{j_1 j_2}$ and $B_{j_1 \tilde{j}_2}$, while for states of the hole–hole or particle–particle type, this is $B_{j_1 \tilde{j}_2}$ and $B_{j_1 j_2}$. In addition, in the absence of pairing correlations, transitions from thermal vacuum to tilde-conjugate two thermal quasiparticle charge-exchange states occur due to operators of the opposite isospin direction. In other words, if the transition to a given two thermal quasiparticle state is carried out under the action of the $\tau \rightarrow -\tau$ operator, then the transition to a

²⁴In what follows, we will call the hole (particle) states that are below (above) the Fermi surface.

tilde-conjugate two thermal quasiparticle state is possible only under the action of the $-\tau \rightarrow \tau$ operator.

The expressions (198), (200), and (201) for the transition strengths to two thermal quasiparticle states can be interpreted in such a way that the system contains $Y^2(\omega)$ thermally excited phonons with energy ω . Therefore, the amplitude of the process, in which a phonon is removed from the system, is proportional to $Y^2(\omega)$, while the amplitude of the inverse process, in which a phonon is added to the system, is proportional to $1 + Y^2(\omega)$ ²⁵. Thus, despite the fact that the initial system is fermionic, when considering excited states under the action of a single-particle operator, the bosonic (i.e., phonon) occupation numbers arise, which relate the transition strength to states with positive energy (a phonon is added) to the transition strength to states with negative energy (the phonon is removed). In this sense, a hot system of fermions exhibits the properties of a hot phonon system. In this case, the bosonic and fermionic distribution functions have the same temperature.

It can be shown that for the Gamow–Teller $\text{GT}_\pm = \sum_i \sigma_i^i t_\pm^i$ and Fermi $F_\pm = \sum_i t_\pm^i$ operators, the total strengths of $n \rightarrow p$ and $p \rightarrow n$ transitions calculated in TQBCS satisfy the model-independent sum rule, which is often called the Ikeda sum rule [111]:

$$S_- - S_+ = \begin{cases} 3(N - Z) & \text{for } \text{GT}_\pm, \\ N - Z & \text{for } F_\pm. \end{cases} \quad (203)$$

Indeed, for the Gamow–Teller operator we have

$$\begin{aligned} S_- - S_+ &= \sum_{j_p j_n} [B_{j_p j_n}(\text{GT}_-) + B_{j_p \tilde{j}_n}(\text{GT}_-) \\ &\quad + B_{j_p \tilde{j}_n}(\text{GT}_+) + B_{j_p j_n}(\text{GT}_+)] \\ &\quad - \sum_{j_p j_n} [B_{j_p j_n}(\text{GT}_+) + B_{j_p \tilde{j}_n}(\text{GT}_+) \\ &\quad + B_{j_p \tilde{j}_n}(\text{GT}_+) + B_{j_p j_n}(\text{GT}_+)] \\ &= \sum_{j_p j_n} |t_{j_p j_n}^{(J)}|^2 [(1 - y_{j_p}^2 - y_{j_n}^2)(u_{j_p}^2 v_{j_n}^2 - v_{j_p}^2 u_{j_n}^2) \\ &\quad + (y_{j_n}^2 - y_{j_p}^2)(u_{j_p}^2 u_{j_n}^2 - v_{j_p}^2 v_{j_n}^2)] \\ &= \sum_{j_p j_n} |t_{j_p j_n}^{(J)}|^2 [(u_{j_n}^2 y_{j_n}^2 + v_{j_n}^2 x_{j_n}^2) \\ &\quad - (u_{j_p}^2 y_{j_p}^2 + v_{j_p}^2 x_{j_p}^2)] = 3(N - Z). \end{aligned} \quad (204)$$

In the last equality, we used the fact that

$$\sum_{j_p(n)} |\langle j_p || \sigma \tau_- || j_n \rangle|^2 = 3(2j_{n(p)} + 1) \quad (205)$$

and took into consideration the conservation of the number of particles in the TQBCS (see Eq. (183)). For

²⁵For bosonic operators $b^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$ and $b |n\rangle = \sqrt{n} |n-1\rangle$.

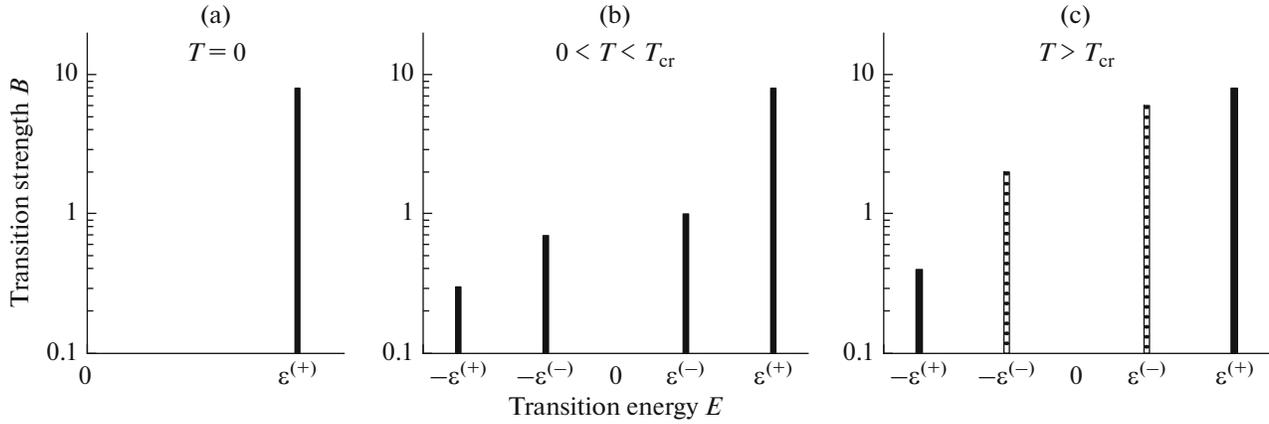


Fig. 1. Temperature evolution of the strength function of charge-neutral transitions to two thermal quasiparticle states (188) with fixed j_1 and j_2 in a system with pairing correlations at $T = 0$. The strength B and energy E of transitions are given in arbitrary units. In panel c, the solid peaks correspond to particle–hole transitions, while the shaded peaks correspond to transitions between the hole or particle states. The notation $\epsilon^{(\pm)} = \epsilon_{j_1} \pm \epsilon_{j_2}$ is used for the transition energy. Other explanations for the figure are given in the text.

the Fermi operator, the proof of the sum rule is similar, with the only difference that

$$\sum_{J_{p(n)}} |\langle j_p \| t_- \| j_n \rangle|^2 = 2j_{n(p)} + 1. \quad (206)$$

The energy and the reduced transition probability to two thermal quasiparticle states (188) determine the strength function $S_{\mathcal{T}_J}(E, T)$ of the operator \mathcal{T}_J in the approximation of independent thermal quasiparticles. Recall that for a charge-neutral operator, the transition energy coincides with the energy of a two thermal quasiparticle state (see Eq. (133)), while in the case of a charge-exchange operator, they differ by the effective threshold value $\pm\Delta_{np}$ (see Eq. (135)).

Let us consider qualitatively the temperature evolution of the strength function. Figure 1 schematically shows the strength distribution of charge-neutral transitions to states (188) with fixed j_1 and j_2 for three temperatures. It is assumed that in the ground state of the system ($T = 0$), there are pairing correlations. At $T = 0$, strength function (130) contains only one peak, corresponding to a \uparrow -transition with energy $E = \epsilon_{j_1 j_2}^{(+)}$ (Fig. 1a). The peak value is equal to reduced probability (198a) of the excitation of two Bogolyubov quasiparticles with energies ϵ_{j_1} and ϵ_{j_2} . Note that if both states j_1 and j_2 are hole (pp -transition) states or particle (hh -transition) states, then at $T = 0$, the corresponding single-particle transition is unblocked due to the presence of pairing correlations. An increase in temperature allows transitions between states with excited quasiparticles to be possible. Eventually, as shown in Fig. 1b, for $0 < T < T_{cr}$, the strength function proves to be fragmented into four peaks symmetrically located with respect to zero energy. The peak at

the energy $E = -\epsilon_{j_1 j_2}^{(+)}$ corresponds to the process of annihilation of two excited Bogolyubov quasiparticles (the probability of this process is given by expression (198b)), and the low-energy peaks at energies $E = \pm\epsilon_{j_1 j_2}^{(-)}$ determine the transition probabilities for an thermally excited quasiparticle going from one state to another (probabilities (198c) and (198d)). In this case, each \uparrow -transition with positive energy corresponds to the inverse \downarrow -transition with negative energy to the tilde-conjugate state. The probabilities of \uparrow - and \downarrow -transitions are related by the principle of detailed balance (199). An increase in temperature leads to a weakening of pairing correlations, and for $T > T_{cr}$, only two of the four peaks survive in the strength function (Fig. 1c). If the states j_1 and j_2 correspond to a particle–hole transition, then peaks with energy $\pm\epsilon_{j_1 j_2}^{(+)}$ are preserved in the strength function; if both states j_1 and j_2 are the hole or particle states, then the peaks with energy $\pm\epsilon_{j_1 j_2}^{(-)}$ are preserved. Consequently, in a system with pairing, an increase in temperature decreases the energy of pp - and hh -transitions from the value $\epsilon_{j_1 j_2}^{(+)}$ to the values $\pm\epsilon_{j_1 j_2}^{(-)}$. If there are no pairing correlations in the ground state of the system, then it is the temperature that leads to the unblocking of the pp - and hh -transitions.

It is easy to see that an increase in temperature has a similar effect on the strength function of charge-exchange transitions. In particular, the fragmentation of the strength function is maximum for $0 < T < T_{cr}$, and an increase in temperature leads to a decrease in the energy of pp - and hh -transitions. The latter effect

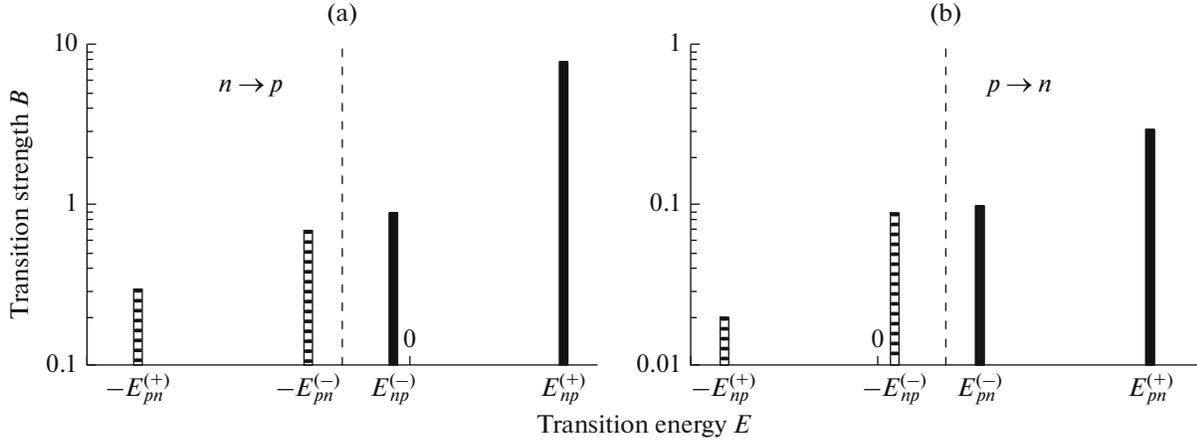


Fig. 2. Temperature evolution of the strength function of charge-exchange transitions to two thermal quasiparticle states (188) with fixed j_p and j_n in a system with pairing correlations at $T = 0$. The strength B and energy E of the transition are given in arbitrary units. The solid peaks correspond to transitions to two thermal quasiparticle states with positive energy, while the shaded peaks correspond to transitions to tilde-conjugate states with negative energy. Dashed lines show the position of the effective threshold $-\Delta_{np}$ (Δ_{np}) of the $n \rightarrow p$ ($p \rightarrow n$) transitions. The following notation is introduced for the transition energies:

$$E_{pn}^{(\pm)} = \varepsilon_{pn}^{(\pm)} + \Delta_{np}, \quad E_{np}^{(\pm)} = \varepsilon_{pn}^{(\pm)} - \Delta_{np}, \quad \text{where } \Delta_{np} = \Delta\mu_{np} + \Delta M_{np} > 0.$$

plays an important role in electron capture by hot neutron-rich nuclei. At the same time, there are two differences between the strength functions of charge-neutral and charge-exchange transitions. The first difference is due to the fact that the energy of the charge-exchange transition and the energy of the corresponding two thermal quasiparticle state differ by the value of the effective threshold $\pm\Delta_{np}$ (135)²⁶. Due to the effective threshold in neutron-rich nuclei, for which $\mu_n > \mu_p$, the strength function of the $p \rightarrow n$ transitions shifts to a region of higher energies, while the strength function of the $n \rightarrow p$ transitions shifts to lower energies. Just this case is depicted in Fig. 2, where the strength distribution of $n \rightarrow p$ and $p \rightarrow n$ transitions in a neutron-rich nucleus for $0 < T < T_{cr}$ is schematically shown. Due to the shift by Δ_{np} , the peaks of strength functions are located asymmetrically with respect to zero energy. However, if the strength function of the $n \rightarrow p$ transition has a peak with energy E , then the strength function of the $p \rightarrow n$ transition has a peak with energy $-E$ corresponding to the transition to the tilde-conjugate state. The second difference lies in the fact that for $T > T_{cr}$, the strength function of the charge-exchange transition contains not two peaks, but one (see the discussion after (202)).

Summing up all of the above, we can draw the following conclusions about the temperature influence on the strength function in the TQBCS approximation. (i) An increase in temperature leads to the frag-

mentation of a strength function of single-particle transitions, which is associated with the unblocking of transitions from excited quasiparticle states. The fragmentation degree depends on temperature and is maximum for $0 < T < T_{cr}$. (ii) For $T \neq 0$, the unblocking of low-energy transitions and negative-energy \downarrow -transitions occurs. Due to these transitions, the concept of a reaction threshold disappears for a hot nucleus. (iii) The thermal smearing of the Fermi surface, as well as pairing correlations, leads to the unblocking of the pp - and hh -transitions, but the transition energies are different. With thermal unblocking, this energy is given by the difference of quasiparticle energies, while with the unblocking due to pairing correlations, it is determined by their sum.

9. CHARGE-NEUTRAL PHONONS IN HOT NUCLEI

According to (191), in the TQBCS approximation, the elementary modes of excitation of a hot system are two thermal quasiparticle states (188). At the next stage of the approximate diagonalization of the thermal Hamiltonian, the interaction between these states, which is due to the residual particle-hole interaction, is considered. Consider first the interaction between charge-neutral states. The multipole and spin-multipole operators (157) included in the definitions of the residual interaction $\mathcal{H}_{\text{ch},n}$ (162), being written in terms of thermal quasi-particles, have the same form as the single-particle transition operator (193). The properties of the reduced matrix elements $f_{j_1 j_2}^{(J;k)} = (-1)^{j_1 - j_2 + J} f_{j_2 j_1}^{(J;k)}$ and $f_{j_1 j_2}^{(LJ;k)} = (-1)^{j_1 + j_2 + J} f_{j_2 j_1}^{(LJ;k)}$

²⁶ Recall that, in contrast to charge-neutral transitions, there is no one-to-one correspondence between the excitation of charge-exchange nontilde (tilde) states and \uparrow (\downarrow)-transitions.

allow expressions (157) to be rewritten in the compact form:

$$\begin{aligned} \mathcal{M}_{JM}^{(k)\dagger}(\tau) &= \hat{J}^{-1} \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(J;k)} \\ &\times \{A_{JM}^{(+)\dagger}(j_1 j_2) + A_{JM}^{(+)}(j_1 j_2) + B_{JM}^{(+)}(j_1 j_2)\}, \\ \mathcal{S}_{LJM}^{(k)\dagger}(\tau) &= \hat{J}^{-1} \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(LJ;k)} \\ &\times \{A_{JM}^{(-)\dagger}(j_1 j_2) - A_{JM}^{(-)}(j_1 j_2) + B_{JM}^{(-)}(j_1 j_2)\}, \end{aligned} \quad (207)$$

where

$$\begin{aligned} &A_{JM}^{(\pm)\dagger}(j_1 j_2) \\ &= \frac{1}{2} u_{j_1 j_2}^{(\pm)}(x_{j_1} x_{j_2} [\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM} \pm y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM}) \\ &\quad + i v_{j_1 j_2}^{(\mp)} x_{j_1} y_{j_2} [\beta_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM}, \\ &A_{JM}^{(\pm)}(j_1 j_2) = (-1)^{J-M} [A_{J-M}^{(\pm)\dagger}(j_1 j_2)]^{\dagger}, \\ &B_{JM}^{(\pm)}(j_1 j_2) = -v_{j_1 j_2}^{(\mp)}(x_{j_1} x_{j_2} [\beta_{j_1}^{\dagger} \beta_{j_2}^{-}]_{JM} \\ &\quad \pm y_{j_1} y_{j_2} [\tilde{\beta}_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{-}]_{JM}) \\ &+ i u_{j_1 j_2}^{(\pm)}(x_{j_1} y_{j_2} [\beta_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{-}]_{JM} \pm y_{j_1} x_{j_2} [\tilde{\beta}_{j_1}^{\dagger} \beta_{j_2}^{-}]_{JM}) \end{aligned} \quad (208)$$

and the following notation is used for combinations of the Bogolyubov transformation coefficients:

$u_{j_1 j_2}^{(\pm)} = u_{j_1} v_{j_2} \pm v_{j_1} u_{j_2}$, $v_{j_1 j_2}^{(\pm)} = u_{j_1} u_{j_2} \pm v_{j_1} v_{j_2}$. Consequently, $\mathcal{H}_{\text{ch.n}}$ (162) contains terms expressed in terms of products of the operators of creation and annihilation of a pair of thermal quasi-particles: $[\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM} [\beta_{j_3}^{\dagger} \beta_{j_4}^{\dagger}]_{JM}$, $[\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM} [\tilde{\beta}_{j_3}^{\dagger} \tilde{\beta}_{j_4}^{\dagger}]_{JM}$, $[\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM} [\beta_{j_3}^{\dagger} \beta_{j_4}^{\dagger}]_{JM}$, etc. These terms describe the interaction between two thermal quasiparticle states.

To consider the interaction between two thermal quasiparticle states, we use the generalization of the quasiparticle random phase approximation (QRPA) [112, 41] to the case $T \neq 0$, that is, we diagonalize (approximately) the thermal Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{BCS}} + \mathcal{H}_{\text{ch.n}} \quad (209)$$

in terms of thermal phonon operators

$$\begin{aligned} Q_{JM_i}^{\dagger} &= \frac{1}{2} \sum_{j_1 j_2}^{\tau} (\psi_{j_1 j_2}^{J_i} [\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM} + \tilde{\psi}_{j_1 j_2}^{J_i} [\tilde{\beta}_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM} \\ &\quad + 2i \eta_{j_1 j_2}^{J_i} [\beta_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM} - \phi_{j_1 j_2}^{J_i} [\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM}^{\dagger} \\ &\quad - \tilde{\phi}_{j_1 j_2}^{J_i} [\tilde{\beta}_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM}^{\dagger} + 2i \xi_{j_1 j_2}^{J_i} [\beta_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM}^{\dagger}). \end{aligned} \quad (210)$$

The phonon operators $\tilde{Q}_{JM_i}^{\dagger}$, \tilde{Q}_{JM_i} , $Q_{JM_i}^{\dagger}$ are obtained from (210) by applying operations of the Hermitian and tilde conjugation. Normal parity phonons ($\pi = (-1)^J$) are generated by multipole and spin-

multipole $L = J$ components of residual interaction, while anomalous parity phonons ($\pi = (-1)^{J+1}$) are generated by spin-multipole components with $L = J \pm 1$.

The method of approximate diagonalization of the thermal Hamiltonian in terms of thermal phonon operators (210) will be called the thermal quasiparticle random phase approximation (TQRPA), thus emphasizing that the phonon operators consist of operators of the creation and annihilation of thermal quasiparticles. The vacuum of thermal phonons $|\psi_0(T)\rangle$ is the thermal vacuum in the TQRPA provided that it satisfies thermal state condition (142).

To find the structure (phonon amplitudes ψ, ϕ , etc.) and the energy of thermal phonons, as in the derivation of the QRPA equations for a cold nucleus, we will use the quasi-boson approximation, that is, we will assume that the operators of creation and annihilation of a pair of thermal quasiparticles obey the bosonic commutation relations²⁷:

$$\begin{aligned} &[[\beta_{j_1}^{\dagger} \beta_{j_2}^{\dagger}]_{JM}^{\dagger}, [\beta_{j_3}^{\dagger} \beta_{j_4}^{\dagger}]_{J'M'}] \\ &\approx \delta_{JJ'} \delta_{MM'} (\delta_{j_1 j_3} \delta_{j_2 j_4} + (-1)^{j_1 - j_2 + J} \delta_{j_1 j_4} \delta_{j_2 j_3}), \\ &[[\tilde{\beta}_{j_1}^{\dagger} \tilde{\beta}_{j_2}^{\dagger}]_{JM}^{\dagger}, [\beta_{j_3}^{\dagger} \beta_{j_4}^{\dagger}]_{J'M'}] \approx \delta_{JJ'} \delta_{MM'} \delta_{j_1 j_3} \delta_{j_2 j_4}, \end{aligned} \quad (211)$$

while all other commutators are equal to zero. In the quasi-boson approximation, the sum of \mathcal{H}_{BCS} (191) and the part $\mathcal{H}_{\text{ch.n}}$, which describes the interaction of two-thermal-quasi-particle states, is a quadratic Hermitian form with respect to the creation and annihilation operators of bosons. This quadratic form can be reduced to a diagonal form

$$\mathcal{H} \approx \sum_{JM_i} \omega_{J_i} (Q_{JM_i}^{\dagger} Q_{JM_i} - \tilde{Q}_{JM_i}^{\dagger} \tilde{Q}_{JM_i}), \quad (212)$$

by a linear transformation of the form (210). For the transformation to be canonical, i.e., to provide bosonic commutation relations between the phonon operators, the phonon amplitudes must satisfy a number of conditions. In particular, from the condition that $[Q_{JM_i}, Q_{JM_i}^{\dagger}] = \delta_{ii'}$ it follows that

$$\begin{aligned} &\frac{1}{2} \sum_{j_1 j_2}^{\tau} \{(\psi_{j_1 j_2}^{J_i} \psi_{j_1 j_2}^{J_i'} - \phi_{j_1 j_2}^{J_i} \phi_{j_1 j_2}^{J_i'}) \\ &+ (\tilde{\psi}_{j_1 j_2}^{J_i} \tilde{\psi}_{j_1 j_2}^{J_i'} - \tilde{\phi}_{j_1 j_2}^{J_i} \tilde{\phi}_{j_1 j_2}^{J_i'}) + (\eta_{j_1 j_2}^{J_i} \eta_{j_1 j_2}^{J_i'} - \xi_{j_1 j_2}^{J_i} \xi_{j_1 j_2}^{J_i'}) \\ &+ (\tilde{\eta}_{j_1 j_2}^{J_i} \tilde{\eta}_{j_1 j_2}^{J_i'} - \tilde{\xi}_{j_1 j_2}^{J_i} \tilde{\xi}_{j_1 j_2}^{J_i'})\} = \delta_{ii'}, \end{aligned} \quad (213)$$

²⁷As well as for $T = 0$, the validity of the quasi-boson approximation is related to the requirement that the number of thermal quasiparticles in the vacuum of thermal phonons be small. This requirement is the main assumption in the TQRPA.

where the notations $\tilde{\eta}_{j_1 j_2}^{J_i} = (-1)^{j_1 - j_2 + J} \eta_{j_2 j_1}^{J_i}$ and $\tilde{\xi}_{j_1 j_2}^{J_i} = (-1)^{j_1 - j_2 + J} \xi_{j_2 j_1}^{J_i}$ are used²⁸. Having considered other commutators ($[Q_{JM_i}, \tilde{Q}_{JM_i}^\dagger] = 0$, etc.), we obtain a number of additional relations between the amplitudes (see (325)–(327) in Appendix B). The obtained relations between the amplitudes imply the normalization and orthogonality of one-phonon states:

$$\begin{aligned} \langle Q_{JM_i} | Q_{J'M'i'} \rangle &= \delta_{JJ'} \delta_{MM'} \delta_{ii'}, \\ \langle Q_{JM_i} | \tilde{Q}_{J'M'i'} \rangle &= 0. \end{aligned} \quad (214)$$

In addition, they can be used to show that the transformations inverse to (210) have the form

$$\begin{aligned} |\beta_{j_1}^\dagger \beta_{j_2}^\dagger\rangle_{JM} &= \sum_i (\psi_{j_1 j_2}^{J_i} Q_{JM_i}^\dagger + \phi_{j_1 j_2}^{J_i} Q_{JM_i}^-) \\ &+ \tilde{\psi}_{j_1 j_2}^{J_i} \tilde{Q}_{JM_i}^\dagger + \tilde{\phi}_{j_1 j_2}^{J_i} \tilde{Q}_{JM_i}^-, \\ |\beta_{j_1}^\dagger \beta_{j_2}^\dagger\rangle_{JM} &= |\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger\rangle_{JM}, \\ |\beta_{j_1}^\dagger \beta_{j_2}^\dagger\rangle_{JM} &= -i \sum_i (\eta_{j_1 j_2}^{J_i} Q_{JM_i}^\dagger + \xi_{j_1 j_2}^{J_i} Q_{JM_i}^-) \\ &+ \tilde{\eta}_{j_1 j_2}^{J_i} \tilde{Q}_{JM_i}^\dagger + \tilde{\xi}_{j_1 j_2}^{J_i} \tilde{Q}_{JM_i}^-, \\ |\beta_{j_1}^\dagger \beta_{j_2}^\dagger\rangle_{JM} &= -|\tilde{\beta}_{j_1}^\dagger \tilde{\beta}_{j_2}^\dagger\rangle_{JM}. \end{aligned} \quad (215)$$

These relations make it possible to express an arbitrary single-particle operator in terms of thermal phonon operators.

So far, the consideration was not different from the standard QRPA. A distinctive feature of the TQRPA method is the fact that the diagonalized Hamiltonian (212) is invariant under the unitary transformation mixing tilde and nontilde phonons

$$\begin{aligned} Q_{JM_i}^\dagger &\rightarrow X_i Q_{JM_i}^\dagger + Y_i \tilde{Q}_{JM_i}, \\ \tilde{Q}_{JM_i}^\dagger &\rightarrow X_i \tilde{Q}_{JM_i}^\dagger + Y_i Q_{JM_i}, \end{aligned} \quad (216)$$

where $X_i^2 - Y_i^2 = 1$. In other words, the diagonalization procedure determines a structure of the thermal phonons and the phonon vacuum only up to unitary transformation (216). Recall that we encountered the same situation when determining a structure of thermal quasiparticles.

Let us obtain additional conditions for phonon amplitudes by requiring that the vacuum of thermal phonons $|\psi_0(T)\rangle$ obeys the thermal state condition (142). As an operator A in condition (142), we first consider the two-quasiparticle operator $A = [\alpha_{j_1}^\dagger \alpha_{j_2}^\dagger]_{JM}$ ($j_{1,2} \in \tau$). Let us express this operator through thermal quasiparticles, and then, using inverse transformations (215),

²⁸Other amplitudes when permuting the indices j_1 and j_2 are multiplied by $(-1)^{j_1 - j_2 + J}$ (i.e., $\psi_{j_2 j_1}^{J_i} = (-1)^{j_1 - j_2 + J} \psi_{j_1 j_2}^{J_i}$ etc.).

through thermal phonon operators. We keep in the resulting expression only one-phonon terms

$$\begin{aligned} A &= \sum_i \{ (x_{j_1} x_{j_2} \psi_{j_1 j_2}^{J_i} + y_{j_1} y_{j_2} \tilde{\psi}_{j_1 j_2}^{J_i}) Q_{JM_i}^\dagger \\ &+ (x_{j_1} x_{j_2} \phi_{j_1 j_2}^{J_i} + y_{j_1} y_{j_2} \tilde{\phi}_{j_1 j_2}^{J_i}) Q_{JM_i}^- \\ &+ (x_{j_1} x_{j_2} \tilde{\psi}_{j_1 j_2}^{J_i} + y_{j_1} y_{j_2} \phi_{j_1 j_2}^{J_i}) \tilde{Q}_{JM_i}^\dagger \\ &+ (x_{j_1} x_{j_2} \tilde{\phi}_{j_1 j_2}^{J_i} + y_{j_1} y_{j_2} \psi_{j_1 j_2}^{J_i}) \tilde{Q}_{JM_i}^- \}. \end{aligned} \quad (217)$$

Substituting this expression into thermal state condition (142) leads to the following relations between tilde $\tilde{\psi}, \tilde{\phi}$ and nontilde ψ, ϕ amplitudes

$$\begin{pmatrix} \tilde{\Psi} \\ \tilde{\Phi} \end{pmatrix}_{j_1 j_2}^{J_i} = \frac{x_{j_1} x_{j_2} e^{-\omega_{j_i}/2T} - y_{j_1} y_{j_2}}{x_{j_1} x_{j_2} - y_{j_1} y_{j_2} e^{-\omega_{j_i}/2T}} \begin{pmatrix} \Phi \\ \Psi \end{pmatrix}_{j_1 j_2}^{J_i}. \quad (218)$$

The same relations can be obtained if we consider the operator $[\alpha_{j_1}^- \alpha_{j_2}^-]_{JM}$ as the operator A . If, however, as A , we use $[\alpha_{j_1}^\dagger \alpha_{j_2}^-]_{JM}$ or $[\alpha_{j_1}^- \alpha_{j_2}^\dagger]_{JM}$, then we obtain the relations between the phonon amplitudes η, ξ and $\tilde{\eta}, \tilde{\xi}$

$$\begin{pmatrix} \tilde{\eta} \\ \tilde{\xi} \end{pmatrix}_{j_1 j_2}^{J_i} = \frac{x_{j_1} y_{j_2} e^{-\omega_{j_i}/2T} - y_{j_1} x_{j_2}}{x_{j_1} y_{j_2} - y_{j_1} x_{j_2} e^{-\omega_{j_i}/2T}} \begin{pmatrix} \xi \\ \eta \end{pmatrix}_{j_1 j_2}^{J_i}. \quad (219)$$

The obtained relations between tilde and nontilde phonon amplitudes unambiguously fix the structure of thermal phonons in such a way that their vacuum is a thermal vacuum in the TQRPA.

Let us fix the “true” structure of thermal phonons when deriving the TQRPA equations by introducing the effective amplitudes Ψ, Φ, H and Ξ :

$$\begin{aligned} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}_{j_1 j_2}^{J_i} &= [X_{J_i} x_{j_1} x_{j_2} - Y_{J_i} y_{j_1} y_{j_2}] \Gamma^{-1} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}_{j_1 j_2}^{J_i} \\ &= [Y_{J_i} x_{j_1} x_{j_2} - X_{J_i} y_{j_1} y_{j_2}] \Gamma^{-1} \begin{pmatrix} \tilde{\Phi} \\ \tilde{\Psi} \end{pmatrix}_{j_1 j_2}^{J_i} \\ \begin{pmatrix} H \\ \Xi \end{pmatrix}_{j_1 j_2}^{J_i} &= [X_{J_i} x_{j_1} y_{j_2} - Y_{J_i} y_{j_1} x_{j_2}] \Gamma^{-1} \begin{pmatrix} \eta \\ \xi \end{pmatrix}_{j_1 j_2}^{J_i} \\ &= [Y_{J_i} x_{j_1} y_{j_2} - X_{J_i} y_{j_1} x_{j_2}] \Gamma^{-1} \begin{pmatrix} \tilde{\xi} \\ \tilde{\eta} \end{pmatrix}_{j_1 j_2}^{J_i}, \end{aligned} \quad (220)$$

where the temperature-dependent functions X_{J_i} and Y_{J_i} are related to the Bose–Einstein distribution function

$$Y_{J_i} = (e^{\omega_{j_i}/T} - 1)^{-1/2}, \quad X_{J_i} = (1 + Y_{J_i}^2)^{1/2}. \quad (221)$$

Thus, the requirement that thermal state condition (142) be satisfied for the vacuum of thermal phonons leads to the fact that phonon amplitudes depend on both fermionic and bosonic occupation numbers. In this case, the direct and tilde-conjugate inverse phonon amplitudes (i.e., Ψ and $\tilde{\Phi}$, $\tilde{\Psi}$ and Φ , η and $\tilde{\xi}$,

$\tilde{\eta}$ and $\tilde{\xi}$ are expressed through the same effective amplitude (Ψ, Φ, H, Ξ) .

It is easy to show that the effective amplitudes satisfy the following relations with permutation of the indices j_1 and j_2 :

$$\begin{aligned} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}_{j_2 j_1}^{J_i} &= (-1)^{j_1 - j_2 + J} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}_{j_1 j_2}^{J_i}, \\ H_{j_2 j_1}^{J_i} &= (-1)^{j_1 + j_2 + J} \Xi_{j_1 j_2}^{J_i}. \end{aligned} \quad (222)$$

In addition, orthonormality condition (213) in this case takes the form

$$\begin{aligned} \frac{1}{2} \sum_{\tau} \sum_{j_1 j_2} \{ (\Psi_{j_1 j_2}^{J_i} \Psi_{j_1 j_2}^{J_i'} - \Phi_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'}) (1 - y_{j_1}^2 - y_{j_2}^2) \\ + (H_{j_1 j_2}^{J_i} H_{j_1 j_2}^{J_i'} - \Xi_{j_1 j_2}^{J_i} \Xi_{j_1 j_2}^{J_i'}) (y_{j_2}^2 - y_{j_1}^2) \} = \delta_{ii'}. \end{aligned} \quad (223)$$

This relation coincides with the normalization condition for the amplitudes of phonon operators, which is satisfied in the method of temperature RPA [113] and when using the temperature Green's functions [114]. However, it should be kept in mind that the phonon definition in [113, 114] includes Bogolyubov quasiparticles, rather than thermal quasiparticles. The comparison of expression (223) with the normalization condition in the mentioned works shows that $\Psi_{j_1 j_2}^{J_i}$ corresponds to the direct phonon amplitude, $\Phi_{j_1 j_2}^{J_i}$ corresponds to the inverse one, while $H_{j_1 j_2}^{J_i}$ and $\Xi_{j_1 j_2}^{J_i}$ are the so-called scattering amplitudes that arise due to thermal smearing of the Fermi surface in the nucleus.

To diagonalize the thermal Hamiltonian in the basis of thermal phonons, i.e., to reduce it to the form (212), we use equation of motion (143), in which we consider the creation and annihilation operators of a pair of thermal quasiparticles as δO , while a role of the vacuum state is played by the thermal vacuum of the TQBCS approximation $|\varphi_0(T)\rangle$. When calculating the commutators, we assume the validity of quasi-boson approximation (211). As a result, we arrive at a system of linear homogeneous TQRPA equations for effective amplitudes (220). For thermal phonons of normal parity, the TQRPA equations take the following form

$$\begin{aligned} \varepsilon_{j_1 j_2}^{(+)} G_{j_1 j_2}^{J_i} - \hat{J}^{-2} u_{j_1 j_2}^{(+)} \sum_{k=1}^N f_{j_1 j_2}^{(J; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} W_{j_1 j_2}^{J_i}, \\ \varepsilon_{j_1 j_2}^{(+)} W_{j_1 j_2}^{J_i} - \hat{J}^{-2} u_{j_1 j_2}^{(-)} \sum_{k=1}^N f_{j_1 j_2}^{(JJ; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} G_{j_1 j_2}^{J_i}, \end{aligned} \quad (224)$$

$$\begin{aligned} \varepsilon_{j_1 j_2}^{(-)} T_{j_1 j_2}^{J_i} - \hat{J}^{-2} v_{j_1 j_2}^{(-)} \sum_{k=1}^N f_{j_1 j_2}^{(J; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} S_{j_1 j_2}^{J_i}, \\ \varepsilon_{j_1 j_2}^{(-)} S_{j_1 j_2}^{J_i} - \hat{J}^{-2} v_{j_1 j_2}^{(+)} \sum_{k=1}^N f_{j_1 j_2}^{(JJ; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} T_{j_1 j_2}^{J_i}. \end{aligned}$$

In the case of phonons of anomalous parity, the system of TQRPA equations is written as [115]

$$\begin{aligned} \varepsilon_{j_1 j_2}^{(+)} G_{j_1 j_2}^{J_i} = \omega_{J_i} W_{j_1 j_2}^{J_i}, \\ \varepsilon_{j_1 j_2}^{(+)} W_{j_1 j_2}^{J_i} - \hat{J}^{-2} u_{j_1 j_2}^{(-)} \sum_{k=1}^N \sum_{L=J \pm 1} f_{j_1 j_2}^{(LJ; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{L J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} G_{j_1 j_2}^{J_i}, \\ \varepsilon_{j_1 j_2}^{(-)} T_{j_1 j_2}^{J_i} = \omega_{J_i} S_{j_1 j_2}^{J_i}, \\ \varepsilon_{j_1 j_2}^{(-)} S_{j_1 j_2}^{J_i} - \hat{J}^{-2} v_{j_1 j_2}^{(+)} \sum_{k=1}^N \sum_{L=J \pm 1} f_{j_1 j_2}^{(LJ; k)} \\ \times \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{L J_i}^{(k)}(\rho\tau) \right) = \omega_{J_i} T_{j_1 j_2}^{J_i}. \end{aligned} \quad (225)$$

In the above equations, the following notation is used for linear combinations of effective amplitudes:

$$\begin{aligned} D_{J_i}^{(k)}(\tau) &= \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(J; k)} \{ u_{j_1 j_2}^{(+)} (1 - y_{j_1}^2 - y_{j_2}^2) G_{j_1 j_2}^{J_i} \\ &\quad + v_{j_1 j_2}^{(-)} (y_{j_2}^2 - y_{j_1}^2) T_{j_1 j_2}^{J_i} \}, \\ D_{L J_i}^{(k)}(\tau) &= \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(LJ; k)} \{ u_{j_1 j_2}^{(-)} (1 - y_{j_1}^2 - y_{j_2}^2) W_{j_1 j_2}^{J_i} \\ &\quad + v_{j_1 j_2}^{(+)} (y_{j_2}^2 - y_{j_1}^2) S_{j_1 j_2}^{J_i} \}, \end{aligned} \quad (226)$$

where

$$\begin{aligned} G_{j_1 j_2}^{J_i} &= \Psi_{j_1 j_2}^{J_i} + \Phi_{j_1 j_2}^{J_i}, & W_{j_1 j_2}^{J_i} &= \Psi_{j_1 j_2}^{J_i} - \Phi_{j_1 j_2}^{J_i}, \\ T_{j_1 j_2}^{J_i} &= H_{j_1 j_2}^{J_i} + \Xi_{j_1 j_2}^{J_i}, & S_{j_1 j_2}^{J_i} &= H_{j_1 j_2}^{J_i} - \Xi_{j_1 j_2}^{J_i}. \end{aligned} \quad (227)$$

The resulting systems of TQRPA equations represent an eigenvalue problem, the matrix of which has a dimension twice as large as the number of two thermal quasiparticle states. As shown in Appendix B, the use of the separable residual interaction makes it possible to reduce the eigenvalue problem to a system of $4N$ linear homogeneous equations for the functions $D_{J_i}^{(k)}(\tau)$ and $D_{L J_i}^{(k)}(\tau)$ ($\tau = n, p$) (Eqs. (330) and (334)). The condition for the existence of a nontrivial solution of this system leads to a secular equation for the temperature-dependent energy ω_{J_i} of thermal phonons (see Eqs. (332) and (335)). Finding for each ω_{J_i} the functions $D_{J_i}^{(k)}(\tau)$, $D_{L J_i}^{(k)}(\tau)$ (with arbitrary normalization) and substituting them into (224), (225), we determine the unnormalized effective amplitudes (220).

The effective amplitudes are normalized using condition (223).

Let us obtain expressions for the transition amplitude from thermal vacuum to one-phonon states. To this end, using (193) and inverse transformations (215), we express the one-particle tensor operator \mathcal{T}_{JM} in terms of thermal phonon operators:

$$\begin{aligned} \mathcal{T}_{JM} = & \hat{J}^{-1} \sum_i X_{Ji} \{ [\Gamma_{Ji}^{(+)}(\mathcal{T}_J) + \Gamma_{Ji}^{(-)}(\mathcal{T}_J)] \\ & \times (Q_{JMi}^\dagger + e^{-\omega_{Ji}/2T} \tilde{Q}_{JMi}) \\ & + [\Gamma_{Ji}^{(+)}(\mathcal{T}_J) - \Gamma_{Ji}^{(-)}(\mathcal{T}_J)] (Q_{JMi} + e^{-\omega_{Ji}/2T} \tilde{Q}_{JMi}^\dagger) \} \\ & + \hat{J}^{-1} \sum_\tau \sum_{j_1 j_2}^\tau t_{j_1 j_2}^{(J)} \{ B_{JM}(j_1 j_2) + B_{JM}^*(j_1 j_2) \}. \end{aligned} \quad (228)$$

Where²⁹

$$\begin{aligned} \Gamma_{Ji}^{(+)}(\mathcal{T}_J) = & \frac{1}{2} \sum_\tau \sum_{j_1 j_2}^\tau t_{j_1 j_2}^{(J)} \{ (1 - y_{j_1}^2 - y_{j_2}^2) \\ & \times u_{j_1 j_2}^{(+)} G_{j_1 j_2}^{Ji} + (y_{j_2}^2 - y_{j_1}^2) v_{j_1 j_2}^{(-)} T_{j_1 j_2}^{Ji} \}, \\ \Gamma_{Ji}^{(-)}(\mathcal{T}_J) = & \frac{1}{2} \sum_\tau \sum_{j_1 j_2}^\tau t_{j_1 j_2}^{(J)} \{ (1 - y_{j_1}^2 - y_{j_2}^2) \\ & \times u_{j_1 j_2}^{(-)} W_{j_1 j_2}^{Ji} + (y_{j_2}^2 - y_{j_1}^2) v_{j_1 j_2}^{(+)} S_{j_1 j_2}^{Ji} \}. \end{aligned} \quad (229)$$

The temperature-dependent functions $\Gamma_{Ji}^{(\pm)}(\mathcal{T}_J)$ determine the transition amplitude to one-phonon states:

$$\begin{aligned} \langle Q_{Ji} \| \mathcal{T}_J \| \Psi_0(T) \rangle = & X_{Ji} [\Gamma_{Ji}^{(+)}(\mathcal{T}_J) + \Gamma_{Ji}^{(-)}(\mathcal{T}_J)], \\ \langle \tilde{Q}_{Ji} \| \mathcal{T}_J \| \Psi_0(T) \rangle = & Y_{Ji} [\Gamma_{Ji}^{(+)}(\mathcal{T}_J) - \Gamma_{Ji}^{(-)}(\mathcal{T}_J)]. \end{aligned} \quad (230)$$

We obtain expressions for the reduced transition probabilities

$$\begin{aligned} B_{Ji}(T_J) = & \langle Q_{Ji} \| \mathcal{T}_J \| \Psi_0(T) \rangle^2 \\ = & X_{Ji}^2 |\Gamma_{Ji}^{(+)}(\mathcal{T}_J) + \Gamma_{Ji}^{(-)}(\mathcal{T}_J)|^2, \\ \tilde{B}_{Ji}(T_J) = & \langle \tilde{Q}_{Ji} \| \mathcal{T}_J \| \Psi_0(T) \rangle^2 \\ = & Y_{Ji}^2 |\Gamma_{Ji}^{(+)}(\mathcal{T}_J) - \Gamma_{Ji}^{(-)}(\mathcal{T}_J)|^2. \end{aligned} \quad (231)$$

If $\mathcal{T}_{JM}^\dagger = \pm(-1)^{J-M} \mathcal{T}_{J-M}$ (see footnote 29), then the transition probabilities to tilde-conjugate one-phonon states are related as

$$\tilde{B}_{Ji}(\mathcal{T}_J) = e^{-\omega_{Ji}/T} B_{Ji}(\mathcal{T}_J). \quad (232)$$

The resulting expressions for the amplitude and strength of transitions to one-phonon states, together with the transition energy

$$E_{Ji} = \omega_{Ji}, \quad \tilde{E}_{Ji} = -\omega_{Ji} \quad (233)$$

²⁹Using relations (222) it is easy to show that if $\mathcal{T}_{JM}^\dagger = (-1)^{J-M} \mathcal{T}_{J-M}$ (and, therefore, $t_{j_2 j_1}^{(J)} = (-1)^{j_1 - j_2 + J} t_{j_1 j_2}^{(J)}$), then $\Gamma_{Ji}^{(-)}(\mathcal{T}_J) = 0$. On the contrary, if $\mathcal{T}_{JM}^\dagger = (-1)^{J-M} \mathcal{T}_{J-M}$ (and, therefore, $t_{j_2 j_1}^{(J)} = (-1)^{j_1 + j_2 + J} t_{j_1 j_2}^{(J)}$), then $\Gamma_{Ji}^{(+)}(\mathcal{T}_J) = 0$.

determine charge-neutral spectral densities (127) and strength functions (130) in the TQRPA. Due to the fact that the TQRPA thermal vacuum satisfies the thermal state condition (142), the principle of detailed balance (119) is valid for the spectral densities and strength functions.

Just as operators of the thermal and Bogolyubov quasi-particles are related by thermal transformation (171), the thermal phonon operators can be represented as a result of the following thermal transformation

$$\begin{aligned} Q_{JMi}^\dagger = & X_{Ji} q_{JMi}^\dagger - Y_{Ji} \tilde{q}_{JMi}, \\ \tilde{Q}_{JMi}^\dagger = & X_{Ji} \tilde{q}_{JMi}^\dagger - Y_{Ji} q_{JMi}, \end{aligned} \quad (234)$$

where the q -phonon operators correspond to the values $X_{Ji} = 1, Y_{Ji} = 0$ in amplitude definition (220). In this case, the one-phonon part of the thermal Hamiltonian is diagonal both in terms of q -phonons and in terms of thermal phonons

$$\begin{aligned} \mathcal{H}_{\text{TQRPA}} = & \sum_{JMi} \omega_{Ji} (Q_{JMi}^\dagger Q_{JMi} - \tilde{Q}_{JMi}^\dagger \tilde{Q}_{JMi}) \\ = & \sum_{JMi} \omega_{Ji} (q_{JMi}^\dagger q_{JMi} - \tilde{q}_{JMi}^\dagger \tilde{q}_{JMi}). \end{aligned} \quad (235)$$

The relationship between the q -phonon vacuum, $|\Psi_0\rangle$, and thermal vacuum $|\Psi_0(T)\rangle$ has the form similar to (177) [37]. Using the standard procedure [41], the TQRPA thermal vacuum can be expressed in terms of the thermal vacuum of the TQBCS approximation, and its tilde invariance can be proved.

In [116, 84, 104, 117], q -phonons were considered as thermal ones, and their vacuum played the role of thermal vacuum. With this approach, the bosonic occupation numbers do not arise in the theory. In addition, the transition probability to tilde states with negative energy turns out to be zero:

$$\begin{aligned} b_{Ji}(\mathcal{T}_J) = & \langle q_{Ji} \| \mathcal{T}_J \| \Psi_0 \rangle^2 \\ = & |\Gamma_{Ji}^{(+)}(\mathcal{T}_J) + \Gamma_{Ji}^{(-)}(\mathcal{T}_J)|^2, \\ \tilde{b}_{Ji}(\mathcal{T}_J) = & \langle \tilde{q}_{Ji} \| \mathcal{T}_J \| \Psi_0 \rangle^2 = 0, \end{aligned} \quad (236)$$

which leads to a violation of the principle of detailed balance, since it makes the exoenergetic processes, associated with the deexcitation of the hot nucleus, impossible. This circumstance was not considered in [84, 104, 116, 117].

The fact that in a system of q -phonons, as well as for a nucleus in the ground state, only an excitation process is possible, allows us to consider q -phonons as ‘‘cold’’ phonons, while thermal transformation (234), as a process of their heating, i.e., a transition to new phonon operators, whose vacuum state is the thermal vacuum. After heating, the thermal vacuum contains thermally excited q -phonons

$$\langle \Psi_0(T) | q_{JMi}^\dagger q_{JMi} | \Psi_0(T) \rangle = Y_{Ji}^2. \quad (237)$$

Therefore, in accordance with expressions (231), the probability of the deexcitation process, in which a q -phonon is removed from the system, is proportional to Y_{ji}^2 , and the probability of the inverse process of excitation, in which a q -phonon is added to the system, is proportional to $X_{ji}^2 = 1 + Y_{ji}^2$.

In [35], using the example of the QPM Hamiltonian with a multipole residual interaction, we have studied how the choice of thermal transformation (171) (real or complex) affects the TQRPA equations. It was found that although the form of the secular equation for the phonon energy does not depend on the choice of thermal transformation, differences arise in the structure of thermal phonons. In particular, it was shown that in order for the thermal phonon to correspond in the limit $H_{\text{res}} = 0$ to the excitation of a two thermal quasiparticle state, while for the TQRPA thermal vacuum to pass into the thermal vacuum of the TQBCS approximation, it is necessary to use exactly the complex transformation.

10. FRAGMENTATION OF CHARGE-NEUTRAL THERMAL PHONONS

In a cold nucleus ($T = 0$), the random phase approximation is successfully used both in studying the basic properties of giant resonances (position, excitation probabilities) and in studying the properties of collective low-lying nuclear states. At the same time, it is known that the assumption of noninteracting collective modes—phonons—does not allow the entire variety of properties of nuclear excitations to be described. In particular, the simple one-phonon approximation fails to reproduce the probabilities of transitions between low-lying vibrational states, the widths of giant resonances, the photoabsorption cross sections, and so on. In microscopic nuclear models, a partial or complete solution of these problems is achieved by complicating the wave function of excited states due to including more and more complex components in its structure. The interaction between the simple and complex components of the wave function occurs due to the part of the residual interaction, which is neglected in RPA when calculating the structure of one-phonon states. One of these models is the quasiparticle-phonon nuclear model, which is based on the coupling of elementary nuclear excitation modes—Bogolyubov quasi-particles and RPA phonons [92, 101, 118, 119]. With the help of QPM, it is possible to describe those properties of nuclear excitations that are related by few-quasiparticle components of the wave functions. In even—even nuclei these are one- and two-phonon configurations, while in odd nuclei, they are one-quasiparticle configurations and configurations of the “quasiparticle + phonon” type. The interaction of these simple configurations with

more complex ones leads to their fragmentation over a large number of states. One of manifestations of the fragmentation is the appearance of large widths at giant resonances and deep hole states [120, 121].

The above presented generalizations of the BCS and QRPA methods to hot nuclei using the method of superoperators, as well as the fact that the thermal Hamiltonian structure inherits a structure of the original physical Hamiltonian of the nucleus, make it possible to consider going beyond the one-phonon approximation at $T \neq 0$ within the method that is traditional for QPM, i.e., by complicating the wave function of excited states due to including two-phonon components in it. The first work in this direction was published in 1994 [104]. Further, the theoretical results of this work were used to calculate the dependence of the giant dipole resonance width on the nucleus temperature [117, 122]. However, in these works, a structure of thermal phonons was found according to [84, 116], i.e., it was assumed that q -phonons are thermal phonons, and their vacuum is a thermal vacuum. As was shown in the previous section, under this assumption the TQRPA vacuum does not satisfy thermal state condition (109). As a result, the detailed balance principle is violated both at the one-phonon level and when the coupling of phonons is considered. To consider the correct structure of the thermal vacuum when going beyond the one-phonon approximation, the results of [104] were revised in [35, 107, 123] in the direction of complicating the probe wave function. As will be shown below, this complication is absolutely necessary if we intend to satisfy the thermal state condition and preserve the detailed balance principle.

It is known that the use of a separable residual interaction in QPM makes it possible to bypass a problem of the configuration space growth as the wave function structure becomes more complex [92, 118, 119]. Separabilization of the Landau–Migdal interaction makes it possible to apply the same calculation scheme when going beyond RPA, which is a promising direction from the viewpoint of self-consistency and possibility of performing global calculations for a large number of nuclei. However, here, for the purpose of clarity and simplification of the result derivation, we restrict ourselves to the QPM Hamiltonian, in which we consider only the multipole residual interaction in the charge-neutral channel. The generalization of the results to the case of separable interaction of a more complex form does not present fundamental difficulty.

If we consider only the multipole interaction and set $N = 1$, then secular equation (332) for determining

the energy ω_{J_i} of one-phonon states of normal parity reduces to the condition:

$$\begin{aligned} & [\mathcal{X}_{mm;p}^{(J)}(\omega) + \mathcal{X}_{mm;n}^{(J)}(\omega)](\chi_0^{(J)} + \chi_1^{(J)}) \\ & - 4\chi_0^{(J)}\chi_1^{(J)}\mathcal{X}_{mm;p}^{(J)}(\omega)\mathcal{X}_{mm;n}^{(J)}(\omega) = 1, \end{aligned} \quad (238)$$

where the functions $\mathcal{X}_{mm;\tau}^{(J)}(\omega)$ are defined in (331). We note that for separable residual strengths, a similar equation was first obtained by Ignatyuk using the temperature Green's functions [124], as well as in a number of later works based on the application of temperature RPA (see, e.g., [125–127]). Equation (238) was obtained in [84] as a special case of a more general equation that considers, along with the particle–hole interaction, the particle–particle multipole residual interaction. In our work [35], Eq. (238) was obtained for the first time using complex thermal transformation (171). In [35], there are also expressions for phonon amplitudes ψ, ϕ , etc., from which the expressions for effective amplitudes follow

$$\begin{aligned} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}_{j_1 j_2}^{J_i} &= \frac{1}{\sqrt{\mathcal{N}_\tau^{J_i}}} \frac{f_{j_1 j_2}^{(J_i)} u_{j_1 j_2}^{(+)}}{\varepsilon_{j_1 j_2}^{(+)} \mp \omega_{J_i}}, \\ \begin{pmatrix} H \\ \Xi \end{pmatrix}_{j_1 j_2}^{J_i} &= \frac{1}{\sqrt{\mathcal{N}_\tau^{J_i}}} \frac{f_{j_1 j_2}^{(J_i)} v_{j_1 j_2}^{(-)}}{\varepsilon_{j_1 j_2}^{(-)} \mp \omega_{J_i}}. \end{aligned} \quad (239)$$

The temperature dependence of the effective amplitudes is contained in the T -dependent energies of thermal quasiparticles and phonons, as well as in the normalization coefficients $\mathcal{N}_\tau^{J_i}$, the analytical form of which is given in [35, Eq. (55)]. It should also be noted that the expressions obtained for the effective amplitudes coincide with the expressions for the phonon amplitudes in [114], where they were obtained using the temperature Green's functions.

After the QPM thermal Hamiltonian part, which is quadratic in the creation and annihilation operators of two thermal quasiparticle states, has been reduced to a diagonal form, the thermal Hamiltonian can be written in the following form³⁰:

$$\mathcal{H} \approx \sum_{JM_i} \omega_{J_i} (Q_{JM_i}^\dagger Q_{JM_i} - \tilde{Q}_{JM_i}^\dagger \tilde{Q}_{JM_i}) + \mathcal{H}_{\text{qph}}. \quad (240)$$

The explicit form of the term \mathcal{H}_{qph} , which describes the interaction of thermal quasiparticles and

³⁰The approximately equal sign in (240) means that in the QPM thermal Hamiltonian we neglect the part containing the products of the creation and annihilation operators of thermal quasiparticles of the form $\beta^\dagger \beta^\dagger \beta$. As with $T = 0$, terms of this form are fourth-order operators in phonon operators, while $\mathcal{H}_{\text{qph}} \sim Q^\dagger Q^\dagger Q$ is the leading correction to the thermal Hamiltonian of noninteracting phonons.

phonons, can be obtained by writing the multipole operator $\mathcal{M}_{JM}^\dagger(\tau)$ in terms of the phonon operators

$$\begin{aligned} \mathcal{M}_{JM}^\dagger(\tau) &= \frac{1}{2} \hat{J}^{-1} \sum_i D_{J_i}(\tau) \{X_{J_i}(Q_{JM_i}^\dagger + \tilde{Q}_{JM_i}) \\ &+ Y_{J_i}(\tilde{Q}_{JM_i}^\dagger + \tilde{Q}_{JM_i})\} + \hat{J}^{-1} \sum_{j_1 j_2}^\tau f_{j_1 j_2}^{(J)} B_{JM}^{(+)}(j_1 j_2). \end{aligned} \quad (241)$$

The substitution of this expression into the thermal Hamiltonian leads to the following formula for \mathcal{H}_{qph} :

$$\begin{aligned} \mathcal{H}_{\text{qph}} &= -\frac{1}{2} \sum_{JM_i} \sum_\tau \sum_{j_1 j_2}^\tau \frac{f_{j_1 j_2}^{(J)}}{\sqrt{\mathcal{N}_\tau^{J_i}}} \\ &\times [\{X_{J_i}(Q_{JM_i}^\dagger + \tilde{Q}_{JM_i}) + Y_{J_i}(\tilde{Q}_{JM_i}^\dagger + \tilde{Q}_{JM_i})\} \\ &\times B_{JM}^{(+)}(j_1 j_2) + (\text{h.c.}) - (\text{t.c.})], \end{aligned} \quad (242)$$

where, for brevity, the terms that are Hermitian- and tilde-conjugate of the indicated terms are denoted as (h.c.) and (t.c.), respectively, and the expression for the operator $B_{JM}^{(+)}(j_1 j_2)$ is given in (208). As in the case of a cold nucleus, the term \mathcal{H}_{qph} mixes states with different numbers of phonons, due to which the fragmentation (broadening) of the strength of transitions to one-phonon states occurs.

Strictly speaking, the thermal Hamiltonian \mathcal{H} , being written in terms of thermal quasiparticles and phonons, contains terms of the type $B^\dagger B$, which describe the interaction of thermal quasiparticles ignored in TQRPA. These terms, as in the standard QPM at zero temperature [118, 92], will be neglected. In addition, when considering the coupling of thermal quasiparticles and thermal phonons, we will neglect the Pauli principle, i.e., consider thermal phonon operators as “true” bosons. In addition, we will use another approximation, namely, we will assume that

$$[B_{JM}^{(+)}(j_1 j_2), \tilde{q}_{J'M'}^\dagger] = [B_{JM}^{(+)}(j_1 j_2), \tilde{q}_{J'M'}] = 0. \quad (243)$$

To clarify the meaning of this approximation, we write \mathcal{H}_{qph} in terms of q -phonons

$$\begin{aligned} \mathcal{H}_{\text{qph}} &= -\frac{1}{2} \sum_{JM_i} \sum_\tau \sum_{j_1 j_2}^\tau \frac{f_{j_1 j_2}^{(J)}}{\sqrt{\mathcal{N}_\tau^{J_i}}} \\ &\times [(q_{JM_i}^\dagger + q_{JM_i}) B_{JM}^{(+)}(j_1 j_2) + (\text{h.c.}) - (\text{t.c.})]. \end{aligned} \quad (244)$$

Comparison of this expression with Eq. (242) shows that approximation (243) switches off the interaction of “cold” q^\dagger , q and \tilde{q}^\dagger , \tilde{q} phonons. The interaction of tilde and nontilde phonon excitations occurs only after “heating” (234).

To satisfy thermal state condition (142) if the coupling of one- and two-phonon configurations are con-

sidered, we will seek the eigenfunctions of the thermal Hamiltonian (240) in the following form:

$$\begin{aligned}
|\mathcal{Q}_{JM\nu}\rangle &= \mathcal{Q}_{JM\nu}^\dagger |\Psi_0(T)\rangle \\
&= \left[\sum_i \{R_i(J\nu)\mathcal{Q}_{JM_i}^\dagger + \tilde{R}_i(J\nu)\tilde{\mathcal{Q}}_{JM_i}^\dagger - N_i(J\nu)\mathcal{Q}_{JM_i} - \tilde{N}_i(J\nu)\tilde{\mathcal{Q}}_{JM_i}\} + \sum_{\substack{\lambda_1\mu_1 \\ \lambda_2\mu_2}} \{P_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\mathcal{Q}_{\lambda_1\mu_1}^\dagger \mathcal{Q}_{\lambda_2\mu_2}^\dagger]_{JM} \right. \\
&\quad + \tilde{P}_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\tilde{\mathcal{Q}}_{\lambda_1\mu_1}^\dagger \tilde{\mathcal{Q}}_{\lambda_2\mu_2}^\dagger]_{JM} + 2S_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\mathcal{Q}_{\lambda_1\mu_1}^\dagger \tilde{\mathcal{Q}}_{\lambda_2\mu_2}^\dagger]_{JM} \\
&\quad \left. - T_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\mathcal{Q}_{\lambda_1\mu_1} \mathcal{Q}_{\lambda_2\mu_2}]_{JM} - \tilde{T}_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\tilde{\mathcal{Q}}_{\lambda_1\mu_1} \tilde{\mathcal{Q}}_{\lambda_2\mu_2}]_{JM} \right. \\
&\quad \left. - 2Z_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)[\mathcal{Q}_{\lambda_1\mu_1} \tilde{\mathcal{Q}}_{\lambda_2\mu_2}]_{JM} \right] |\Psi_0(T)\rangle, \quad (245)
\end{aligned}$$

where, as before, square brackets denote the coupling of two angular momenta:

$$\begin{aligned}
[\mathcal{Q}_{\lambda_1\mu_1}^\dagger \mathcal{Q}_{\lambda_2\mu_2}^\dagger]_{JM} &= \sum_{\mu_1\mu_2} \langle \lambda_1\mu_1 \lambda_2\mu_2 | JM \rangle \mathcal{Q}_{\lambda_1\mu_1\mu_1}^\dagger \mathcal{Q}_{\lambda_2\mu_2\mu_2}^\dagger, \\
[\mathcal{Q}_{\lambda_1\mu_1}^\dagger \tilde{\mathcal{Q}}_{\lambda_2\mu_2}^\dagger]_{JM} &= \sum_{\mu_1\mu_2} \langle \lambda_1\mu_1 \lambda_2\mu_2 | JM \rangle \mathcal{Q}_{\lambda_1\mu_1\mu_1}^\dagger \tilde{\mathcal{Q}}_{\lambda_2\mu_2\mu_2}^\dagger
\end{aligned}$$

and so on. The wave function (245) must be normalized. Therefore, the one- and two-phonon amplitudes in expansion (245) satisfy the condition

$$\begin{aligned}
\langle \mathcal{Q}_{JM\nu} | \mathcal{Q}_{JM\nu} \rangle &= \sum_i \{ [R_i(J\nu)]^2 + [\tilde{R}_i(J\nu)]^2 \\
&\quad - [N_i(J\nu)]^2 - [\tilde{N}_i(J\nu)]^2 \} \\
&\quad + 2 \sum_{\substack{\lambda_1\mu_1 \\ \lambda_2\mu_2}} \{ [P_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 + [\tilde{P}_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 \\
&\quad + 2[S_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 - [T_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 - [\tilde{T}_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 \\
&\quad - 2[Z_{\lambda_2\mu_2}^{\lambda_1\mu_1}(J\nu)]^2 \} = 1. \quad (246)
\end{aligned}$$

As before, we will assume that nontilde state (245) corresponds to the positive energy $E_{J\nu}$. Then the tilde conjugate state corresponds to the negative energy $-E_{J\nu}$. The new thermal vacuum is defined as the vacuum with respect to the annihilation operators

$$\mathcal{Q}_{JM\nu} |\Psi_0(T)\rangle = \tilde{\mathcal{Q}}_{JM\nu} |\Psi_0(T)\rangle = 0. \quad (247)$$

We emphasize that the presence of thermal phonon annihilation operators in (245) indicates that the thermal vacuum is redefined when the coupling of one- and two-phonon configurations is considered. Recall that in the standard QPM, when the fragmentation of one-phonon states is considered, the wave function of the ground state is not redefined but remains identical to the QRPA phonon vacuum. A similar assumption was used in [35, 104, 107, 117] when considering the fragmentation of thermal one-phonon states. Also note that, in contrast to [104], the wave function (245) contains mixed components of the type $Q^\dagger \tilde{Q}^\dagger$. The

presence of these components leads to additional poles of spectral densities and strength functions³¹.

Let us obtain additional conditions on the structure of the operator $\mathcal{Q}_{JM\nu}^\dagger$, requiring that the new vacuum satisfy condition (142). To this end, as when considering the structure of the thermal vacuum TQRPA, we use as A the two-quasiparticle operators $[\alpha_{j_1}^\dagger \alpha_{j_2}^\dagger]_{JM}$, $[\alpha_{j_1}^\dagger \alpha_{j_2}]_{JM}$, and their Hermitian conjugates. Expressing the two-quasiparticle operators through thermal phonon operators, it is easy to show that the amplitudes at one-phonon terms in (245) must satisfy the condition

$$\begin{pmatrix} \tilde{N} \\ \tilde{R} \end{pmatrix}_i (J\nu) = \frac{X_{J_i} e^{-E_{J\nu}/2T} - Y_{J_i}}{X_{J_i} - Y_{J_i} e^{-E_{J\nu}/2T}} \begin{pmatrix} R \\ N \end{pmatrix}_i (J\nu), \quad (248)$$

where $E_{J\nu}$ is the eigenvalue of thermal Hamiltonian (240) corresponding to wave function (245). Thus, we have obtained an important result regarding the structure of wave function (245): if we require that the thermal state condition for the vacuum of the operators $\mathcal{Q}_{JM\nu}$ be satisfied, then wave function (245) must contain both direct one-phonon terms, i.e., terms consisting of the phonon creation operator, and inverse tilde-conjugate terms consisting of the phonon annihilation operator. In this connection, it is logical to include in wave function (245) the inverse two-phonon terms as well.

By analogy with TQRPA, in order to fix the correct structure of wave function (245), we determine the effective amplitudes

$$\begin{aligned}
\begin{pmatrix} \mathbb{R} \\ \mathbb{N} \end{pmatrix}_i (J\nu) &= [X_{J\nu} X_{J_i} - Y_{J\nu} Y_{J_i}]^{-1} \begin{pmatrix} R \\ N \end{pmatrix}_i (J\nu) \\
&= [Y_{J\nu} X_{J_i} - X_{J\nu} Y_{J_i}]^{-1} \begin{pmatrix} \tilde{N} \\ \tilde{R} \end{pmatrix}_i (J\nu), \quad (249)
\end{aligned}$$

where $X_{J\nu}^2 - Y_{J\nu}^2 = 1$ and $X_{J\nu}/Y_{J\nu} = e^{-E_{J\nu}/2T}$. Using the equality

$$\begin{aligned}
[R_i(J\nu)]^2 + [\tilde{R}_i(J\nu)]^2 - [N_i(J\nu)]^2 - [\tilde{N}_i(J\nu)]^2 \\
= [\mathbb{R}_i(J\nu)]^2 - [\mathbb{N}_i(J\nu)]^2 \quad (250)
\end{aligned}$$

normalization condition (246) can be written in terms of effective amplitudes.

³¹ In TQRPA (see Eq. (210)), the analogs of these mixed components in the structure of a thermal phonon are two thermal quasiparticle states of the form $\beta^\dagger \beta^\dagger$, which describe the scattering of thermally excited Bogolyubov quasiparticles. By analogy, terms of the form $Q^\dagger \tilde{Q}^\dagger$ correspond to the scattering of thermally excited q -phonons.

To find the eigenstates of thermal Hamiltonian (240) and their energies, we again use the equation of motion (139) in the form

$$\begin{aligned} & \langle \Psi_0(T) | [\delta O, \mathcal{H}, \mathcal{Q}_{JM\nu}^\dagger] | \Psi_0(T) \rangle \\ &= E_{J\nu} \langle \Psi_0(T) | [\delta O, \mathcal{Q}_{JM\nu}^\dagger] | \Psi_0(T) \rangle, \end{aligned} \quad (251)$$

where $|\Psi_0(T)\rangle$ is the TQRPA phonon vacuum, and the operators included in the definition of the right-hand side of (245) are considered as δO operators, i.e., $\delta O = Q_{JM}, Q_{JM}^\dagger, [Q_{\lambda_1 i_1}, Q_{\lambda_2 i_2}]_{JM}$, and so on. As a result, we arrive at a system of linear equations for one- and two-phonon amplitudes in expansion (245) [123]. The dimension of the resulting system of equations can be significantly reduced by excluding from it two-phonon amplitudes. Then, using (249), we obtain a system of linear homogeneous equations for effective amplitudes \mathbb{R}_i and \mathbb{N}_i [123]:

$$\begin{pmatrix} \mathbb{M}^{(1)}(E) & \mathbb{M}^{(2)}(E) \\ \mathbb{M}^{(2)}(-E) & \mathbb{M}^{(1)}(-E) \end{pmatrix} \begin{pmatrix} \mathbb{R} \\ \mathbb{N} \end{pmatrix} = 0. \quad (252)$$

The expressions for the matrix elements $\mathbb{M}_{ii'}^{(1,2)}$ is the following:

$$\begin{aligned} & \mathbb{M}_{ii'}^{(1)}(E) = \delta_{ii'}(\omega_{Ji} - E) \\ & - \frac{1}{2} \sum_{\lambda_1 i_1} \left\{ \left(\frac{\mathbb{U}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{U}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} - E} + \frac{\mathbb{V}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{V}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} + E} \right) \right. \\ & \times (1 + Y_{\lambda_1 i_1}^2 + Y_{\lambda_2 i_2}^2) + \left. \left(\frac{\mathbb{W}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{W}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} - \omega_{\lambda_2 i_2} - E} \right. \right. \\ & \left. \left. + \frac{\mathbb{G}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{G}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} - \omega_{\lambda_2 i_2} + E} \right) (Y_{\lambda_2 i_2}^2 - Y_{\lambda_1 i_1}^2) \right\}, \end{aligned} \quad (253)$$

$$\begin{aligned} & \mathbb{M}_{ii'}^{(2)}(E) \\ &= \frac{1}{2} \sum_{\lambda_1 i_1} \left\{ \left(\frac{\mathbb{U}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{V}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} - E} + \frac{\mathbb{V}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{U}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} + E} \right) \right. \\ & \times (1 + Y_{\lambda_1 i_1}^2 + Y_{\lambda_2 i_2}^2) + \left. \left(\frac{\mathbb{W}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{G}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} - \omega_{\lambda_2 i_2} - E} \right. \right. \\ & \left. \left. + \frac{\mathbb{G}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji) \mathbb{W}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji')}{\omega_{\lambda_1 i_1} - \omega_{\lambda_2 i_2} + E} \right) (Y_{\lambda_2 i_2}^2 - Y_{\lambda_1 i_1}^2) \right\}. \end{aligned} \quad (254)$$

The quantities $\mathbb{U}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji)$, $\mathbb{V}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji)$, $\mathbb{W}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji)$, and $\mathbb{G}_{\lambda_2 i_2}^{\lambda_1 i_1}(Ji)$ are related to the matrix elements of the operator \mathcal{H}_{qph} between the one- and two-phonon states and are expressed through the effective TQRPA amplitudes (220) and fermionic thermal occupation numbers [123]. We note the dependence of the matrix elements $\mathbb{M}_{ii'}^{(1,2)}$ not only on fermionic, but also on phonon thermal occupation numbers. In this sense,

the equations obtained have something in common with the results of [26], where the bosonic occupation numbers arise due to special properties of the temperature Green's functions.

The condition for existence of a nontrivial solution of system (252) leads to a secular equation $\det \mathbb{M} = 0$ for the eigenvalues $E_{J\nu}$ of thermal Hamiltonian (240). Solving system (252) for each positive eigenvalue $E_{J\nu}$, we find the unnormalized effective amplitudes $\mathbb{R}_i(J\nu)$ and $\mathbb{N}_i(J\nu)$. The normalization is carried out using conditions (246) and (250). Thus, we completely define the structure of the operator $\mathcal{Q}_{JM\nu}^\dagger$. The structure of the operator $\tilde{\mathcal{Q}}_{JM\nu}^\dagger$, corresponding to the negative eigenvalue $-E_{J\nu}$, is found using the tilde-conjugation operation, i.e., replacing nontilde phonons in expression (245) with tilde ones and vice versa.

After the structure of the eigenstates of thermal Hamiltonian (240) has been determined, we calculate the reduced transition probabilities for the one-particle multipole operator \mathcal{T}_{JM}

$$\begin{aligned} & \mathcal{B}_{J\nu}(\mathcal{T}_J) = \langle \mathcal{Q}_{J\nu} \mathcal{T}_J \Psi_0(T) \rangle^2 \\ &= X_{J\nu}^2 \left| \sum_i \Gamma_{Ji} [\mathbb{R}_i(J\nu) + \mathbb{N}_i(J\nu)] \right|^2, \\ & \tilde{\mathcal{B}}_{J\nu}(\mathcal{T}_J) = \langle \tilde{\mathcal{Q}}_{J\nu} \mathcal{T}_J \Psi_0(T) \rangle^2 \\ &= Y_{J\nu}^2 \left| \sum_i \Gamma_{Ji} [\mathbb{R}_i(J\nu) + \mathbb{N}_i(J\nu)] \right|^2. \end{aligned} \quad (255)$$

The expressions for the reduced probabilities obtained in our work [123] satisfy the detailed balance principle (134). Thus, by requiring for the thermal vacuum that the thermal state condition be satisfied at each stage of diagonalization of the thermal Hamiltonian, we succeeded in constructing a thermodynamically consistent method for describing the fragmentation of one-phonon states in hot nuclei. In [104, 117], the thermal state condition was satisfied only in the TQBCS approximation, but already at the TQRPA level, the detailed balance principle was violated, since the strength function did not have terms describing \downarrow -transitions. In subsequent papers [35, 107], the consistent construction of the thermal vacuum and thermal phonons ensured the satisfaction of the detailed balance principle in TQRPA. However, for considering the interaction of one- and two-phonon configurations, the TQRPA vacuum was used as the thermal vacuum, with the result that the detailed balance principle was satisfied only on average, i.e., after averaging the strength function over a certain energy interval.

Thus, using the example of the quasiparticle-phonon nuclear model, we have shown that a thermodynamically consistent consideration of the coupling between one- and two-phonon configurations in a hot

nucleus requires a consistent redefinition of the thermal vacuum. According to the equations obtained, the matrix elements of the interaction of phonons of a hot nucleus depend on both quasiparticle (fermionic) and phonon (bosonic) thermal occupation numbers. The procedure presented here can be easily generalized to the case of spin–isospin excitations of a hot nucleus (magnetic dipole, Gamow–Teller, etc.), which is important from the viewpoint of astrophysical applications.

11. CHARGE-EXCHANGE PHONONS IN HOT NUCLEI

Let us apply the TQRPA method to finding the eigenstates of the charge-exchange part of the thermal Hamiltonian. To this end, we approximately diagonalize

$$\mathcal{H} = \mathcal{H}_{\text{BCS}} + \mathcal{H}_{\text{ch.ex}} \quad (256)$$

in terms of phonon operators. For cold nuclei, charge-exchange phonons were considered in [97, 128–130]. In the approximation of independent thermal quasiparticles, the charge-exchange modes of thermal Hamiltonian \mathcal{H}_{BCS} (191) are described as proton–neutron pairs of thermal quasiparticles. The interaction between elementary excitation modes arises due to the charge-exchange part of thermal Hamiltonian (163). The multipole $\mathcal{M}_{JM}^{(k)\dagger}$ and spin–multipole $S_{LJM}^{(k)\dagger}$ operators (157) included in the definition of the residual interaction $H_{\text{ch.ex}}$, being written in terms of thermal quasiparticles, have the same form as the single-particle transition operator (193)³².

Let us perform a linear transformation from the operators of creation and annihilation of proton–neutron two thermal quasiparticle states to the operators of creation and annihilation of charge-exchange thermal phonons:

$$\begin{aligned} \Omega_{JM}^\dagger = & \sum_{j_p j_n} (\psi_{j_p j_n}^{Ji} [\beta_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM} + \tilde{\psi}_{j_p j_n}^{Ji} [\tilde{\beta}_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM} \\ & + i\tilde{\eta}_{j_p j_n}^{Ji} [\beta_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM} + i\tilde{\eta}_{j_p j_n}^{Ji} [\tilde{\beta}_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM} \\ & - \phi_{j_p j_n}^{Ji} [\beta_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM}^\dagger - \tilde{\phi}_{j_p j_n}^{Ji} [\tilde{\beta}_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM}^\dagger \\ & + i\xi_{j_p j_n}^{Ji} [\beta_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM}^\dagger + i\xi_{j_p j_n}^{Ji} [\tilde{\beta}_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM}^\dagger). \end{aligned} \quad (257)$$

As in the case of charge-neutral phonons, the operators $\tilde{\Omega}_{JM}^\dagger$, Ω_{JM}^\dagger , and $\tilde{\Omega}_{JM}^\dagger$ are obtained from (257) by applying the operation of Hermitian- and tilde-conjugation. The multipole and spin–multipole with $L = J$

components of the residual interaction $\mathcal{H}_{\text{ch.ex}}$ generate charge-exchange phonons of normal parity ($\pi = (-1)^J$), while the spin–multipole interaction with $L = J \pm 1$ generates phonons of anomalous parity ($\pi = (-1)^{J+1}$).

Requiring the fulfillment of bosonic commutation rules for thermal charge-exchange phonons and assuming that the quasi-boson approximation for the creation and annihilation operators of proton-neutron pairs of thermal quasiparticles is valid, we obtain orthonormalization relations for phonon amplitudes ψ, ϕ , etc., which are included in the definition of a thermal phonon (see Eqs. (336)–(339)) in Appendix C). Using these relations, it is easy to show that the transformations inverse to (257) have the form:

$$\begin{aligned} [\beta_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM} = & \sum_i (\psi_{j_p j_n}^{Ji} \Omega_{JM}^\dagger + \phi_{j_p j_n}^{Ji} \Omega_{JM}^\dagger \\ & + \tilde{\psi}_{j_p j_n}^{Ji} \tilde{\Omega}_{JM}^\dagger + \tilde{\phi}_{j_p j_n}^{Ji} \tilde{\Omega}_{JM}^\dagger), \end{aligned} \quad (258)$$

$$[\beta_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM} = \widetilde{[\beta_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM}}, \quad (259)$$

$$\begin{aligned} [\beta_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM} = & -i \sum_i (\eta_{j_p j_n}^{Ji} \Omega_{JM}^\dagger + \xi_{j_p j_n}^{Ji} \Omega_{JM}^\dagger \\ & + \tilde{\eta}_{j_p j_n}^{Ji} \tilde{\Omega}_{JM}^\dagger + \tilde{\xi}_{j_p j_n}^{Ji} \tilde{\Omega}_{JM}^\dagger), \end{aligned} \quad (260)$$

$$[\tilde{\beta}_{j_p}^\dagger \beta_{j_n}^\dagger]_{JM} = -\widetilde{[\beta_{j_p}^\dagger \tilde{\beta}_{j_n}^\dagger]_{JM}}. \quad (261)$$

We further require that thermal Hamiltonian (256) be diagonal in terms of the phonon operators

$$\mathcal{H} \approx \sum_{JM} \omega_{JM} (\Omega_{JM}^\dagger \Omega_{JM} - \tilde{\Omega}_{JM}^\dagger \tilde{\Omega}_{JM}), \quad (262)$$

and the phonon vacuum was the thermal vacuum in the TQRPA. To this end, the phonon operators must satisfy equation of motion (143), and the phonon vacuum must satisfy the thermal state condition (142). As an operator A in condition (142), we consider the proton–neutron two quasiparticle operators

$$[\alpha_{j_p}^\dagger \alpha_{j_n}^\dagger]_{JM}, [\alpha_{j_p}^- \alpha_{j_n}^-]_{JM}, [\alpha_{j_p}^\dagger \alpha_{j_n}^-]_{JM}, [\alpha_{j_p}^- \alpha_{j_n}^\dagger]_{JM}. \quad (263)$$

Expressing these operators first in terms of the operators of creation and annihilation of thermal quasiparticles, and then through charge-exchange thermal phonons, we arrive at relations between nontilde and tilde amplitudes similar to those considered in the charge-neutral case ((218), (219)). Let us introduce the effective amplitudes

³²To obtain expressions for $\mathcal{M}_{JM}^{(k)\dagger}$ and $S_{LJM}^{(k)\dagger}$ from (193), it suffices to make the substitutions: $j_{1,2} \rightarrow j_{p,n}$ and $t_{j_1 j_2}^{(J)} \rightarrow f_{j_p j_n}^{(J;k)}, f_{j_p j_n}^{(LJ;k)}$.

$$\begin{aligned}
\Psi_{j_p j_n}^{J_i} &= \frac{\Psi_{j_p j_n}^{J_i}}{X_{J_i} x_{j_p} x_{j_n} - Y_{J_i} y_{j_p} y_{j_n}} \\
&= \frac{\tilde{\Phi}_{j_p j_n}^{J_i}}{Y_{J_i} x_{j_p} x_{j_n} - X_{J_i} y_{j_p} y_{j_n}}, \\
\Phi_{j_p j_n}^{J_i} &= \frac{\Phi_{j_p j_n}^{J_i}}{X_{J_i} x_{j_p} x_{j_n} - Y_{J_i} y_{j_p} y_{j_n}} \\
&= \frac{\tilde{\Psi}_{j_p j_n}^{J_i}}{Y_{J_i} x_{j_p} x_{j_n} - X_{J_i} y_{j_p} y_{j_n}}, \\
H_{j_p j_n}^{J_i} &= \frac{\eta_{j_p j_n}^{J_i}}{X_{J_i} x_{j_p} y_{j_n} - Y_{J_i} y_{j_p} x_{j_n}} \\
&= \frac{\xi_{j_p j_n}^{J_i}}{Y_{J_i} x_{j_p} y_{j_n} - X_{J_i} y_{j_p} x_{j_n}}, \\
\Xi_{j_p j_n}^{J_i} &= \frac{\xi_{j_p j_n}^{J_i}}{X_{J_i} x_{j_p} y_{j_n} - Y_{J_i} y_{j_p} x_{j_n}} \\
&= \frac{\tilde{\eta}_{j_p j_n}^{J_i}}{Y_{J_i} x_{j_p} y_{j_n} - X_{J_i} y_{j_p} x_{j_n}}.
\end{aligned} \tag{264}$$

For them, the orthonormalization condition takes the form

$$\begin{aligned}
&\sum_{j_p j_n} \{ (\Psi_{j_p j_n}^{J_i} \Psi_{j_p j_n}^{J_i'} - \Phi_{j_p j_n}^{J_i} \Phi_{j_p j_n}^{J_i'}) \\
&\times (1 - y_{j_p}^2 - y_{j_n}^2) + (H_{j_p j_n}^{J_i} H_{j_p j_n}^{J_i'} \\
&- \Xi_{j_p j_n}^{J_i} \Xi_{j_p j_n}^{J_i'}) (y_{j_n}^2 - y_{j_p}^2) \} = \delta_{ii'}.
\end{aligned} \tag{265}$$

As in the case of charge-neutral phonons, the requirement to satisfy the thermal state condition for the vacuum of charge-exchange phonons leads to the fact that phonon amplitudes depend on both fermionic and bosonic thermal occupation numbers.

Equation of motion (143) leads to the following system of homogeneous linear equations for effective amplitudes [131]:

$$\begin{aligned}
&\varepsilon_{j_p j_n}^{(+)} G_{j_p j_n}^{J_i} - 2\hat{J}^{-2} u_{j_p j_n}^{(+)} \\
&\times \sum_{k=1}^{2N} d_{j_p j_n}^{(J;k)} \chi_1^{(k)} \mathcal{D}_{J_i}^{(+;k)} = \omega_{J_i} W_{j_p j_n}^{J_i}, \\
&\varepsilon_{j_p j_n}^{(+)} W_{j_p j_n}^{J_i} - 2\hat{J}^{-2} u_{j_p j_n}^{(-)} \\
&\times \sum_{k=1}^{2N} d_{j_p j_n}^{(J;k)} \chi_1^{(k)} \mathcal{D}_{J_i}^{(-;k)} = \omega_{J_i} G_{j_p j_n}^{J_i}, \\
&\varepsilon_{j_p j_n}^{(-)} T_{j_p j_n}^{J_i} - 2\hat{J}^{-2} v_{j_p j_n}^{(-)} \\
&\times \sum_{k=1}^{2N} d_{j_p j_n}^{(J;k)} \chi_1^{(k)} \mathcal{D}_{J_i}^{(+;k)} = \omega_{J_i} S_{j_p j_n}^{J_i}, \\
&\varepsilon_{j_p j_n}^{(-)} S_{j_p j_n}^{J_i} - 2\hat{J}^{-2} v_{j_p j_n}^{(+)} \\
&\times \sum_{k=1}^{2N} d_{j_p j_n}^{(J;k)} \chi_1^{(k)} \mathcal{D}_{J_i}^{(-;k)} = \omega_{J_i} T_{j_p j_n}^{J_i}.
\end{aligned} \tag{266}$$

The resulting system of TQRPA equations applies to both parity types (normal and anomalous) of charge-exchange phonons. For the sake of brevity, the following notation is used:

$$\begin{aligned}
\chi_1^{(k)} &= \chi_1^{(m;k)}, \quad d_{j_p j_n}^{(J;k)} = f_{j_p j_n}^{(J;k)}, \\
\mathcal{D}_{J_i}^{(\pm;k)} &= D_{J_i}^{(\pm;k)} \quad (1 \leq k \leq N), \\
\chi_1^{(k)} &= \chi_1^{(s;k-N)}, \quad d_{j_p j_n}^{(J;k)} = f_{j_p j_n}^{(JJ;k-N)}, \\
\mathcal{D}_{J_i}^{(\pm;k)} &= D_{J_i}^{(\pm;k-N)} \quad (N+1 \leq k \leq 2N)
\end{aligned}$$

for phonons of normal parity, and

$$\begin{aligned}
\chi_1^{(k)} &= \chi_1^{(s;k)}, \quad d_{j_p j_n}^{(J;k)} = f_{j_p j_n}^{(J-1J;k)}, \\
\mathcal{D}_{J_i}^{(\pm;k)} &= D_{J-1J_i}^{(\pm;k)} \quad (1 \leq k \leq N), \\
\chi_1^{(k)} &= \chi_1^{(s;k-N)}, \quad d_{j_p j_n}^{(J;k)} = f_{j_p j_n}^{(J+1J;k-N)}, \\
\mathcal{D}_{J_i}^{(\pm;k)} &= D_{J+1J_i}^{(\pm;k-N)} \quad (N+1 \leq k \leq 2N)
\end{aligned}$$

for anomalous parity phonons. In addition, the following linear combinations of effective amplitudes are defined:

$$\begin{aligned}
D_{J_i}^{(+;k)} &= \sum_{j_p j_n} f_{j_p j_n}^{(J;k)} \{ u_{j_p j_n}^{(+)} (1 - y_{j_p}^2 - y_{j_n}^2) \\
&\times G_{j_p j_n}^{J_i} + v_{j_p j_n}^{(-)} (y_{j_n}^2 - y_{j_p}^2) T_{j_p j_n}^{J_i} \}, \\
D_{J_i}^{(-;k)} &= \sum_{j_p j_n} f_{j_p j_n}^{(J;k)} \{ u_{j_p j_n}^{(-)} (1 - y_{j_p}^2 - y_{j_n}^2) \\
&\times W_{j_p j_n}^{J_i} + v_{j_p j_n}^{(+)} (y_{j_n}^2 - y_{j_p}^2) S_{j_p j_n}^{J_i} \},
\end{aligned} \tag{267}$$

where

$$\begin{aligned}
G_{j_p j_n}^{J_i} &= \Psi_{j_p j_n}^{J_i} + \Phi_{j_p j_n}^{J_i}, \\
W_{j_p j_n}^{J_i} &= \Psi_{j_p j_n}^{J_i} - \Phi_{j_p j_n}^{J_i}, \\
T_{j_p j_n}^{J_i} &= H_{j_p j_n}^{J_i} + \Xi_{j_p j_n}^{J_i}, \\
S_{j_p j_n}^{J_i} &= H_{j_p j_n}^{J_i} - \Xi_{j_p j_n}^{J_i}.
\end{aligned} \tag{268}$$

The expressions for $D_{LJ_i}^{(\pm;k)}$ have exactly the same form up to replacement $f_{j_p j_n}^{(J;k)}$ by $f_{j_p j_n}^{(LJ;k)}$.

The dimension of the system of TQRPA equations (266) for charge-exchange thermal phonons is twice the number of basic proton-neutron two thermal quasiparticle states. The separable form of the residual interaction makes it possible to reduce this system to a system of $4N$ linear homogeneous equations for the functions $D_{J_i}^{(\pm;k)}$, $D_{LJ_i}^{(\pm;k)}$, (see Eqs. (342) in Appendix C). The condition for the existence of a nontrivial solution to this system leads to secular equation (345) for the energy ω_{J_i} of thermal phonons.

Finding for each ω_{J_i} the functions $D_{J_i}^{(\pm;k)}$, $D_{LJ_i}^{(\pm;k)}$ (with arbitrary normalization) and substituting them into (266), we determine the unnormalized sums $G_{j_p j_n}^{J_i}$, $T_{j_p j_n}^{J_i}$ and differences $W_{j_p j_n}^{J_i}$, $S_{j_p j_n}^{J_i}$ of effective ampli-

tudes. The effective amplitudes are then normalized using condition (265).

Let us obtain expressions for the amplitudes and probabilities of charge-exchange transitions from thermal vacuum to the one-phonon state. To express the multipole operator $\mathcal{T}_{JM}^{(-)}$ of $n \rightarrow p$ transition through thermal phonons, in expression (228) it suffices to replace the operators of charge-neutral phonons with the operators of charge-exchange phonons, and to carry out the summation over proton–neutron states. As a result, the amplitudes of $n \rightarrow p$ transitions take the form

$$\begin{aligned} \langle \Omega_{Ji} \| \mathcal{T}_{JM}^{(-)} \| 0(T) \rangle &= X_{Ji} [\Gamma_{Ji}^{(+)}(\mathcal{T}_{JM}^{(-)}) + \Gamma_{Ji}^{(-)}(\mathcal{T}_{JM}^{(-)})], \\ \langle \tilde{\Omega}_{Ji} \| \mathcal{T}_{JM}^{(-)} \| 0(T) \rangle &= Y_{Ji} [\Gamma_{Ji}^{(+)}(\mathcal{T}_{JM}^{(-)}) - \Gamma_{Ji}^{(-)}(\mathcal{T}_{JM}^{(-)})], \end{aligned} \quad (269)$$

where

$$\begin{aligned} \Gamma_i^{(+)}(\mathcal{T}_{JM}^{(-)}) &= \frac{1}{2} \sum_{j_p j_n} t_{j_p j_n}^{(J)} \{ (1 - y_{j_p}^2 - y_{j_n}^2) \\ &\quad \times u_{j_p j_n}^{(+)} G_{j_p j_n}^{Ji} + (y_{j_n}^2 - y_{j_p}^2) v_{j_p j_n}^{(-)} T_{j_p j_n}^{Ji} \}, \\ \Gamma_i^{(-)}(\mathcal{T}_{JM}^{(-)}) &= \frac{1}{2} \sum_{j_p j_n} t_{j_p j_n}^{(J)} \{ (1 - y_{j_p}^2 - y_{j_n}^2) \\ &\quad \times u_{j_p j_n}^{(-)} W_{j_p j_n}^{Ji} + (y_{j_n}^2 - y_{j_p}^2) v_{j_p j_n}^{(+)} S_{j_p j_n}^{Ji} \}. \end{aligned} \quad (270)$$

For the $p \rightarrow n$ transition operator $\mathcal{T}_{JM}^{(+)}$, we use the fact that

$$\begin{aligned} \mathcal{T}_{JM}^{(+)} &= -\hat{J}^{-1} \sum_{j_p j_n} t_{j_p j_n}^{(J)} [a_{j_n}^{\dagger} a_{j_p}^{-}]_{JM} \\ &= -\hat{J}^{-1} \sum_{j_p j_n} \bar{t}_{j_p j_n}^{(J)} [a_{j_p}^{\dagger} a_{j_n}^{-}]_{JM}^{\dagger}, \end{aligned} \quad (271)$$

where $\bar{t}_{j_p j_n}^{(J)} = (-1)^{j_n - j_p + J} t_{j_p j_n}^{(J)}$. Therefore, the amplitudes of $p \rightarrow n$ transitions are

$$\begin{aligned} \langle \Omega_{Ji} \| \mathcal{T}_{JM}^{(+)} \| 0(T) \rangle &= X_{Ji} [\bar{\Gamma}_i^{(+)}(\mathcal{T}_{JM}^{(+)}) - \bar{\Gamma}_i^{(-)}(\mathcal{T}_{JM}^{(+)})], \\ \langle \tilde{\Omega}_{Ji} \| \mathcal{T}_{JM}^{(+)} \| 0(T) \rangle &= Y_{Ji} [\bar{\Gamma}_i^{(+)}(\mathcal{T}_{JM}^{(+)}) + \bar{\Gamma}_i^{(-)}(\mathcal{T}_{JM}^{(+)})]. \end{aligned} \quad (272)$$

The functions $\bar{\Gamma}_i^{(\pm)}(\mathcal{T}_{JM}^{(+)})$ are obtained from (270) by replacing the reduced matrix element $t_{j_p j_n}^{(J)}$ with $\bar{t}_{j_p j_n}^{(J)}$. The squares of the modulus of the right-hand side of (269) and (272) are equal to the reduced probability (strength) of charge-exchange transitions:

$$\begin{aligned} B_{Ji}(\mathcal{T}_{JM}^{(-)}) &= X_{Ji}^2 |\Gamma_i^{(+)}(\mathcal{T}_{JM}^{(-)}) + \Gamma_i^{(-)}(\mathcal{T}_{JM}^{(-)})|^2, \\ \tilde{B}_{Ji}(\mathcal{T}_{JM}^{(-)}) &= Y_{Ji}^2 |\Gamma_i^{(+)}(\mathcal{T}_{JM}^{(-)}) - \Gamma_i^{(-)}(\mathcal{T}_{JM}^{(-)})|^2, \end{aligned} \quad (273)$$

and

$$\begin{aligned} B_{Ji}(\mathcal{T}_{JM}^{(+)}) &= X_{Ji}^2 |\bar{\Gamma}_i^{(+)}(\mathcal{T}_{JM}^{(+)}) - \bar{\Gamma}_i^{(-)}(\mathcal{T}_{JM}^{(+)})|^2, \\ \tilde{B}_{Ji}(\mathcal{T}_{JM}^{(+)}) &= Y_{Ji}^2 |\bar{\Gamma}_i^{(+)}(\mathcal{T}_{JM}^{(+)}) + \bar{\Gamma}_i^{(-)}(\mathcal{T}_{JM}^{(+)})|^2. \end{aligned} \quad (274)$$

If the multipole charge-exchange operators $\mathcal{T}_{JM}^{(\pm)}$ are such that $(\mathcal{T}_{JM}^{(+)})^{\dagger} = \pm \mathcal{T}_{JM}^{(-)}$, then the reduced prob-

abilities of the $n \rightarrow p$ and $p \rightarrow n$ transitions to tilde-conjugate states are related by the principle of detailed balance

$$\tilde{B}_{Ji}(\mathcal{T}_{JM}^{(\pm)}) = e^{-\omega_{Ji}/T} B_{Ji}(\mathcal{T}_{JM}^{(\mp)}). \quad (275)$$

This relation, in particular, is valid for the Fermi and Gamow–Teller transitions.

The above expressions for the amplitude and strength of transitions to one-phonon states together with the transition energy determine the charge-exchange spectral densities (128) and strength functions (131) in TQRPA. Once again, we note that the energy of the charge-exchange transition is not equal to the energy of the phonon—they are related as follows:

$$E_{Ji}^{(\pm)} = \omega_{Ji} \pm \Delta_{np}, \quad \tilde{E}_{Ji}^{(\pm)} = -E_{Ji}^{(\mp)}. \quad (276)$$

Here $E_{Ji}^{(\pm)}$ ($\tilde{E}_{Ji}^{(\pm)}$) is the transition energy to a non-tilde (tilde) one-phonon state. Due to the fact that the vacuum of charge-exchange phonons satisfies thermal state condition (142), principle of detailed balance (120) is valid for spectral densities and strength functions.

Let us show that a total strength of the Fermi and Gamow–Teller transitions calculated in TQRPA satisfies Ikeda sum rule (203). In the case of Gamow–Teller ($J^{\pi} = 1^{+}$) transitions, we have

$$\begin{aligned} S_{-} - S_{+} &= \sum_i [B_i(GT_{-}) + \tilde{B}_i(GT_{-})] \\ &\quad - \sum_i [B_i(GT_{+}) + \tilde{B}_i(GT_{+})] \\ &= \sum_i [B_i(GT_{-}) - B_i(GT_{+})] (1 - e^{-\omega_i/T}) \\ &= \sum_i \left[|\Gamma_i^{(+)}(GT_{-}) + \Gamma_i^{(-)}(GT_{-})|^2 \right. \\ &\quad \left. - |\Gamma_i^{(+)}(GT_{+}) + \Gamma_i^{(-)}(GT_{+})|^2 \right] \\ &= \sum_i \sum_{j_p j_n} t_{j_p j_n} [(1 - y_{j_p}^2 - y_{j_n}^2) u_{j_p j_n}^{(-)} W_{j_p j_n}^{ji} \\ &\quad - (y_{j_p}^2 - y_{j_n}^2) v_{j_p j_n}^{(+)} S_{j_p j_n}^{ji}] \\ &\quad \times \sum_{j_p' j_n'} \bar{t}_{j_p' j_n'} [(1 - y_{j_p'}^2 - y_{j_n'}^2) u_{j_p' j_n'}^{(+)} G_{j_p' j_n'}^{ji} \\ &\quad - (y_{j_p'}^2 - y_{j_n'}^2) v_{j_p' j_n'}^{(-)} T_{j_p' j_n'}^{ji}] \\ &= \sum_{j_p j_n} |t_{j_p j_n}|^2 [(1 - y_{j_p}^2 - y_{j_n}^2) u_{j_p j_n}^{(+)} u_{j_p j_n}^{(-)} \\ &\quad + (y_{j_n}^2 - y_{j_p}^2) v_{j_p j_n}^{(+)} v_{j_p j_n}^{(-)}]. \end{aligned} \quad (277)$$

In the last equality, we used the fact that the effective amplitudes satisfy completeness condition (341). Since the last line is nothing else than expression (204) for $S_{-} - S_{+}$ in the independent thermal quasiparticle approximation, then we have thus proved the fulfillment of the Ikeda sum rule in TQRPA. The validity of the sum rule for the Fermi operator is proved similarly.

In the conclusion to this section, we note that in our papers [132–134] the TQRPA equations for charge-exchange one-phonon excitations were obtained for the QPM Hamiltonian. The formally similar equations for a separable residual interaction were obtained in [135–137] in the context of thermal RPA. However, these works did not consider the processes of deexcitation of the hot nucleus, and, as a result, the principle of detailed balance was violated.

12. CROSS SECTIONS OF WEAK REACTIONS WITH HOT NUCLEI

Further, we will apply the developed statistical approach to the calculation of spectral densities and strength functions to describe weak reactions of leptons with hot nuclei under astrophysical conditions. The standard way to describe semileptonic nuclear processes is the Donnelly–Walecka method [138, 139], which is based on the analogy with the scattering of electrons by nuclei. The use of the current–current form of the weak interaction Hamiltonian \hat{H}_W makes it possible to obtain a general expression for the matrix elements $\langle f | \hat{H}_W | i \rangle$ between the initial and final states for all semileptonic processes, while the multipole expansion of the nucleon current makes it possible to formulate selection rules for the parity and total momentum of a nucleus. The Donnelly–Walecka method is widely used in calculating cross sections for neutrino–nuclear processes (see, e.g., [140–145]), as well as in studying the rates of muon capture [146].

Let us present the basic information about the calculation of cross sections for semileptonic processes involving atomic nuclei in the context of the Donnelly–Walecka approach. A more detailed discussion and details of the derivation of cross section are given in books [139, 147] and papers [138, 148]. For generality, we will consider the following reaction

$$l + {}^Z_N A \rightarrow {}^{Z'}_{N'} A + l'. \quad (278)$$

Here, l is the lepton incident on the parent nucleus ${}^Z_N A$, l' is the scattered lepton, while ${}^{Z'}_{N'} A$ is the daughter nucleus. In charge-neutral reactions of the inelastic scattering of neutrino ($l = l' = \nu$) and antineutrino ($l = l' = \bar{\nu}$), the number of nucleons of each type in the nucleus does not change, i.e., $Z' = Z$ and $N' = N$. The change in the number of nucleons in the nucleus occurs in charge-exchange reactions: $Z' = Z - 1$ and $N' = N + 1$ in the reactions of capture of an electron ($l = e^-, l' = \nu_e$) and an antineutrino ($l = \bar{\nu}_e, l' = e^+$); $Z' = Z + 1$ and $N' = N - 1$ when capturing a neutrino ($l = \nu_e, l' = e^-$) or a positron ($l = e^+, l' = \bar{\nu}_e$). We will assume that the states of the

incident and scattered leptons are described by a plane wave³³. Let us denote the energy and momentum of the incident (scattered) lepton as $\varepsilon_l, \mathbf{p}_l$ ($\varepsilon_{l'}, \mathbf{p}_{l'}$). Then $\mathbf{q} = \mathbf{p}_{l'} - \mathbf{p}_l$ is the three-momentum transferred to the lepton in the scattering at the angle θ , while $\omega = \varepsilon_l - \varepsilon_{l'}$ is the energy transferred to the nucleus.

The Donnelly–Walecka method assumes that the states of the parent $|J_i \pi_i\rangle$ and daughter $|J_f \pi_f\rangle$ nuclei are characterized by certain values of the total momentum and parity. Using the multipole expansion of the matrix elements of the lepton weak current, the differential cross section for reaction (278) can be represented in the following form:³⁴

$$\frac{d\sigma_{if}(\varepsilon_l)}{d \cos \theta} = \frac{2(G_F')^2}{\hbar^4 c^4} S_l \left(\frac{\varepsilon_l}{p_l} \right) \times p_{l'} \varepsilon_{l'} \left\{ \sum_{J \geq 0} \eta_J^{CL}(if) + \sum_{J \geq 1} \eta_J^T(if) \right\}, \quad (280)$$

where the summation over J is constrained by the momentum selection rules $|J_i - J_f| \leq J \leq J_i + J_f$. For convenience, a general notation for the weak interaction constant is introduced

$$G_F' = \begin{cases} G_F V_{ud} & \text{for charged currents,} \\ G_F & \text{for neutral currents,} \end{cases} \quad (281)$$

where $G_F/(\hbar c)^3 \approx 1.166 \times 10^{-5} \text{ GeV}^{-2}$ [150] is the Fermi constant of weak interaction, while $V_{ud} = 0.9740$ [150] is the Cabibbo–Kobayashi–Maskawa matrix element, which is associated with the mixing of two components of the charged nucleon current: the one that preserves strangeness and another that does not preserve it. The factor $S_l = \frac{1}{2}(S_l = 1)$ for $l = e^\pm$ ($l = \nu, \bar{\nu}$) in (280) considers the need for averaging the electron or positron spin over the initial states.

The functions $\eta_J^{CL,T}$ are expressed in terms of the reduced matrix elements of the nucleon current multipole operators:

³³To consider a distortion of the wave function of a charged lepton in the Coulomb field of the nucleus, see below.

³⁴As shown in [149], the nuclear recoil can be neglected provided that the energy of incident lepton and the energy of nucleus excitation are much less than the nuclear mass M_A . If this condition is omitted, then the largest correction will be a coefficient for the density of final states (recoil factor)

$$f_R = \left[1 + \frac{\varepsilon_l p_{l'} - \varepsilon_{l'} p_l \cos \theta}{p_{l'} M_A c^2} \right]^{-1} \approx \left[1 + \frac{2\varepsilon_l \sin^2(\theta/2)}{M_A c^2} \right]^{-1}, \quad (279)$$

by which the right-hand side of (280) is multiplied.

Table 1. Expressions for kinematic factors used in the definition of functions $\eta_J^{CL,T}$. In the second column, using the designations in [139, Table 2] (see also [147, Table 46.2]), the combinations of matrix elements of the lepton current are indicated. The explanation of notations a, b, c is given in the text (see expressions (283)); $S = -1(+1)$, if a neutrino (antineutrino) is involved in the reaction; $q_\mu^2 = q^2 - \omega^2$ is the transferred four-momentum squared

		Charge-exchange reactions	Charge-neutral reactions
v_{TT}	$\frac{1}{2}(\mathbf{1} \cdot \mathbf{I}^* - l_3 l_3^*)$	$1 - a \cos \theta + b \sin^2 \theta$	$\frac{q_\mu^2}{q^2} \cos^2 \left(\frac{\theta}{2}\right) + 2 \sin^2 \left(\frac{\theta}{2}\right)$
v_{TT^*}	$-\frac{i}{2}(\mathbf{1} \times \mathbf{I}^*)_3$	$S \left[\frac{\varepsilon_l + \varepsilon_l'}{q\hbar c} (1 - a \cos \theta) - c \right]$	$2S \sin \left(\frac{\theta}{2}\right) \left[1 - \frac{\omega^2}{q^2} \cos^2 \left(\frac{\theta}{2}\right) \right]^{1/2}$
v_{CC}	$l_0 l_0^*$	$1 + a \cos \theta$	$2 \cos^2 \left(\frac{\theta}{2}\right)$
v_{LL}	$l_3 l_3^*$	$1 + a \cos \theta - 2b \sin^2 \theta$	$\frac{\omega^2}{q^2} \times 2 \cos^2 \left(\frac{\theta}{2}\right)$
v_{CL}	$-l_3 l_0^*$	$\frac{\omega}{q} (1 + \cos \theta) + c$	$\frac{\omega}{q} \times 2 \cos^2 \left(\frac{\theta}{2}\right)$

$$\begin{aligned} \eta_J^{CL}(if) &= \frac{1}{2J_i + 1} \left\{ v_{LL} \left| \langle J_f \parallel \hat{\mathcal{L}}_J \parallel J_i \rangle \right|^2 \right. \\ &\quad + v_{CC} \left| \langle J_f \parallel \hat{\mathcal{M}}_J \parallel J_i \rangle \right|^2 \\ &\quad \left. + v_{CL} 2 \operatorname{Re} \left(\langle J_f \parallel \hat{\mathcal{L}}_J \parallel J_i \rangle \langle J_f \parallel \hat{\mathcal{M}}_J \parallel J_i \rangle^* \right) \right\}, \end{aligned} \quad (282a)$$

$$\begin{aligned} \eta_J^T(if) &= \frac{1}{2J_i + 1} \left\{ v_{TT} \left(\left| \langle J_f \parallel \hat{\mathcal{T}}_J^{\text{mag}} \parallel J_i \rangle \right|^2 \right. \right. \\ &\quad \left. \left. + \left| \langle J_f \parallel \hat{\mathcal{T}}_J^{\text{el}} \parallel J_i \rangle \right|^2 \right) \right. \\ &\quad \left. + v_{TT^*} 2 \operatorname{Re} \left(\langle J_f \parallel \hat{\mathcal{T}}_J^{\text{mag}} \parallel J_i \rangle \langle J_f \parallel \hat{\mathcal{T}}_J^{\text{el}} \parallel J_i \rangle^* \right) \right\}. \end{aligned} \quad (282b)$$

The charge multipole operator $\hat{\mathcal{M}}_{JM}$ is related to the distribution of the zero component of the weak nucleon current in the nucleus, while the longitudinal $\hat{\mathcal{L}}_{JM}$, transverse electric $\hat{\mathcal{T}}_{JM}^{\text{el}}$ and transverse magnetic $\hat{\mathcal{T}}_{JM}^{\text{mag}}$ multipole operators are related to the distribution of its spatial component [147, Eqs. 45.13]. Kinematic factors v_{LL} , v_{CC} , etc. are the result of averaging the various combinations of matrix elements of the lepton current over lepton polarizations. Their values are given in Table 1 in a form convenient for numerical calculations. To this end, the following notations are used for charge-exchange reactions

$$\begin{aligned} a &\equiv \frac{p_e c}{\varepsilon_e} = \sqrt{1 - \left(\frac{m_e c^2}{\varepsilon_e} \right)^2}, \\ b &\equiv \frac{\varepsilon_e \varepsilon_v a^2}{(q\hbar c)^2}, \quad c \equiv \frac{(m_e c^2)^2}{\varepsilon_e (q\hbar c)}, \end{aligned} \quad (283)$$

where q is the value of the transferred three-momentum

$$\begin{aligned} q\hbar c &= \sqrt{E_{if}^2 + 2\varepsilon_e \varepsilon_v (1 - a \cos \theta) - (m_e c^2)^2} \\ &= \sqrt{(\varepsilon_v - p_e c)^2 + 4\varepsilon_v p_e c \sin^2 \frac{\theta}{2}}, \end{aligned} \quad (284)$$

while $E_{if} = \omega$ corresponds to the transition energy from the initial nuclear state i to final state f . If we neglect the electron mass ($\varepsilon_e \gg m_e c^2$), then $a = 1, c = 0$, and the charge-exchange kinematic factors coincide with the charge-neutral ones. In this case

$$q\hbar c = \sqrt{E_{if}^2 + 4\varepsilon_v \varepsilon_v \sin^2 \frac{\theta}{2}}. \quad (285)$$

Note that the interference term between the electric and magnetic components of the function η_J^T has a different sign for reactions involving neutrinos and antineutrinos.

Since the nucleon weak current includes the vector and axial-vector parts, then each multipole operator in (282) consists of two components of opposite parity: $\hat{\mathcal{M}}_{JM} = \hat{M}_{JM} + \hat{M}_{JM}^5$, $\hat{\mathcal{L}}_{JM} = \hat{L}_{JM} + \hat{L}_{JM}^5$, $\hat{\mathcal{T}}_{JM}^{\text{el}} = \hat{T}_{JM}^{\text{el}} + \hat{T}_{JM}^{\text{el}5}$, and $\hat{\mathcal{T}}_{JM}^{\text{mag}} = \hat{T}_{JM}^{\text{mag}} + \hat{T}_{JM}^{\text{mag}5}$. The operators \hat{M}_{JM} , \hat{L}_{JM} , \hat{T}_{JM}^{el} , and $\hat{T}_{JM}^{\text{mag}5}$ have the parity $\pi = (-1)^J$, while the operators \hat{M}_{JM}^5 , \hat{L}_{JM}^5 , $\hat{T}_{JM}^{\text{el}5}$, and $\hat{T}_{JM}^{\text{mag}}$ have the parity $\pi = (-1)^{J+1}$. Consequently, for the given values of J and $\pi = \pi_i \pi_f$, the contribution to the matrix elements (282) is made by either the vector or axial-vector component of the nucleon current multipole operator. Note that, in contrast to electromagnetic processes (photoexcitation, electron scattering), in semileptonic processes, 0^- transitions are possible in nuclei due to the axial component of the nucleon current.

To obtain an explicit form of the multipole operators \hat{L}_{JM} , \hat{L}_{JM}^5 , etc., which makes it possible to perform calculations with nonrelativistic wave functions, but taking into account relativistic corrections, in [139, 147, 151] a method based on the expansion in powers of the inverse mass of nucleon M_N^{-1} of matrix element of the nucleon current for free nucleons was applied. In this approach, the relativistic, or small, component of the wave function is expressed through the nonrelativistic component, while the required expressions for multipole operators, considering relativistic corrections, are obtained by retaining the terms of zero and first orders. We present the final expressions for the multipole operators of the weak nucleon current obtained in this way [138, 148, 152]:

$$\hat{M}_{JM} = F_1 M_{JM}(q\mathbf{x}), \quad (286a)$$

$$\hat{M}_{JM}^5 = -\frac{iq}{M_N} \times \left\{ F_A \Omega_{JM}(q\mathbf{x}) + \frac{1}{2} (F_A^{(T)} - \omega F_P) \Sigma_{JM}''(q\mathbf{x}) \right\}, \quad (286b)$$

$$\hat{L}_{JM} = -\frac{\omega}{q} \hat{M}_{JM}(q\mathbf{x}), \quad (286c)$$

$$\hat{L}_{JM}^5 = i \left\{ F_A - \frac{q^2}{2M_N} F_P \right\} \Sigma_{JM}''(q\mathbf{x}), \quad (286d)$$

$$\hat{T}_{JM}^{\text{el}} = \frac{q}{M_N} \times \left\{ F_1 \Delta_{JM}'(q\mathbf{x}) + \frac{1}{2} (F_1 + 2M_N F_2) \Sigma_{JM}'(q\mathbf{x}) \right\}, \quad (286e)$$

$$\hat{T}_{JM}^{\text{el}5} = i F_A \Sigma_{JM}'(q\mathbf{x}), \quad (286f)$$

$$\hat{T}_{JM}^{\text{mag}} = -\frac{iq}{M_N} \times \left\{ F_1 \Delta_{JM}(q\mathbf{x}) - \frac{1}{2} (F_1 + 2M_N F_2) \Sigma_{JM}'(q\mathbf{x}) \right\}, \quad (286g)$$

$$\hat{T}_{JM}^{\text{mag}5} = F_A \Sigma_{JM}(q\mathbf{x}). \quad (286h)$$

In turn, seven basis operators $M, \Omega, \Delta, \Delta', \Sigma, \Sigma'$ and Σ'' are expressed in terms of spherical Bessel functions $j_L(qx)$, spherical $Y_{lm}(\Omega_x)$ and vector spherical $\mathcal{Y}_{Jl}^M(\Omega_x)$ harmonics. In [153–155], expressions are given for the one-particle matrix elements of the basis operators. We emphasize that not only kinematic factors (see Table 1), but also matrix elements of the nucleon current multipole operators are functions of the transferred three-momentum q .

The values of the form factors F_X ($X = 1, 2, A, P$) involved in the expressions for multipole operators (286) are determined based on the hypotheses of the conserved vector current [156, 157] and the partially conserved axial current [158, 159]. Conservation of the vector current leads to the fact that the vector form factors of the charged weak current coincide with the form factors of the electromagnetic current, i.e., $F_{1,2}(0) = F_{1,2}^V(0)$, where [151, 160]

$$F_1^V(0) = g_V = 1, \quad (287)$$

$$F_2^V(0) = \frac{\mu_p - \mu_n - 1}{2M_N} \quad (288)$$

($\mu_p = 2.79$ and $\mu_n = -1.91$ are magnetic moments of the proton and neutron in Bohr magnetons). For the vector form factors of neutral weak currents, the Glashow–Weinberg–Salam electroweak interaction theory gives the values [161, 160]

$$F_1(0) = \begin{cases} \frac{1}{2}(1 - 4 \sin^2 \theta_W), & \text{for protons,} \\ -\frac{1}{2}, & \text{for neutrons,} \end{cases} \quad (289)$$

$$F_2(0) = \frac{1}{2M_N} \begin{cases} \frac{1}{2}(\mu_p - 1 - \mu_n - 4 \sin^2 \theta_W (\mu_p - 1)), & \text{for protons,} \\ -\frac{1}{2}(\mu_p - 1 - \mu_n - 4 \sin^2 \theta_W \mu_n), & \text{for neutrons,} \end{cases} \quad (290)$$

where θ_W is the Weinberg angle ($\sin^2 \theta_W = 0.2325$). The hypothesis of partial conservation of the axial current establishes the dependence of the axial and pseudoscalar form factors on the pion characteristics and the parameters of the pion–nucleon interaction. In particular, the axial form factor of the charged current satisfies the Goldberger–Treiman relation [139, 160]

$$F_A(0) = -\frac{f_\pi g_{\pi N}}{\sqrt{2} M_N}, \quad (291)$$

where f_π is a constant determined by the lifetime of charged pions, and $g_{\pi N}$ is the pion–nucleon coupling constant. Substituting the numerical values for f_π and $g_{\pi N}$ leads to a value $F_A(0)$ that is in good agreement with the value obtained by averaging the results of numerous measurements of the characteristics of β -transitions [162]

$$F_A(0) = g_A = -1.269 \pm 0.003. \quad (292)$$

Using relation (291) together with the one-pole approximation for $F_p(q_\mu^2)$ gives an expression relating the axial and pseudoscalar form factors [139, 160]

$$F_p(q_\mu^2) = \frac{2M_N F_A(q_\mu^2)}{q_\mu^2 + m_\pi^2}, \quad (293)$$

where $m_\pi = 139.57$ MeV is the pion mass. The corresponding form factors of neutral weak currents have the form [160, 161]

$$F_A(0) = \pm \frac{1}{2} F_A(0), \quad F_p(q_\mu^2) = \pm \frac{1}{2} F_p(q_\mu^2), \quad (294)$$

where the upper sign corresponds to protons and the lower sign, to neutrons. Following [138], to take into account the dependence of the form factors on the transferred four-momentum q_μ^2 , the static values of the form factors $F_{1,2}(0)$ and $F_A(0)$ are multiplied by the one-nucleon form factor

$f_{SN}(q_\mu^2) = [1 + q_\mu^2 / (855 \text{ MeV})^2]^{-2}$. For astrophysical calculations with good accuracy, $f_{SN}(q_\mu^2) = 1$.

The expressions for the reaction cross section (280) were derived by assuming that the lepton wave function corresponds to a plane wave. However, for charge-exchange processes where a charged lepton is present in the initial or final states, it is necessary to consider the distortion of its wave function in the Coulomb field of the nucleus. Depending on the lepton charge sign, either an increase or a decrease in the value of its wave function occurs near the nucleus.

This leads to a growth (for e^-) or a suppression (for e^+) of the reaction cross section. To consider the influence of the Coulomb field of the nucleus, cross section (280) is multiplied by the Fermi function $F(\pm Z^*, \varepsilon_e)$. Depending on the type of reaction, Z^* either coincides with the charge Z of the parent nucleus or with the charge of the daughter nucleus Z' ; the sign “+” (“−”) corresponds to the case when the charged lepton is an electron (positron). The exact value of $F(Z, \varepsilon_e)$ can be calculated by solving the relativistic Dirac equation with the Coulomb potential of a nucleus with radius R [163]. However, at a low charged-lepton energy ($p_e R / \hbar \ll 1$), the expression [62, 140, 163] is usually used as an approximate value of the Fermi function:

$$F(Z, \varepsilon_e) = 2(1 + s) \left(\frac{2p_e R}{\hbar} \right)^{2(s-1)} \left| \frac{\Gamma(s + i\eta)}{\Gamma(2s + 1)} \right|^2 e^{\pi\eta}, \quad (295)$$

where $s = \sqrt{1 - (\alpha Z)^2}$, $\eta = \alpha Z \varepsilon_e / (c p_e)$, $\alpha \equiv e^2 / (\hbar c)$ is the fine structure constant while $\Gamma(z)$ is the gamma function. At large values of ε_e , an effect of the Coulomb field of a nucleus can be considered by replacing the momentum and energy of the charged lepton with

effective values (effective momentum approximation [140, 141, 164])

$$\begin{aligned} \varepsilon_e^{\text{eff}} &= \varepsilon_e - V_C^{\text{eff}}, \\ p_e^{\text{eff}} c &= \sqrt{(\varepsilon_e^{\text{eff}})^2 - (m_e c^2)^2}, \end{aligned} \quad (296)$$

where V_C^{eff} is the effective Coulomb potential. As shown in [165], a good agreement with the exact solution to the Dirac equation is achieved by using $V_C^{\text{eff}} = 4V_C(0)/5$, where $V_C(0) = \mp 3Ze^2 / (2R)$ is the electrostatic potential at the center of the nucleus.

Expression (280) corresponds to the differential cross section of the exclusive reaction, in which the nucleus passes from the state i to the state f . The cross section for an inclusive reaction is obtained by summing over all possible final states f , such that $E_{if} \leq \varepsilon_i - m_\nu c^2$, and by integrating over the scattering angle. In a hot stellar medium, thermal occupation of excited nuclear states takes place. Let us occupation the temperature-dependent cross section for reaction (278) as the result of averaging over all thermally excited states of the nucleus:

$$\begin{aligned} \sigma(\varepsilon_i, T) &= \sum_{if} p_i(T) \sigma_{if}(\varepsilon_i) \\ &= \frac{2(G_F')^2}{\hbar^4 c^4} S_l \left(\frac{\varepsilon_l}{p_l} \right)^{\varepsilon_l - m_l c^2} \int_{-\infty}^{\varepsilon_l - m_l c^2} dE \varepsilon_l' p_l' \\ &\times \int_{-1}^1 d(\cos \theta) \left\{ \sum_{J \geq 0} \eta_J^{CL}(E, T) + \sum_{J \geq 1} \eta_J^T(E, T) \right\}, \end{aligned} \quad (297)$$

where $\varepsilon_l' = \varepsilon_l - E$, while the entire temperature dependence is contained in the charge longitudinal and transverse multipole functions

$$\eta_J^{CL,T}(E, T) = \sum_{if} p_i(T) \eta_J^{CL,T}(if) \delta(E - E_{if}). \quad (298)$$

Using the explicit form of the functions $\eta_J^{CL,T}(if)$ (282), we express $\eta_J^{CL,T}(E, T)$ in terms of the spectral densities of the charge \hat{M}_J , longitudinal $\hat{\mathcal{L}}_J$, transverse electric $\hat{\mathcal{T}}_J^{\text{el}}$, and transverse magnetic $\hat{\mathcal{T}}_J^{\text{mag}}$ multipole operators of the nucleon current:

$$\begin{aligned} \eta_{CL}^J(E, T) &= v_{LL} S_{\mathcal{L}_J \mathcal{L}_J} \\ &+ v_{CC} S_{\mathcal{M}_J \mathcal{M}_J} + v_{LC} 2 \text{Re} \{ S_{\mathcal{M}_J \mathcal{L}_J} \} \end{aligned} \quad (299)$$

and

$$\begin{aligned} \eta_T^J(E, T) &= v_{TT} [S_{\mathcal{T}_J^{\text{mag}} \mathcal{T}_J^{\text{mag}}} + S_{\mathcal{T}_J^{\text{el}} \mathcal{T}_J^{\text{el}}}] \\ &+ v_{TT'} 2 \text{Re} \{ S_{\mathcal{T}_J^{\text{mag}} \mathcal{T}_J^{\text{el}}} \}. \end{aligned} \quad (300)$$

Kinematic factors v_{LL}, v_{CC} , etc. do not depend on temperature, while the spectral densities $S_{A_j B_j}(E, T)$ of multipole operators are determined according to

(165). Thus, within the statistical approach, the calculation of the cross sections for weak reactions with hot nuclei is reduced to the calculation of spectral densities for multipole operators (286) of the nucleon current, which depend on the transferred momentum q . To consider the Coulomb corrections, the cross section (297) is multiplied by the Fermi function (295), and the nuclear recoil is taken into consideration by using the factor f_R (279).

Using the dependence of the multipole operators of nucleon current (286) on the transferred momentum q , we can directly from (297) obtain an expression for the cross section $\sigma(\varepsilon_l, T)$ at small values of ε_l . Indeed, since the maximum value of the momentum transferred in reaction (278) is equal to $q_{\max} = (2\varepsilon_l - E_{if})/\hbar c$, then at a low energy of the initial lepton $\varepsilon_l \leq 10$ MeV, the long-wave approximation condition becomes valid $qR \ll 1$, where $R \approx 5$ fm for nuclei with $A = 50-80$. Using the property of the Bessel function

$$j_J(qx) \approx \frac{(qx)^J}{(2J+1)!!} \text{ for } qx \ll 1 \quad (301)$$

and considering the nucleons in the nucleus to be slow, $v_{\text{nucl}}/c \ll 1$, it can be shown [139, 147] that, in the limit $q \rightarrow 0$, only the allowed transitions of the Fermi ($J^\pi = 0^+$) and Gamow–Teller ($J^\pi = 1^+$) types contribute to the cross section. For charge-exchange reactions, the corresponding multipole operators of current take the form:

$$\hat{M}_{00} = \frac{1}{\sqrt{4\pi}} g_V \sum_{j=1}^A t_{\pm}^{(j)} = \frac{1}{\sqrt{4\pi}} F_{\pm}, \quad (302)$$

$$\hat{L}_{1M}^5 = \frac{1}{\sqrt{2}} \hat{T}_{1M}^{\text{el5}} = \frac{i}{\sqrt{12\pi}} g_A \sum_{j=1}^A t_{\pm}^{(j)} \sigma_M^{(j)} = \frac{i}{\sqrt{12\pi}} \text{GT}_{\pm}. \quad (303)$$

In a charge-neutral channel, the operator \hat{M}_{00} contributes only to the elastic scattering of (anti)neutrinos. Since $F_1(0) \approx 0$ for protons, then to a good approximation, we can assume that

$$\hat{M}_{00} \approx -\frac{1}{2\sqrt{4\pi}} \hat{N}, \quad (304)$$

where \hat{N} is the operator of the number of neutrons in the nucleus. Therefore, only operators of $J^\pi = 1^+$ transition that are proportional to the zero component of the Gamow–Teller operator contribute to the inelastic scattering of (anti)neutrinos in the long-wavelength approximation:

$$\hat{L}_{1M}^5 = \frac{1}{\sqrt{2}} \hat{T}_{1M}^{\text{el5}} = \frac{i}{\sqrt{12\pi}} g_A \sum_{j=1}^A t_0^{(j)} \sigma_M^{(j)} = \frac{i}{\sqrt{12\pi}} \text{GT}_0, \quad (305)$$

where $t_0 = \tau_3/2$ is the operator of isospin projection.

Substitution of the given expressions for \hat{M}_{00} , \hat{L}_{1M}^5 , and $\hat{T}_{1M}^{\text{el5}}$, in (297) and integration over the scattering angle lead to the following expressions for the cross section of semileptonic reactions on hot nuclei in the long-wavelength approximation:

- capture of an electron or positron

$$\begin{aligned} \sigma(\varepsilon_e, T) &= \frac{(G_F V_{ud})^2}{2\pi(\hbar c)^4} \left(\frac{\varepsilon_e}{p_e c} \right) F(\pm Z, \varepsilon_e) \\ &\times \int_{-\infty}^{\varepsilon_e} (\varepsilon_e - E)^2 [S_{F_{\pm}}(E, T) + S_{G_{T_{\pm}}}(E, T)] dE; \end{aligned} \quad (306)$$

- capture of an electron (anti)neutrino

$$\begin{aligned} \sigma(\varepsilon_\nu, T) &= \frac{(G_F V_{ud})^2}{\pi(\hbar c)^4} \int_{-\infty}^{\varepsilon_\nu - m_e c^2} F(\pm Z \pm 1, \varepsilon_e) \\ &\times (\varepsilon_e p_e c) [S_{F_{\pm}}(E, T) + S_{G_{T_{\pm}}}(E, T)] dE, \end{aligned} \quad (307)$$

where $\varepsilon_e = \varepsilon_\nu - E$, $p_e c = (\varepsilon_e - m_e c^2)^{1/2}$;

- inelastic scattering of (anti)neutrinos

$$\sigma(\varepsilon_\nu, T) = \frac{G_F^2}{\pi(\hbar c)^4} \int_{-\infty}^{\varepsilon_\nu} (\varepsilon_\nu - E)^2 S_{G_{T_0}}(E, T) dE. \quad (308)$$

Thus, in the long-wavelength approximation, the cross sections for weak reactions on a hot nucleus are expressed in terms of the temperature-dependent strength functions (115) of the Fermi and Gamow–Teller transition operators.

The above expressions (297), (306)–(308) for the temperature-dependent cross section $\sigma(\varepsilon_l, T)$ are exact in the sense that no additional assumptions about the structure of the spectral densities and strength functions were made when they were derived from (280). In the TQRPA, the spectral densities and strength functions of multipole operators are expressed in terms of the reduced matrix elements between the thermal vacuum and thermal one-phonon states (see Eqs. (230), (269), (272)). Substituting the spectral functions calculated in TQRPA into (297) and integrating over the transferred energy E , we obtain a multipole expansion of the total cross section $\sigma(\varepsilon_l, T)$ in the form of the sum of contributions from individual thermal one-phonon states:

$$\begin{aligned} \sigma(\varepsilon_l, T) &= \sum_{Jk} \sigma_{Jk}(\varepsilon_l, T) = \frac{2(G_F')^2}{\hbar^4 c^4} S_l \left(\frac{\varepsilon_l}{p_l} \right) \\ &\times \sum_{Jk} \varepsilon_l p_l \int_{-1}^1 d(\cos \theta) \{ \eta_{Jk}^{\text{CL}}(k, T) + \eta_{Jk}^T(k, T) \}, \end{aligned} \quad (309a)$$

where

$$\eta_J^{CL}(k, T) = v_{LL} \left| \langle Jk \|\hat{\mathcal{L}}_J \|\Psi_0(T) \rangle \right|^2 + v_{CC} \left| \langle Jk \|\hat{\mathcal{M}}_J \|\Psi_0(T) \rangle \right|^2 \quad (309b)$$

$$+ v_{CL} 2 \operatorname{Re} \left(\langle Jk \|\hat{\mathcal{L}}_J \|\Psi_0(T) \rangle \langle J_f \|\hat{\mathcal{M}}_J \|\Psi_0(T) \rangle^* \right)$$

and

$$\eta_J^T(k, T) = v_{TT} \left(\left| \langle Jk \|\hat{\mathcal{G}}_J^{\text{mag}} \|\Psi_0(T) \rangle \right|^2 + \left| \langle Jk \|\hat{\mathcal{G}}_J^{\text{el}} \|\Psi_0(T) \rangle \right|^2 \right) + v_{TT} 2 \operatorname{Re} \left(\langle Jk \|\hat{\mathcal{G}}_J^{\text{mag}} \|\Psi_0(T) \rangle \langle Jk \|\hat{\mathcal{G}}_J^{\text{el}} \|\Psi_0(T) \rangle^* \right). \quad (309c)$$

Here, the summation extends to all one-phonon (nontilde and tilde) states with energies below the threshold $\varepsilon_i - m_i c^2$. The appearance of one-phonon states with negative energy for $T \neq 0$ leads to a situation that $\sigma(\varepsilon_i, T)$ is different from zero at an arbitrarily small energy of an incident lepton. Since at zero temperature the TQRPA method reduces to the quasiparticle random phase approximation, then at $T = 0$, expression (309) corresponds to the cross section of the semileptonic reaction on the ground state of the nucleus.

13. CONCLUSIONS

In the present work, using the formalism of superoperators and the method of the equation of motion, we construct a thermodynamically consistent method for calculating the spectral densities and strength functions in hot nuclei within the grand canonical ensemble. For this, a new definition of right fermionic superoperators in the Liouville space is introduced. As a consequence of this definition, it is shown that the thermal state condition depends only on whether the superoperator is fermion-like or boson-like. Relations are obtained connecting matrix elements and vacuum expectation values of tilde-conjugate superoperators.

For a model of a nucleus with a separabelized Skyrme interaction in a particle–hole channel, the equations of the thermal quasiparticle random phase approximation are obtained that describe the charge-neutral and charge-exchange one-phonon states in hot nuclei. The fulfillment of the model-independent Ikeda sum rule in this approximation is proved. Using the example of the Hamiltonian of the quasiparticle-phonon nuclear model, going beyond the random phase approximation in hot nuclei is proposed by considering the coupling of one- and two-phonon configurations. It is shown that the principle of detailed balance requires a redefinition of the thermal phonon vacuum with using the fragmentation of one-phonon states in hot nuclei.

A statistical approach is proposed for calculating the cross sections and rates of weak nuclear reactions with hot nuclei under astrophysical conditions, based

on a combination of the superoperator formalism and the Donnelly–Walecka method describing semileptonic nuclear processes.

APPENDICES

APPENDIX A:

Finding functions $\alpha(m, n)$ and $\beta(m, n)$

For the right superoperators defined according to (47), the conditions $[\tilde{a}_i, \tilde{a}_j]_\sigma = 0$, $[\tilde{a}_i^\dagger, \tilde{a}_j^\dagger]_\sigma = 0$ are satisfied regardless of the choice of the functions $\alpha(m, n)$ and $\beta(m, n)$. From the condition $[\tilde{a}_i, \tilde{a}_j^\dagger]_\sigma = 0$ for $i \neq j$ and relations

$$\begin{aligned} \tilde{a}_i \tilde{a}_j^\dagger \|mn\rangle\rangle &= \alpha(m, n+1) \beta(m, n) \| |m\rangle \langle n | a_j a_i^\dagger \rangle\rangle, \\ \tilde{a}_j^\dagger \tilde{a}_i \|mn\rangle\rangle &= \beta(m, n-1) \alpha(m, n) \| |m\rangle \langle n | a_i^\dagger a_j \rangle\rangle \end{aligned} \quad (310)$$

we obtain

$$\alpha(m, n) \beta(m, n-1) = \alpha(m, n+1) \beta(m, n). \quad (311)$$

With allowance for this relation, from $[\tilde{a}_j, \tilde{a}_j^\dagger]_\sigma = 1$ it follows that

$$\alpha(m, n) \beta(m, n-1) = 1. \quad (312)$$

Consequently, $\tilde{a}_i^\dagger \tilde{a}_i$ satisfies condition (45), i.e., is the superoperator of the number of particles.

Since

$$\begin{aligned} \tilde{a}_j \tilde{a}_i^\dagger \|mn\rangle\rangle &= \alpha(m+1, n) \| |a_i^\dagger |m\rangle \langle n | a_j^\dagger \rangle\rangle, \\ \tilde{a}_i^\dagger \tilde{a}_j \|mn\rangle\rangle &= \alpha(m, n) \| |a_i^\dagger |m\rangle \langle n | a_j \rangle\rangle. \end{aligned} \quad (313)$$

Then the requirement $[\tilde{a}_j, \tilde{a}_j^\dagger]_\sigma = 0$ leads to

$$\alpha(m+1, n) = -\sigma \alpha(m, n), \quad (314)$$

whence it follows that

$$\alpha(m, n) = (-\sigma)^m \alpha(0, n). \quad (315)$$

The same relation follows from $[\tilde{a}_j, \tilde{a}_i]_\sigma = 0$. Proceeding similarly, from the conditions $[\tilde{a}_j^\dagger, \tilde{a}_i^\dagger]_\sigma = 0$ and $[\tilde{a}_j^\dagger, \tilde{a}_i]_\sigma = 0$, we get

$$\beta(m+1, n) = -\sigma \beta(m, n) \quad (316)$$

or

$$\beta(m, n) = (-\sigma)^m \beta(0, n). \quad (317)$$

Consider now the following chains of equalities:

$$\begin{aligned} \langle \langle m_1 n_1 | \tilde{a}_i^\dagger | m_2 n_2 \rangle \rangle &= \beta(m_2, n_2) \delta_{m_1 m_2} \langle n_2 | a_i | n_1 \rangle \\ &= \beta(m_2, n_2) \delta_{m_1 m_2} \delta_{n_1, n_2-1} \langle n_2 | a_i | n_1 \rangle \end{aligned} \quad (318)$$

and

$$\begin{aligned} \langle\langle m_2 n_2 | \bar{a}_i^\dagger | m_1 n_1 \rangle\rangle &= \alpha(m_1, n_1) \delta_{m_1 m_2} \langle n_1 | a_i^\dagger | n_2 \rangle \\ &= \alpha(m_1, n_1) \delta_{m_1 m_2} \delta_{n_1, n_2-1} \langle n_1 | a_i^\dagger | n_2 \rangle \\ &= \alpha(m_2, n_2 - 1) \delta_{m_1 m_2} \delta_{n_1, n_2-1} \langle n_1 | a_i^\dagger | n_2 \rangle. \end{aligned} \quad (319)$$

Then from the condition $\langle\langle m_1 n_1 | \bar{a}_i^\dagger | m_2 n_2 \rangle\rangle = \langle\langle m_2 n_2 | \bar{a}_i | m_1 n_1 \rangle\rangle^*$, it follows that

$$\beta(m, n) = \alpha^*(m, n - 1). \quad (320)$$

Consider what the last of the conditions listed on page 892 leads to. Since

$$\langle\langle mn | \bar{a}_j^\dagger | I \rangle\rangle = \beta(m, m) \langle m | a_j | n \rangle \quad (321)$$

and $\langle\langle mn | a_j \rangle\rangle = \langle m | a_j | n \rangle$, then the condition $\langle\langle \bar{a}_j^\dagger | I \rangle\rangle = c | | a_j \rangle\rangle$ means that

$$\beta(m, m) = c. \quad (322)$$

Comparing (322) and (317), we obtain

$$\beta(m, n) = c(-\sigma)^{m+n}. \quad (323)$$

Using this equality on the right-hand side of (320), we get

$$\alpha(m, n) = c^*(-\sigma)^{m+n+1}, \quad (324)$$

which is consistent with (320). Substituting the expressions obtained for $\alpha(m, n)$ and $\beta(m, n)$ into (312), we arrive at the condition $cc^* = 1$.

APPENDIX B:

Secular Equation

for Charge-Neutral Thermal Phonons

In addition to condition (213), the amplitudes of charge-neutral thermal phonons satisfy the following relations:

• from $[Q_{JM_i}, Q_{JM_i}] = 0$, it follows that

$$\begin{aligned} \sum_{j_1 j_2} \{ & (\Psi_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'} - \Phi_{j_1 j_2}^{J_i} \Psi_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\Psi}_{j_1 j_2}^{J_i} \tilde{\Phi}_{j_1 j_2}^{J_i'} - \tilde{\Phi}_{j_1 j_2}^{J_i} \tilde{\Psi}_{j_1 j_2}^{J_i'}) \\ & + (\eta_{j_1 j_2}^{\lambda_i} \xi_{j_1 j_2}^{J_i'} - \xi_{j_1 j_2}^{J_i} \eta_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\eta}_{j_1 j_2}^{J_i} \tilde{\xi}_{j_1 j_2}^{J_i'} - \tilde{\xi}_{j_1 j_2}^{J_i} \tilde{\eta}_{j_1 j_2}^{J_i'}) \} = 0; \end{aligned} \quad (325)$$

• from $[Q_{JM_i}, \tilde{Q}_{JM_i}^\dagger] = 0$, it follows that

$$\begin{aligned} \sum_{j_1 j_2} \{ & (\Psi_{j_1 j_2}^{J_i} \tilde{\Psi}_{j_1 j_2}^{J_i'} - \Phi_{j_1 j_2}^{J_i} \tilde{\Phi}_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\Psi}_{j_1 j_2}^{J_i} \Psi_{j_1 j_2}^{J_i'} - \tilde{\Phi}_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'}) \\ & + (\eta_{j_1 j_2}^{\lambda_i} \tilde{\eta}_{j_1 j_2}^{J_i'} - \xi_{j_1 j_2}^{J_i} \tilde{\xi}_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\eta}_{j_1 j_2}^{J_i} \eta_{j_1 j_2}^{J_i'} - \tilde{\xi}_{j_1 j_2}^{J_i} \xi_{j_1 j_2}^{J_i'}) \} = 0; \end{aligned} \quad (326)$$

• from $[Q_{JM_i}, \tilde{Q}_{JM_i}^\dagger] = 0$, it follows that

$$\begin{aligned} \sum_{j_1 j_2} \{ & (\Psi_{j_1 j_2}^{J_i} \tilde{\Phi}_{j_1 j_2}^{J_i'} - \Psi_{j_1 j_2}^{J_i} \tilde{\Phi}_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\Psi}_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'} - \tilde{\Phi}_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'}) \\ & + (\eta_{j_1 j_2}^{\lambda_i} \xi_{j_1 j_2}^{J_i'} - \xi_{j_1 j_2}^{J_i} \tilde{\eta}_{j_1 j_2}^{J_i'}) \\ & + (\tilde{\eta}_{j_1 j_2}^{J_i} \xi_{j_1 j_2}^{J_i'} - \tilde{\xi}_{j_1 j_2}^{J_i} \eta_{j_1 j_2}^{J_i'}) \} = 0. \end{aligned} \quad (327)$$

With the help of effective amplitudes (220) four orthonormalization conditions (Eqs. (213), (325)–(327)) can be written as two relations: (223) and

$$\begin{aligned} \sum_{\tau} \sum_{j_1 j_2} \{ & (\Psi_{j_1 j_2}^{J_i} \Phi_{j_1 j_2}^{J_i'} - \Phi_{j_1 j_2}^{J_i} \Psi_{j_1 j_2}^{J_i'}) \\ & \times (1 - y_{j_1}^2 - y_{j_2}^2) + \\ & + (H_{j_1 j_2}^{J_i} \Xi_{j_1 j_2}^{J_i'} - \Xi_{j_1 j_2}^{J_i} H_{j_1 j_2}^{J_i'}) (y_{j_1}^2 - y_{j_2}^2) \} = 0. \end{aligned} \quad (328)$$

The separable form of the residual interaction allows the TQRPA equations (224) and (225) to be reduced to a system of $4N$ linear homogeneous equations. Indeed, for charge-neutral phonons of normal parity, the formal solution to the problem (224) can be represented in the following form

$$\begin{aligned} G_{j_1 j_2}^{J_i}(\tau) &= \frac{\hat{j}^{-2}}{(\epsilon_{j_1 j_2}^{(+)})^2 - \omega_{J_i}^2} \\ &\times \left\{ \epsilon_{j_1 j_2}^{(+)} u_{j_1 j_2}^{(+)} \sum_k f_{j_1 j_2}^{(J; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right. \\ &\left. + \omega_{J_i} u_{j_1 j_2}^{(-)} \sum_k f_{j_1 j_2}^{(JJ; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right\}, \\ W_{j_1 j_2}^{J_i}(\tau) &= \frac{\hat{j}^{-2}}{(\epsilon_{j_1 j_2}^{(+)})^2 - \omega_{J_i}^2} \\ &\times \left\{ \omega_{J_i} u_{j_1 j_2}^{(+)} \sum_k f_{j_1 j_2}^{(J; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right. \\ &\left. + \epsilon_{j_1 j_2}^{(+)} u_{j_1 j_2}^{(-)} \sum_k f_{j_1 j_2}^{(JJ; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right\}, \\ T_{j_1 j_2}^{J_i}(\tau) &= \frac{\hat{j}^{-2}}{(\epsilon_{j_1 j_2}^{(-)})^2 - \omega_{J_i}^2} \\ &\times \left\{ \epsilon_{j_1 j_2}^{(-)} v_{j_1 j_2}^{(-)} \sum_k f_{j_1 j_2}^{(J; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right. \\ &\left. + \omega_{J_i} v_{j_1 j_2}^{(+)} \sum_k f_{j_1 j_2}^{(JJ; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right\}, \\ S_{j_1 j_2}^{J_i}(\tau) &= \frac{\hat{j}^{-2}}{(\epsilon_{j_1 j_2}^{(-)})^2 - \omega_{J_i}^2} \\ &\times \left\{ \omega_{J_i} v_{j_1 j_2}^{(-)} \sum_k f_{j_1 j_2}^{(J; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(m; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right. \\ &\left. + \epsilon_{j_1 j_2}^{(-)} v_{j_1 j_2}^{(+)} \sum_k f_{j_1 j_2}^{(JJ; k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s; k)} D_{J_i}^{(k)}(\rho\tau) \right) \right\}. \end{aligned} \quad (329)$$

Substitution of obtained expressions in (226) leads to a system of $4N$ homogeneous equations for the functions $D_{ji}^{(k)}(\tau)$ and $D_{JJi}^{(k)}(\tau)$ ($1 \leq k \leq N$, $\tau = p, n$). In matrix notation, the resulting system has the form:

$$\begin{pmatrix} \mathbb{M}_{mm} - 1 & \mathbb{M}_{ms} \\ \mathbb{M}_{sm} & \mathbb{M}_{ss} - 1 \end{pmatrix} \begin{pmatrix} \mathbb{D}_J \\ \mathbb{D}_{JJ} \end{pmatrix} = 0. \quad (330)$$

The vectors \mathbb{D}_J and \mathbb{D}_{JJ} of dimension $2N$ consist of the elements

$$\mathbb{D}_J^{(k)} = \begin{pmatrix} D_J^{(k)}(p) \\ D_J^{(k)}(n) \end{pmatrix},$$

$$\mathbb{D}_{JJ}^{(k)} = \begin{pmatrix} D_{JJ}^{(k)}(p) \\ D_{JJ}^{(k)}(n) \end{pmatrix} \quad (1 \leq k \leq N),$$

while the matrices $\mathbb{M}_{\alpha\beta}$ ($\alpha, \beta = m, s$) are the $2N \times 2N$ matrices, composed of 2×2 units

$$\mathbb{M}_{\alpha\beta}^{kk'} = \begin{pmatrix} \chi_{+1}^{(\beta;k')} \mathcal{X}_{\alpha\beta;p}^{(J;kk')}(\omega) & \chi_{-1}^{(\beta;k')} \mathcal{X}_{\alpha\beta;p}^{(J;kk')}(\omega) \\ \chi_{-1}^{(\beta;k')} \mathcal{X}_{\alpha\beta;n}^{(J;kk')}(\omega) & \chi_{+1}^{(\beta;k')} \mathcal{X}_{\alpha\beta;n}^{(J;kk')}(\omega) \end{pmatrix} \quad (1 \leq k, k' \leq N).$$

Here the following notation for functions of ω are introduced:

$$\begin{aligned} \mathcal{X}_{mm;\tau}^{(J;kk')}(\omega) &= \hat{J}^{-2} \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(J;k)} f_{j_1 j_2}^{(J;k')} \\ &\times \left\{ \frac{\epsilon_{j_1 j_2}^{(+)} (u_{j_1 j_2}^{+})^2}{(\epsilon_{j_1 j_2}^{+})^2 - \omega^2} (1 - y_{j_1}^2 - y_{j_2}^2) \right. \\ &\quad \left. + \frac{\epsilon_{j_1 j_2}^{(-)} (v_{j_1 j_2}^{-})^2}{(\epsilon_{j_1 j_2}^{-})^2 - \omega^2} (y_{j_2}^2 - y_{j_1}^2) \right\}, \\ \mathcal{X}_{ss;\tau}^{(J;kk')}(\omega) &= \hat{J}^{-2} \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(JJ;k)} f_{j_1 j_2}^{(JJ;k')} \\ &\times \left\{ \frac{\epsilon_{j_1 j_2}^{(+)} (u_{j_1 j_2}^{-})^2}{(\epsilon_{j_1 j_2}^{+})^2 - \omega^2} (1 - y_{j_1}^2 - y_{j_2}^2) \right. \\ &\quad \left. + \frac{\epsilon_{j_1 j_2}^{(-)} (v_{j_1 j_2}^{+})^2}{(\epsilon_{j_1 j_2}^{-})^2 - \omega^2} (y_{j_2}^2 - y_{j_1}^2) \right\}, \\ \mathcal{X}_{ms;\tau}^{(J;kk')}(\omega) &= \hat{J}^{-2} \omega \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(J;k)} f_{j_1 j_2}^{(JJ;k')} \\ &\times \left\{ \frac{u_{j_1 j_2}^{(+)} u_{j_1 j_2}^{(-)}}{(\epsilon_{j_1 j_2}^{+})^2 - \omega^2} (1 - y_{j_1}^2 - y_{j_2}^2) \right. \\ &\quad \left. + \frac{v_{j_1 j_2}^{(+)} v_{j_1 j_2}^{(-)}}{(\epsilon_{j_1 j_2}^{-})^2 - \omega^2} (y_{j_2}^2 - y_{j_1}^2) \right\} \end{aligned} \quad (331)$$

and $\mathcal{X}_{sm;\tau}^{(J;kk')}(\omega) = \mathcal{X}_{ms;\tau}^{(J;k'k)}(\omega)$. The solvability condition for the system of homogeneous equations (330) leads

to a secular equation for finding the energy ω_{ji} of thermal phonons

$$\det \begin{pmatrix} \mathbb{M}_{mm} - 1 & \mathbb{M}_{ms} \\ \mathbb{M}_{sm} & \mathbb{M}_{ss} - 1 \end{pmatrix} = 0. \quad (332)$$

For thermal phonons of anomalous parity, the formal solution of the system of TQRPA equations (225) has the form

$$\begin{aligned} W_{j_1 j_2}^{Ji}(\tau) &= \frac{\hat{J}^{-2}}{(\epsilon_{j_1 j_2}^{+})^2 - \omega_{ji}^2} \epsilon_{j_1 j_2}^{(+)} u_{j_1 j_2}^{(-)} \\ &\times \sum_k \sum_{L=J \pm 1} f_{j_1 j_2}^{(LJ;k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s;k)} D_{LJi}^{(k)}(\rho\tau) \right), \\ S_{j_1 j_2}^{Ji}(\tau) &= \frac{\hat{J}^{-2}}{(\epsilon_{j_1 j_2}^{-})^2 - \omega_{ji}^2} \epsilon_{j_1 j_2}^{(-)} v_{j_1 j_2}^{(+)} \\ &\times \sum_k \sum_{L=J \pm 1} f_{j_1 j_2}^{(LJ;k)} \left(\sum_{\rho=\pm 1} \chi_{\rho}^{(s;k)} D_{LJi}^{(k)}(\rho\tau) \right). \end{aligned} \quad (333)$$

As in the case of the normal parity phonons, a substitution of the obtained expressions in (226) leads to a system of $4N$ homogeneous equations for the functions $D_{J \pm 1 J}^{(k)}(\tau)$ ($1 \leq k \leq N$, $\tau = p, n$):

$$\begin{pmatrix} \mathbb{M}_{J-1J-1} - 1 & \mathbb{M}_{J-1J+1} \\ \mathbb{M}_{J+1J-1} & \mathbb{M}_{J+1J+1} - 1 \end{pmatrix} \begin{pmatrix} \mathbb{D}_{J-1J} \\ \mathbb{D}_{J+1J} \end{pmatrix} = 0. \quad (334)$$

Here $\mathbb{M}_{LL'}$ are the $2N \times 2N$ matrices, composed of 2×2 units

$$\mathbb{M}_{LL'}^{(kk')} = \begin{pmatrix} \chi_{+1}^{(s;k')} \mathcal{X}_{LL';p}^{(J;kk')}(\omega) & \chi_{-1}^{(s;k')} \mathcal{X}_{LL';p}^{(J;kk')}(\omega) \\ \chi_{-1}^{(s;k')} \mathcal{X}_{LL';n}^{(J;kk')}(\omega) & \chi_{+1}^{(s;k')} \mathcal{X}_{LL';n}^{(J;kk')}(\omega) \end{pmatrix} \quad (1 \leq k, k' \leq N),$$

with the matrix elements

$$\begin{aligned} \mathcal{X}_{LL';\tau}^{(J;kk')}(\omega) &= \hat{J}^{-2} \sum_{j_1 j_2}^{\tau} f_{j_1 j_2}^{(LJ;k)} f_{j_1 j_2}^{(L'J;k')} \\ &\times \left\{ \frac{\epsilon_{j_1 j_2}^{(+)} (u_{j_1 j_2}^{-})^2}{(\epsilon_{j_1 j_2}^{+})^2 - \omega^2} (1 - y_{j_1}^2 - y_{j_2}^2) \right. \\ &\quad \left. + \frac{\epsilon_{j_1 j_2}^{(-)} (v_{j_1 j_2}^{+})^2}{(\epsilon_{j_1 j_2}^{-})^2 - \omega^2} (y_{j_2}^2 - y_{j_1}^2) \right\}, \end{aligned}$$

while the vector \mathbb{D}_{LJ} of $2N$ dimension has the following components:

$$\mathbb{D}_{LJ}^{(k)} = \begin{pmatrix} D_{LJ}^{(k)}(p) \\ D_{LJ}^{(k)}(n) \end{pmatrix}, \quad 1 \leq k \leq N.$$

The thermal phonon energy is found from the condition for the existence of a nontrivial solution for the system (334), therefore, it is a solution to the secular equation

$$\det \begin{pmatrix} \mathbb{M}_{J-1,J-1} - 1 & \mathbb{M}_{J-1,J+1} \\ \mathbb{M}_{J+1,J-1} & \mathbb{M}_{J+1,J+1} - 1 \end{pmatrix} = 0. \quad (335)$$

APPENDIX C:

*Secular Equation
for Charge-Exchange Thermal Phonons*

The requirement to preserve the bosonic commutation relations for charge-exchange thermal phonons leads to four orthonormalization conditions for the amplitudes:

- from $[\Omega_{JM_i}, \Omega_{J'M'i'}^\dagger] = \delta_{JJ'} \delta_{MM'} \delta_{ii'}$, it follows that

$$\begin{aligned} & \sum_{J_p J_n} \{ (\psi_{J_p J_n}^{J_i} \psi_{J_p J_n}^{J_i'} - \phi_{J_p J_n}^{J_i} \phi_{J_p J_n}^{J_i'}) \\ & + (\tilde{\psi}_{J_p J_n}^{J_i} \tilde{\psi}_{J_p J_n}^{J_i'} - \tilde{\phi}_{J_p J_n}^{J_i} \tilde{\phi}_{J_p J_n}^{J_i'}) \\ & + (\eta_{J_p J_n}^{\lambda i} \eta_{J_p J_n}^{J_i'} - \xi_{J_p J_n}^{J_i} \xi_{J_p J_n}^{J_i'}) \\ & + (\tilde{\eta}_{J_p J_n}^{J_i} \tilde{\eta}_{J_p J_n}^{J_i'} - \tilde{\xi}_{J_p J_n}^{J_i} \tilde{\xi}_{J_p J_n}^{J_i'}) \} = \delta_{ii'}; \end{aligned} \quad (336)$$

- from $[\Omega_{JM_i}, \Omega_{J'M'i'}] = 0$, it follows that

$$\begin{aligned} & \sum_{J_p J_n} \{ (\psi_{J_p J_n}^{J_i} \phi_{J_p J_n}^{J_i'} - \phi_{J_p J_n}^{J_i} \psi_{J_p J_n}^{J_i'}) \\ & + (\tilde{\psi}_{J_p J_n}^{J_i} \tilde{\phi}_{J_p J_n}^{J_i'} - \tilde{\phi}_{J_p J_n}^{J_i} \tilde{\psi}_{J_p J_n}^{J_i'}) \\ & + (\eta_{J_p J_n}^{\lambda i} \xi_{J_p J_n}^{J_i'} - \xi_{J_p J_n}^{J_i} \eta_{J_p J_n}^{J_i'}) \\ & + (\tilde{\eta}_{J_p J_n}^{J_i} \tilde{\xi}_{J_p J_n}^{J_i'} - \tilde{\xi}_{J_p J_n}^{J_i} \tilde{\eta}_{J_p J_n}^{J_i'}) \} = 0; \end{aligned} \quad (337)$$

- from $[\Omega_{JM_i}, \tilde{\Omega}_{J'M'i'}^\dagger] = 0$, it follows that

$$\begin{aligned} & \sum_{J_p J_n} \{ (\psi_{J_p J_n}^{J_i} \tilde{\psi}_{J_p J_n}^{J_i'} - \phi_{J_p J_n}^{J_i} \tilde{\phi}_{J_p J_n}^{J_i'}) \\ & + (\tilde{\psi}_{J_p J_n}^{J_i} \psi_{J_p J_n}^{J_i'} - \tilde{\phi}_{J_p J_n}^{J_i} \phi_{J_p J_n}^{J_i'}) \\ & + (\eta_{J_p J_n}^{\lambda i} \tilde{\eta}_{J_p J_n}^{J_i'} - \xi_{J_p J_n}^{J_i} \tilde{\xi}_{J_p J_n}^{J_i'}) \\ & + (\tilde{\eta}_{J_p J_n}^{J_i} \eta_{J_p J_n}^{J_i'} - \tilde{\xi}_{J_p J_n}^{J_i} \xi_{J_p J_n}^{J_i'}) \} = 0; \end{aligned} \quad (338)$$

- from $[\Omega_{JM_i}, \tilde{\Omega}_{J'M'i'}] = 0$, it follows that

$$\begin{aligned} & \sum_{J_p J_n} \{ (\psi_{J_p J_n}^{J_i} \tilde{\phi}_{J_p J_n}^{J_i'} - \psi_{J_p J_n}^{J_i} \tilde{\phi}_{J_p J_n}^{J_i'}) \\ & + (\tilde{\psi}_{J_p J_n}^{J_i} \phi_{J_p J_n}^{J_i'} - \tilde{\phi}_{J_p J_n}^{J_i} \psi_{J_p J_n}^{J_i'}) \\ & + (\eta_{J_p J_n}^{\lambda i} \tilde{\xi}_{J_p J_n}^{J_i'} - \xi_{J_p J_n}^{J_i} \tilde{\eta}_{J_p J_n}^{J_i'}) \\ & + (\tilde{\eta}_{J_p J_n}^{J_i} \xi_{J_p J_n}^{J_i'} - \tilde{\xi}_{J_p J_n}^{J_i} \eta_{J_p J_n}^{J_i'}) \} = 0. \end{aligned} \quad (339)$$

For effective amplitudes, the above conditions take the form of two relations: (265) and

$$\begin{aligned} & \sum_{J_p J_n} \{ (\Psi_{J_p J_n}^{J_i} \Phi_{J_p J_n}^{J_i'} - \Phi_{J_p J_n}^{J_i} \Psi_{J_p J_n}^{J_i'}) (1 - y_{j_1}^2 - y_{j_2}^2) \\ & + (H_{J_p J_n}^{J_i} \Xi_{J_p J_n}^{J_i'} - \Xi_{J_p J_n}^{J_i} H_{J_p J_n}^{J_i'}) (y_{j_n}^2 - y_{j_p}^2) \} = 0. \end{aligned} \quad (340)$$

In proving the fulfillment of the Ikeda sum rule in TQRPA approximation (277), we used the completeness properties of effective amplitudes

$$\begin{aligned} \sum_i G_{J_p J_n}^{J_i} W_{J_p J_n}^{J_i} &= \frac{\delta_{j_p j_p'} \delta_{j_n j_n'}}{1 - y_{j_p}^2 - y_{j_n}^2}, \\ \sum_i T_{J_p J_n}^{J_i} S_{J_p J_n}^{J_i} &= \frac{\delta_{j_p j_p'} \delta_{j_n j_n'}}{y_{j_n}^2 - y_{j_p}^2}, \\ \sum_i G_{J_p J_n}^{J_i} S_{J_p J_n}^{J_i} &= \sum_i T_{J_p J_n}^{J_i} W_{J_p J_n}^{J_i} = 0. \end{aligned} \quad (341)$$

These properties can be easily obtained by writing down the completeness conditions for phonon amplitudes and then expressing ϕ, ψ , etc. through effective amplitudes.

As in the case of charge-neutral phonons, the separable form of the residual interaction makes it possible to reduce the system of TQRPA equations (266) to $4N$ homogeneous equations

$$\begin{pmatrix} \mathbb{M}_{+-} - 1 & \mathbb{M}_{+-} \\ \mathbb{M}_{+-} & \mathbb{M}_{--} - 1 \end{pmatrix} \begin{pmatrix} \mathbb{D}_+ \\ \mathbb{D}_- \end{pmatrix} = 0. \quad (342)$$

Here \mathbb{M}_σ ($\sigma = +, -, +-$) are the $2N \times 2N$ matrices, composed of 2×2 units

$$\mathbb{M}_\sigma^{kk'} = \begin{pmatrix} \chi_1^{(a;k)} \mathcal{X}_\sigma^{(aa;kk')}(\omega) & \chi_1^{(b;k)} \mathcal{X}_\sigma^{(ab;kk')}(\omega) \\ \chi_1^{(a;k')} \mathcal{X}_\sigma^{(ba;kk')}(\omega) & \chi_1^{(b;k')} \mathcal{X}_\sigma^{(bb;kk')}(\omega) \end{pmatrix}, \quad (343)$$

$1 \leq k, k' \leq N.$

For the normal parity phonons, the indices a, b assume the values $a = J, b = JJ$, while for the anomalous parity phonons $a = (J-1)J, b = (J+1)J$. In addition, $\chi_1^{(J;k)} = \chi_1^{(m;k)}$ and $\chi_1^{(LJ;k)} = \chi_1^{(s;k)}$. The functions $\mathcal{X}_\sigma^{(cd;kk')}(\omega)$ ($c = a, b, d = a, b$) are defined as

$$\begin{aligned} \mathcal{X}_\pm^{(cd;kk')}(\omega) &= 2\hat{J}^{-2} \sum_{J_p J_n} f_{J_p J_n}^{(c;k)} f_{J_p J_n}^{(d;k')} \\ &\times \left\{ \frac{\epsilon_{J_p J_n}^{(+)} (u_{J_p J_n}^{(\pm)})^2}{(\epsilon_{J_p J_n}^{(+)})^2 - \omega^2} (1 - y_{j_p}^2 - y_{j_n}^2) \right. \\ &\left. + \frac{\epsilon_{J_p J_n}^{(-)} (v_{J_p J_n}^{(\mp)})^2}{(\epsilon_{J_p J_n}^{(-)})^2 - \omega^2} (y_{j_n}^2 - y_{j_p}^2) \right\}, \\ \mathcal{X}_{+-}^{(cd;kk')}(\omega) &= 2\omega \hat{J}^{-2} \sum_{J_p J_n} f_{J_p J_n}^{(c;k)} f_{J_p J_n}^{(d;k')} \\ &\times \left\{ \frac{u_{J_p J_n}^{(+)} u_{J_p J_n}^{(-)}}{(\epsilon_{J_p J_n}^{(+)})^2 - \omega^2} (1 - y_{j_p}^2 - y_{j_n}^2) \right. \\ &\left. + \frac{v_{J_p J_n}^{(+)} v_{J_p J_n}^{(-)}}{(\epsilon_{J_p J_n}^{(-)})^2 - \omega^2} (y_{j_p}^2 - y_{j_n}^2) \right\}. \end{aligned} \quad (344)$$

The vectors $\mathbb{D}^{(\pm)}$ of the $2N$ dimension consist of the functions $D_J^{(\pm;k)}$, $D_{LJ}^{(\pm;k)}$ (267)

$$\mathbb{D}_k^{(\pm)} = \begin{pmatrix} D_a^{(\pm;k)} \\ D_b^{(\pm;k)} \end{pmatrix}, \quad 1 \leq k \leq N.$$

The condition for the existence of a nontrivial solution for system (342) leads to a secular equation for finding the energy of charge-exchange thermal phonons

$$\det \begin{pmatrix} M_{++} - 1 & M_{+-} \\ M_{-+} & M_{--} - 1 \end{pmatrix} = 0. \quad (345)$$

For the QPM Hamiltonian, the secular equation for determining the energy of charge-exchange phonons in hot nuclei is given in our paper [134].

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