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Generalized inequalities for the Bogoliubov-Duhamel inner product with applications in the Approximating Hamiltonian Method*

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Infinite sets of inequalities which generalize all the known inequalities that can be used in the majorization step of the Approximating Hamiltonian method are derived. They provide upper bounds on the difference between the quadratic fluctuations of intensive observables of a N-particle system and the corresponding Bogoliubov-Duhamel inner product. The novel feature is that, under sufficiently mild conditions, the upper bounds have the same form and order of magnitude with respect to N for all the quantities derived by a finite number of commutations of an original intensive observable with the Hamiltonian. The results are illustrated on two types of exactly solvable model systems: one with bounded separable attraction and the other containing interaction of a boson field with matter.

Key words: *correlation functions, Bogoliubov-Duhamel inner product, statistical-mechanical inequalities, approximating Hamiltonian method, exactly solved models*

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1. Introduction

The Approximating Hamiltonian Method (AHM) provides a rigorous approach to the study of some classes of statistical mechanical systems in the thermodynamic limit. The method consists of the following interrelated ingredients:

(i) Description of classes of model systems which admit a rigorous treatment in terms of a more simple approximating Hamiltonian;

(ii) Rules according to which the approximating Hamiltonian is constructed from the original one;

(iii) Mathematical techniques for derivation of bounds which prove the thermodynamic equivalence of the approximating and original Hamiltonians;

(iv) Investigation of the thermodynamic and statistical properties of the system described by the approximating Hamiltonian.

For the first time, the idea of the Approximating Hamiltonian method (AHM) has been suggested on a heuristic level by N.N. Bogoliubov in his paper on the theory of the weakly non-ideal Bose-gas [1]. He conjectured that, under the existence of Bose condensate in the system, the normalized (by the square root of the volume) creation/annihilation operators for bosons with zero

*The paper is dedicated to the 70th jubilee of N.N. Bogoliubov Jr.
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momentum can be replaced by c-numbers in the model Hamiltonian. The value of these complex-conjugate numbers was determined by thermodynamic arguments. Thus, the initial model Hamiltonian was replaced by an approximating (trial) one, which has the advantage to be easily diagonalized by a canonical u-v transformation. The further development of the AHM took place in the framework of the Bardeen-Cooper-Schrieffer (BCS) reduced model of superconductivity [2]. In 1957 the corresponding approximating Hamiltonian was suggested and diagonalized by means of a u-v canonical transformation [3]. A little later, N.N. Bogoliubov [4] rigorously proved that the ground state energy density and the zero-temperature Green functions for the model and approximating Hamiltonians coincide in the thermodynamic limit.

The foundations of the modern formulation of the AHM have been laid down by N.N. Bogoliubov (Jr.), see [5] and references therein. The essential generalization to classes of quantum systems with separable interaction, considered at nonzero temperatures, has been achieved by using the Bogoliubov variational principle for the free energy density and a special majorization technique based on integration over external sources. Some major restrictions on the applicability of the method, such as the quadratic form of the interaction Hamiltonian and its boundedness, were removed by further extensions of the AHM, see the review article [6] and the books [7, 8].

In this paper we generalize all the known inequalities which have been, or could have been, used in the majorization step (iii) of the AHM. They set different lower and upper bounds on the quadratic fluctuations, proportional to the difference between the original and approximating Hamiltonians, by terms involving new functionals of which the Bogoliubov-Duhamel inner product is a special case. Their place and role (not only in the AHM) is illustrated by the derivation of some new consequences pertaining to the infinitely coordinated anisotropic Heisenberg model and the Dicke superradiance model. These inequalities can be used for estimating the closeness of the Gibbs average values to the corresponding Bogoliubov-Duhamel inner product for a special class of observables. In some sense they are complementary to the Bogoliubov inequality [9] which has been used to exclude conventional superfluid and superconducting long-range order in one- and two-dimensional systems with gage invariant interactions. By exploiting it for setting upper bounds on the spontaneous magnetization or sublattice magnetization, Mermin and Wagner [10] have rigorously proved the absence of long-range order in one- and two-dimensional isotropic Heisenberg models with finite-range interactions. Harris [11] has derived a lower bound on the symmetrized average value of the product of an operator A and its conjugate $A^{\dagger}$, which is a special case of the Bogoliubov inequality, but turns out to be sufficient for the derivation of the result of Mermin and Wagner. Alternative inequalities, setting a lower bound on the Bogoliubov-Duhamel inner product, have been used in the proof of the existence of spontaneous magnetization in a variety of quantum spin systems [12–15]. In the physical literature, the Bogoliubov-Duhamel inner product is also known as the Bogoliubov-Kubo-Mori scalar product. In addition, it plays an important role in the linear response theory [16], Kondo problem [12], the so-called parameter estimation problem in quantum statistical mechanics and noncommutative probability theory [17], see also [18] and references therein.

2. Systems with bounded separable attraction

Here we consider a special class of quantum statistical models which are defined initially in a finite region Λ of the d-dimensional Euclidean space R^d or the integer lattice Z^d. By $|\Lambda|$ we denote the volume of Λ in the first case, or the number of lattice sites in the latter case. The Hamiltonian $\mathcal{H}_\Lambda$ is defined as a self-adjoint operator in a separable Hilbert space $\mathbf{H}$, and the corresponding free energy density $f_\Lambda[\mathcal{H}_\Lambda]$ is assumed to exist. For the sake of simplicity, we do not explicitly distinguish between a Hamiltonian $\mathcal{H}_\Lambda$, describing a system with fixed number of particles N in Λ, and the statistical operator $\mathcal{H}_\Lambda - \mu\mathcal{N}$ in the grand canonical ensemble, where μ is the chemical potential and $\mathcal{N}$ is the number operator of particles. The density of the corresponding thermodynamic potential is given by

$$f_\Lambda[\mathcal{H}_\Lambda] = -(\beta|\Lambda|)^{-1} \ln Z[\mathcal{H}_\Lambda], \tag{2.1}$$

where $Z[\mathcal{H}_\Lambda]$ is the partition function; in all cases the thermodynamic limit is denoted by t$-$lim. The norm of a bounded operator A is $\|A\|$, the symbol $A^{\#}$ remains for both the operator A and its adjoint $A^{\dagger}$. As usual, $[A,B]=AB-BA$ is the commutator of two operators. Average values in the Gibbs ensemble with the Hamiltonian $\mathcal{H}_\Lambda$ are defined as

$$\langle\cdots\rangle_{\mathcal{H}_\Lambda}\equiv \mathrm{Tr}(\mathrm{e}^{-\beta\mathcal{H}_\Lambda}\cdots)/Z[\mathcal{H}_\Lambda]. \tag{2.2}$$

Let the Hamiltonian of the system in Λ be defined as a sum of two self-adjoint operators,

$$\mathcal{H}_\Lambda=\mathcal{T}_\Lambda+\mathcal{U}_\Lambda\,, \tag{2.3}$$

where $\mathcal{T}_\Lambda=\mathcal{T}_\Lambda^{\dagger}$ is a trace-class operator which generates the Gibbs semigroup $\{\exp(-\beta\mathcal{T}_\Lambda)\}_{\beta\geqslant 0}$. In addition, we impose the condition that the density of the thermodynamic potential corresponding to $\mathcal{T}_\Lambda$ is bounded uniformly with respect to the volume of the system $|\Lambda|$,

$$|f_\Lambda[\mathcal{T}_\Lambda]|\leqslant M_0\,. \tag{2.4}$$

A distinguishing feature of the models with bounded separable attraction is that the interaction Hamiltonian can be written as an extensive self-adjoint operator of the form [5]

$$\mathcal{U}_\Lambda=-|\Lambda|\sum_{s=1}^{n}g_{\mathrm{s}}A_{\Lambda,s}A_{\Lambda,s}^{\dagger}\,. \tag{2.5}$$

Here $g_{\mathrm{s}}>0$, $s=1,\ldots,n$, are interaction parameters and the intensive observables $A_{\Lambda,s}$, $A_{\Lambda,s}^{\dagger}$ represent uniformly bounded local operators averaged over a region of the space (real space or conjugate momentum space). The uniform boundedness of these operators,

$$\|A_{\Lambda,s}\|=\|A_{\Lambda,s}^{\dagger}\|\leqslant M_1\,,\qquad s=1,\ldots,n, \tag{2.6}$$

where the constant M_1 is independent of the volume $|\Lambda|$, is essential for the applicability of the method in the case under consideration. In the general framework one does not need explicit expressions for the operators $\mathcal{T}_\Lambda$ and $A_{\Lambda,s}$. It suffices to impose, in addition to (2.4) and (2.6), the following general constraints ($s,s'=1,\ldots,n$):

$$\|[A_{\Lambda,s},\mathcal{T}_\Lambda]\|\ \leqslant\ M_{1,T}\,, \tag{2.7}$$
$$\|[A_{\Lambda,s},A_{\Lambda,s'}^{\#}]\|\ \leqslant\ M_2|\Lambda|^{-1}. \tag{2.8}$$

The heuristic rule for construction of the approximating Hamiltonian $\mathcal{H}_\Lambda^{(0)}(\mathrm{a})$ consists in linearization of the original interaction Hamiltonian with respect to the deviations of the intensive operators $A_{\Lambda,s}$, $A_{\Lambda,s}^{\dagger}$ from some complex numbers:

$$\mathcal{H}_\Lambda^{(0)}(\mathrm{a})=\mathcal{T}_\Lambda-|\Lambda|\sum_{s=1}^{n}g_{\mathrm{s}}(a_{\mathrm{s}}A_{\Lambda,s}^{\dagger}+a_{\mathrm{s}}^{\star}A_{\Lambda,s}-a_{\mathrm{s}}a_{\mathrm{s}}^{\star}), \tag{2.9}$$

where $\mathrm{a}=(a_1,\ldots,a_n)\in\mathbf{C}^n$, and $a_{\mathrm{s}}^{\star}$ is the complex conjugate of a_{s}. The latter numbers are considered to be variational parameters, chosen so as to minimize the contribution in the free energy density of the residual interaction Hamiltonian

$$\mathcal{H}_\Lambda^{(1)}(\mathrm{a})\equiv\mathcal{H}_\Lambda-\mathcal{H}_\Lambda^{(0)}(\mathrm{a})=-|\Lambda|\sum_{s=1}^{n}g_{\mathrm{s}}(A_{\Lambda,s}-a_{\mathrm{s}})(A_{\Lambda,s}^{\dagger}-a_{\mathrm{s}}^{\star})\leqslant 0. \tag{2.10}$$

The main result of the AHM for this class of model systems is summarized in the absolute minimum principle for the approximating free energy density:

$$0\leqslant\min_{\mathrm{a}}f_\Lambda[\mathcal{H}_\Lambda^{(0)}(\mathrm{a})]-f_\Lambda[\mathcal{H}_\Lambda]\leqslant\epsilon(|\Lambda|), \tag{2.11}$$

where $\epsilon(|\Lambda|) \to 0$ as $|\Lambda| \to \infty$. This establishes the thermodynamic equivalence of the free energy densities for the model Hamiltonian (2.3), (2.5), and the approximating one (2.9).

The proof of (2.11) is carried out with the majorization technique developed by Bogoliubov Jr. [5]. It starts with the introduction of auxiliary external fields ν_{s} and $\nu_{\mathrm{s}}^{\star}$ conjugate to the operators $A_{\Lambda,s}^{\dagger}$ and $A_{\Lambda,s}$, respectively,

$$\mathcal{H}_{\Lambda}(\nu) \equiv \mathcal{H}_{\Lambda} - |\Lambda| \sum_{s=1}^{n} (\nu_{\mathrm{s}} A_{\Lambda,s}^{\dagger} + \nu_{\mathrm{s}}^{\star} A_{\Lambda,s}), \qquad \mathcal{H}_{\Lambda}^{(0)}(\mathrm{a},\nu) \equiv \mathcal{H}_{\Lambda}^{(0)}(\mathrm{a}) - |\Lambda| \sum_{s=1}^{n} (\nu_{\mathrm{s}} A_{\Lambda,s}^{\dagger} + \nu_{\mathrm{s}}^{\star} A_{\Lambda,s}). \tag{2.12}$$

Next, lower and upper bounds on the difference in the free energy densities for the original and approximating Hamiltonians are set by the Bogoliubov variational principle and the inequalities following from it. In view of the non-positive definiteness of the residual interaction Hamiltonian $\mathcal{H}_{\Lambda}^{(1)}(\mathrm{a}) \equiv \mathcal{H}_{\Lambda}(\nu) - \mathcal{H}_{\Lambda}^{(0)}(\mathrm{a},\nu)$, the application of the Bogoliubov inequalities yields the bounds

$$\begin{aligned} 0 &\leqslant \min_{\mathrm{a}} f_{\Lambda}[\mathcal{H}_{\Lambda}^{(0)}(\mathrm{a},\nu)] - f_{\Lambda}[\mathcal{H}_{\Lambda}(\nu)] \\ &\leqslant \sum_{s=1}^{n} g_{\mathrm{s}} \langle (A_{\Lambda,s} - \langle A_{\Lambda,s}\rangle_{\mathcal{H}_{\Lambda}(\nu)})(A_{\Lambda,s}^{\dagger} - \langle A_{\Lambda,s}^{\dagger}\rangle_{\mathcal{H}_{\Lambda}(\nu)})\rangle_{\mathcal{H}_{\Lambda}(\nu)}\,, \end{aligned} \tag{2.13}$$

valid for all complex fields ν_{s}, $s = 1, 2, \ldots n$.

The fact that the absolute minimum of the free energy density $f_{\Lambda}[\mathcal{H}_{\Lambda}^{(0)}(\mathrm{a},\nu))]$ is attained at a finite value $a = \bar{a}_{\Lambda}(\nu)$, which depends on the thermodynamic parameters of the Gibbs ensemble as well as on the size and shape of the domain Λ, has been proved by using the conditions (2.4) and (2.6).

Here it is in place to mention that the attempt to prove directly that the correlation functions in the right-hand side of inequalities (2.13) tends to zero as $|\Lambda| \to \infty$ may happen to be an impossible task. An efficient means for solving the problem provides the majorization technique of Bogoliubov (Jr.), see [5]. Instead of direct evaluation of the above correlation function, it uses inequalities which set upper bounds to averages of the form

$$\langle \delta A_{\Lambda,s} \delta A_{\Lambda,s}^{\dagger} \rangle_{\mathcal{H}_{\Lambda}(\nu)}\,, \qquad \delta A_{\Lambda,s} \equiv A_{\Lambda,s} - \langle A_{\Lambda,s} \rangle_{\mathcal{H}_{\Lambda}(\nu)}\,, \tag{2.14}$$

in terms involving second derivatives of the free energy density with respect to external fields ν_{s}:

$$\frac{\partial^2 f_{\Lambda}[\mathcal{H}_{\Lambda}(\nu)]}{\partial \nu_{\mathrm{s}}^{\star} \nu_{\mathrm{s}}} = -\beta|\Lambda|(\delta A_{\Lambda,s}; \delta A_{\Lambda,s}). \tag{2.15}$$

Here $(A;B)$ denotes the Bogoliubov-Duhamel inner product on the algebra of observables A, $B, \ldots$, defined as

$$(A;B)_{\mathcal{H}} \equiv (Z[\mathcal{H}])^{-1} \int_0^1 \mathrm{d}\tau \, \mathrm{Tr}\left[\mathrm{e}^{-\beta(1-\tau)\mathcal{H}} A^{\dagger} \mathrm{e}^{-\beta\tau\mathcal{H}} B\right]. \tag{2.16}$$

In the remainder we consider the given observables $A, B, C, \ldots$ and fixed Hamiltonian $\mathcal{H}$ pertaining to a quantum system in a finite region Λ. Whenever no confusion could arise, for brevity of notation we will omit the subscripts $\mathcal{H}$ and Λ and the argument of the partition function Z.

2.1. The Bogoluibov-Duhamel inner product

The general properties of the functional (2.16) are considered in the book [19] and in the articles [12–14, 17, 18]. We warn the reader that some authors use definitions which differ from (2.16) by a factor of β and/or by involving the operator A instead of its adjoint $A^{\dagger}$. For our purposes it suffices to mention the following. The inner product $(A;B)$ is conjugate symmetric, $(A;B) = (B^{\dagger};A^{\dagger})$, antilinear (linear) in the first (second) argument, $(A + \alpha C; B) = (A;B) + \alpha^{\star}(C;B)$ $((A; B + \alpha C) = (A;B) + \alpha(A;C))$, it satisfies the relationship

$$\beta(A;[\mathcal{H},B])_{\mathcal{H}} = \langle [A^{\dagger},B] \rangle_{\mathcal{H}}\,. \tag{2.17}$$

The inner product $(A;A)$ is nonnegative, $(A;A) \geqslant 0$, and convex,

$$(A;A) \leqslant (1/2)\langle AA^\dagger + A^\dagger A\rangle. \tag{2.18}$$

Finally, in the case when either A or B (or both) commute with the Hamiltonian, the inner product $(A;B)$ reduces to the bilinear complex-valued functional

$$\langle A;B\rangle_{\mathcal{H}} = \langle A^\dagger B\rangle_{\mathcal{H}}\,. \tag{2.19}$$

Note that in some works the operator metric in the algebra of physical observables defined by (2.19) is called Kubo-Martin-Schwinger metric, and the one defined by (2.16) is called Bogoliubov-Kubo-Mori metric [18, 20].

The further considerations are conveniently carried out by using the spectral representation of the Bogoliubov-Duhamel inner product. We assume that the Hamiltonian $\mathcal{H}$ has a simple discrete spectrum only, $\{E_n, n = 1,2,3\ldots\}$ and denote the corresponding eigenfunctions by $|n\rangle$, i.e., $\mathcal{H}|n\rangle = E_n|n\rangle$, $n = 1,2,3\ldots$. By $A_{mn} = \langle m|A|n\rangle$ we denote the corresponding matrix element of an operator A. Then, the right-hand side of (2.16) can be written as

$$(A;B)_{\mathcal{H}} = (Z_\Lambda[\mathcal{H}])^{-1}\sum_{m,n}{}' A^*_{mn}B_{mn}\frac{\mathrm{e}^{-\beta E_m} - \mathrm{e}^{-\beta E_n}}{\beta(E_n - E_m)} + (Z_\Lambda[\mathcal{H}])^{-1}\sum_n \mathrm{e}^{-\beta E_n}A^*_{nn}B_{nn}\,, \tag{2.20}$$

where the prime in the double sum means that the term $n = m$ is excluded.

Our aim is to majorize the quadratic fluctuations

$$\langle \delta A^\dagger \delta A\rangle = \langle A^\dagger A\rangle_{\mathcal{H}} - |\langle A\rangle|^2 \tag{2.21}$$

by terms proportional to some power of the inner product

$$\begin{aligned}(\delta A;\delta A) &= (A;A) - |\langle A\rangle|^2\\ &= Z_\Lambda^{-1}\sum_{m,n}{}'|A_{mn}|^2\frac{\mathrm{e}^{-\beta E_m} - \mathrm{e}^{-\beta E_n}}{\beta(E_n - E_m)} + (Z_\Lambda[\mathcal{H}])^{-1}\sum_n \mathrm{e}^{-\beta E_n}|A_{nn}|^2 - |\langle A\rangle|^2.\end{aligned} \tag{2.22}$$

Instead of (2.21) it is more convenient to consider the symmetrized form

$$\frac{1}{2}\langle \delta A^\dagger\delta A + \delta A\delta A^\dagger\rangle = \frac{1}{2}\langle A^\dagger A + AA^\dagger\rangle - |\langle A\rangle|^2. \tag{2.23}$$

Here we have

$$\begin{aligned}\frac{1}{2}\langle A^\dagger A + AA^\dagger\rangle &= Z^{-1}\sum_{m,n}\mathrm{e}^{-\beta E_n}\frac{1}{2}(|A_{mn}|^2 + |A_{nm}|^2)\\ &= Z^{-1}\sum_{m,n}{}'|A_{mn}|^2\frac{1}{2}(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m}) + Z^{-1}\sum_n |A_{nn}|^2\mathrm{e}^{-\beta E_n}.\end{aligned} \tag{2.24}$$

By comparing equations (2.22), (2.23) and (2.24) we obtain

$$\frac{1}{2}\langle A^\dagger A + AA^\dagger\rangle - (A;A) = Z^{-1}\sum_{m,n}{}'|A_{mn}|^2\left\{\frac{1}{2}(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m}) - \frac{\mathrm{e}^{-\beta E_m} - \mathrm{e}^{-\beta E_n}}{\beta(E_n - E_m)}\right\}. \tag{2.25}$$

Now, by using the identity

$$\mathrm{e}^{-\beta E_m} + \mathrm{e}^{-\beta E_n} = (\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m})\coth\frac{\beta(E_m - E_n)}{2} \tag{2.26}$$

we can express the difference (2.25) in two equivalent forms:

$$\frac{1}{2}\langle A^\dagger A + AA^\dagger\rangle - (A;A) = Z^{-1}\sum_{m,n}{}'|A_{mn}|^2\frac{\mathrm{e}^{-\beta E_m} - \mathrm{e}^{-\beta E_n}}{\beta(E_n - E_m)}(X_{mn}\coth X_{mn} - 1), \tag{2.27}$$

and

$$\frac{1}{2}\langle A^\dagger A + AA^\dagger\rangle - (A;A) = Z^{-1}\sum_{m,n}{}'|A_{mn}|^2\frac{1}{2}(\mathrm{e}^{-\beta E_n}+\mathrm{e}^{-\beta E_m})\left(1-\frac{1}{X_{mn}\coth X_{mn}}\right), \qquad (2.28)$$

where

$$X_{mn} = \frac{1}{2}\beta(E_m - E_n). \qquad (2.29)$$

The application of the elementary inequality $x\coth x \geqslant 1$ to the right-hand side of (2.27) immediately yields the convexity property (2.18).

Different choices of the upper bound on the right-hand side of (2.27) generate different inequalities. Thus, the inequality of Brooks Harris [11],

$$(A;A) \leqslant \frac{1}{2}\langle AA^+ + A^+A\rangle \leqslant (A;A) + \frac{\beta}{12}\langle[[A^+,\mathcal{H}],A]\rangle \qquad (2.30)$$

is obtained by setting

$$1 \leqslant x\coth x \leqslant 1 + \frac{1}{3}x^2. \qquad (2.31)$$

On the other hand, if one uses another elementary inequality,

$$1 \leqslant x\coth x \leqslant 1 + |x|, \qquad (2.32)$$

and subsequently applies the Hölder inequality, one obtains the result due to Ginibre [22]:

$$(A;A) \leqslant \frac{1}{2}\langle AA^+ + A^+A\rangle \leqslant (A;A) + \frac{1}{2}\{(A;A)\beta\langle[[A^+,\mathcal{H}],A]\rangle\}^{\frac{1}{2}}. \qquad (2.33)$$

A different choice of the parameters in the Hölder inequality, followed by the implementation of the upper bound

$$|\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}| < |\mathrm{e}^{-\beta E_l} + \mathrm{e}^{-\beta E_m}|, \qquad (2.34)$$

generates a symmetric version of the inequality due to Bogoliubov (Jr.) [5]:

$$\frac{1}{2}\langle AA^+ + A^+A\rangle \leqslant (A;A) + \frac{1}{2}[(A;A)\beta]^{2/3}\{\langle[A^+,\mathcal{H}][\mathcal{H},A] + [\mathcal{H},A][A^+,\mathcal{H}]\rangle\}^{1/3}. \qquad (2.35)$$

Due to relation (2.15), each of the above inequalities can be used in the AHM to majorize the quadratic fluctuations (2.14) in terms involving second derivatives of the free energy density with respect to the external fields ν_{s}. However, note that in the zero temperature limit $\beta \to \infty$ the right-hand side of the simplest inequality (2.30) diverges.

3. Main inequalities

To derive generalizations of the known inequalities involving the Bogoliubov-Duhamel inner product, a set of new functionals $F_k(J;J)$, $k = 0,1,2,\ldots$, is defined by their spectral representation:

$$F_k(J;J) := Z^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l} - (-1)^k\mathrm{e}^{-\beta E_m}|(\beta|E_m - E_l|)^{k-1}. \qquad (3.1)$$

The specific choice of $k = 0,1,2,\ldots$ is motivated by the relation of functionals (3.1) to the Gibbs average values of some commutators and anticommutators involving the given operators J and Hamiltonian $\mathcal{H}$. Indeed,

(i) If $k = 2n$, $n = 0,1,2,3,\ldots$, then

$$\begin{aligned} F_{2n}(J;J) &\equiv Z^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}|(\beta|E_m - E_l|)^{2n-1} \\ &= \beta^{2n}(R_n;R_n) = \beta^{2n-1}\langle[R_n^+R_{n-1} - R_{n-1}R_n^+]\rangle, \end{aligned} \qquad (3.2)$$

where, by definition, $R_{-1} \equiv X_{J\mathcal{H}}$ is a solution of the operator equation $J = [X_{J\mathcal{H}}, \mathcal{H}]$, and

$$R_0 \equiv R_0(J) = J, \quad R_1 \equiv R_1(J) = [\mathcal{H}, J], \quad R_n \equiv R_n(J) = [\mathcal{H}, R_{n-1}(J)], \quad n = 1, 2, 3, \ldots \tag{3.3}$$

These observables have been introduced in [23].

(ii) If $k = 2n + 1$, $n = 0, 1, 2, 3, \ldots$, then

$$\begin{aligned} F_{2n+1}(J; J) &\equiv Z^{-1} \sum_{ml} |J_{ml}|^2 (\mathrm{e}^{-\beta E_l} + \mathrm{e}^{-\beta E_m}) [\beta(E_m - E_l)]^{2n} \\ &= \beta^{2n} \langle [R_n R_n^+ + R_n^+ R_n] \rangle. \end{aligned} \tag{3.4}$$

In particular,

$$\begin{aligned} &F_0(J; J) = (J; J), \qquad F_1(J; J) = \langle J J^+ + J^+ J \rangle, \qquad F_2(J; J) = \beta \langle [[J^+, \mathcal{H}], J] \rangle, \\ &F_3(J; J) = \beta^2 \langle [J^+, \mathcal{H}][\mathcal{H}, J] + [\mathcal{H}, J][J^+, \mathcal{H}] \rangle. \end{aligned} \tag{3.5}$$

The functionals (3.1) will be used to generalize all the known inequalities used in the AHM.

3.1. Generalization of the Harris inequality

By using the identity (2.26), one can rewrite the equality (3.4) in the form

$$F_{2n+1}(J; J) \equiv Z^{-1} \sum_{ml} |J_{ml}|^2 (\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}) \coth \frac{\beta(E_m - E_l)}{2} [\beta(E_m - E_l)]^{2n}. \tag{3.6}$$

Now, from the elementary inequalities (2.31) it follows that

$$F_{2n}(J; J) \leqslant \frac{1}{2} F_{2n+1}(J; J) \leqslant F_{2n}(J; J) + \frac{1}{12} F_{2n+2}(J; J). \tag{3.7}$$

This is a generalization of the Brooks Harris inequality (2.30), since the latter is recovered in the particular case of $n = 0$.

3.2. Generalization of the Plechko inequalities

The application of the elementary inequalities (2.32) to the right-hand side of (3.6) leads to

$$F_{2n}(J; J) \leqslant \frac{1}{2} F_{2n+1}(J; J) \leqslant F_{2n}(J; J) + (2Z)^{-1} \sum_{ml} |J_{ml}|^2 |\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}| [\beta(E_m - E_l)]^{2n}. \tag{3.8}$$

The problem now is that, due to the absolute value of the difference of the two Gibbs exponents, there is no apparent interpretation of the sum in the right-hand side of (3.8) in terms of average values. A known way to overcome this difficulty is based on the application of the Hölder inequality

$$\sum_k |x_k y_k| \leqslant \left(\sum_k |x_k|^p \right)^{1/p} \left(\sum_k |y_k|^q \right)^{1/q}, \qquad p, q > 1, \qquad 1/p + 1/q = 1. \tag{3.9}$$

By setting $k = (m, l)$ and

$$\begin{aligned} |x_{ml}| &= \left\{ |J_{ml}|^2 \frac{\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}}{\beta(E_m - E_l)} \right\}^{1/p}, \\ |y_{ml}| &= \left\{ |J_{ml}|^2 \frac{\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}}{\beta(E_m - E_l)} [\beta |E_m - E_l)|]^{(2n+1)q} \right\}^{1/q}, \end{aligned} \tag{3.10}$$

we obtain

$$(2Z)^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}|[\beta(E_m-E_l)]^{2n}$$
$$\leqslant \frac{1}{2}(J;J)^{1/p}\left\{Z^{-1}\sum_{ml}|J_{ml}|^2\frac{\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}}{\beta(E_m-E_l)}[\beta|E_m-E_l|]^{(2n+1)q}\right\}^{1/q}. \qquad (3.11)$$

One of the possible choices of p and q here, namely even integer $q=2k$ (hence, $p=2k/(2k-1)$) leads to the set of generalized Ginibre inequalities ($k=1,2,3,\ldots$):

$$F_{2n}(J;J)\leqslant \frac{1}{2}F_{2n+1}(J;J)\leqslant F_{2n}(J;J)+\frac{1}{2}(J;J)^{(2k-1)/2k}[F_{2k(2n+1)}(J;J)]^{1/2k}. \qquad (3.12)$$

At $n=0$ the above set reduces to a symmetric version of the inequalities obtained by Plechko [21]:

$$(J;J)\leqslant\frac{1}{2}\langle JJ^+ + J^+J\rangle\leqslant (J;J)+\frac{1}{2}(J;J)^{(2k-1)/2k}\beta(R_k;R_k)^{1/2k}, \quad (k=1,2,3,\ldots). \qquad (3.13)$$

Hence, in the particular case of $k=1$ one obtains the Ginibre inequality (2.33).

3.3. Generalization of the Bogoliubov (Jr.)-Plechko-Repnikov inequalities

If in (3.11) one chooses odd $q=2k+1$, hence, $p=(2k+1)/2k$, then for the sum in the right-hand side one can use the upper bound

$$Z^{-1}\sum_{ml}|J_{ml}|^2\frac{\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}}{\beta(E_m-E_l)}[\beta|E_m-E_l)|]^{(2n+1)(2k+1)}$$
$$\leqslant Z^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l}+\mathrm{e}^{-\beta E_m}|[\beta|E_m-E_l)|]^{2(2nk+n+k)}=F_{2(2nk+n+k)+1}(J;J). \qquad (3.14)$$

Thus one obtains the set of inequalities ($k=1,2,3,\ldots$)

$$\frac{1}{2}F_{2n+1}(J;J)\leqslant F_{2n}(J;J)+\frac{1}{2}(J;J)^{2k/(2k+1)}[F_{2(2nk+n+k)+1}(J;J)]^{1/(2k+1)}. \qquad (3.15)$$

At $n=0$ these reduce to a symmetric version of the set of inequalities obtained by Bogoliubov Jr., Plechko and Repnikov [23]:

$$\frac{1}{2}\langle JJ^+ + J^+J\rangle\leqslant (J;J)+\frac{1}{2}(J;J)^{2k/(2k+1)}\{\beta^{2k}\langle R_kR_k^+ + R_k^+R_k\rangle\}^{1/(2k+1)}. \qquad (3.16)$$

The symmetric version of the Bogoliubov's (Jr.) inequality (2.35) follows from here in the particular case of $k=1$.

3.4. Alternative sets of inequalities

By applying the Hölder inequality (3.9) to the second term in the right-hand side of (3.7) under the substitution

$$|x_{ml}|=\left\{|J_{ml}|^2\frac{\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}}{\beta(E_m-E_l)}[\beta(E_m-E_l)]^{2n}\right\}^{1/p},$$
$$|y_{ml}|=\left\{|J_{ml}|^2|\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}|[\beta|E_m-E_l|]^{2n+q/p}\right\}^{1/q}, \qquad (3.17)$$

instead of (3.10), one can in parallel derive two new sets of inequalities. Thus we obtain first

$$(2Z)^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}|[\beta(E_m-E_l)]^{2n}$$
$$\leqslant\frac{1}{2}[F_{2n}(J;J)]^{1/p}\left\{Z^{-1}\sum_{ml}|J_{ml}|^2\frac{\mathrm{e}^{-\beta E_l}-\mathrm{e}^{-\beta E_m}}{\beta(E_m-E_l)}[\beta|E_m-E_l|]^{2n+1/(p-1)}\right\}^{(p-1)/p}. \qquad (3.18)$$

Now there are two choices of p, one of which yields $1/(p-1)$ odd integer, and the other – even integer. In the first case we set $1/(p-1) = 2k-1$, $k = 1, 2, 3, \ldots$, which implies $p = 2k/(2k-1)$, $q = 2k$. Then, from (3.18) and (3.7) the following set of inequalities follows

$$\frac{1}{2}F_{2n+1}(J;J) \leqslant F_{2n}(J;J) + \frac{1}{2}[F_{2n}(J;J)]^{(2k-1)/2k}[F_{2(n+k)}(J;J)]^{1/2k}, \qquad (k = 1, 2, 3, \ldots). \quad (3.19)$$

In the second case we set $1/(p-1) = 2k$, $k = 1, 2, 3, \ldots$, which implies $p = (2k+1)/2k$, $q = 2k+1$. Then we can use the upper bound

$$\begin{aligned} &Z^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l} - \mathrm{e}^{-\beta E_m}|[\beta|E_m - E_l)|]^{2(n+k)} \\ &\quad\leqslant Z^{-1}\sum_{ml}|J_{ml}|^2|\mathrm{e}^{-\beta E_l} + \mathrm{e}^{-\beta E_m}|[\beta|E_m - E_l)|]^{2(n+k)} = F_{2(n+k)+1}(J;J), \end{aligned} \qquad (3.20)$$

to obtain another set of inequalities

$$\frac{1}{2}F_{2n+1}(J;J) \leqslant F_{2n}(J;J) + \frac{1}{2}[F_{2n}(J;J)]^{2k/(2k+1)}[F_{2(n+k)+1}(J;J)]^{1/(2k+1)}, \qquad (k = 1, 2, 3, \ldots). \quad (3.21)$$

Note that (3.19) is different from (3.12) but at $n = 0$ it reduces to the Plechko inequalities (3.13). Therefore, this set of inequalities can also be considered as a generalization of the Ginibre inequality (2.33).

Similarly, for general n, equation (3.21) differs from (3.15) but reduces to the Bogoliubov (Jr.)-Plechko-Repnikov inequalities (3.16) at $n = 0$. Hence, the set of inequalities (3.21) is also a generalization of the Bogoliubov (Jr.) inequality (2.35).

A comment is in order here. Due to the property $R_{n+k}(J) = R_k(R_n(J))$, in terms of the operators $B_n \equiv R_n(J)$ one has

$$\begin{aligned} &F_{2n}(J;J) = \beta^{2n}(B_n;B_n), \quad F_{2n+1}(J;J) = \beta^{2n}\langle B_n B_n^+ + B_n^+ B_n\rangle, \\ &F_{2(n+k)}(J;J) = \beta^{2(n+k)}(R_k(B_n);R_k(B_n)), \\ &F_{2(n+k)+1}(J;J) = \beta^{2(n+k)}\langle R_k(B_n)R_k^{\dagger}(B_n) + R_k^{\dagger}(B_n)R_k(B_n)\rangle. \end{aligned} \qquad (3.22)$$

Therefore, inequalities (3.7) take exactly the form of the inequality of Brooks Harris (2.30) with A replaced by B_n, inequalities (3.19), respectively (3.21), take exactly the form of a symmetric version of the Plechko inequalities (3.13), respectively, the Bogoliubov (Jr.)-Plechko-Repnikov inequalities (3.16), with J replaced by B_n.

Notably, under the above substitution, the generalized Ginibre inequalities (3.12) and the generalized Bogoliubov (Jr.)-Plechko-Repnikov inequalities (3.15) do not reduce to any of the known types of inequalities, except in the particular case of $n = 0$.

3.5. General features and comparison of upper bounds

Obviously, the main inequalities have been derived under different approximations. The most direct is the derivation of generalized Harris inequalities - it is based upon the single elementary upper bound (2.31). Next, the generalized Ginibre inequalities are derived by first using the elementary upper bound (2.32), followed by the application of the Hölder inequality (3.9) under a special choice of the parameters: $p = 2k/(2k-1)$ and $q = 2k$. An alternative choice of these parameters, $p = (2k+1)/2k$ and $q = 2k+1$, requires the use of an additional, rather crude upper bound (2.34), in order to derive the Bogoliubov (Jr.)-Plechko-Repnikov inequalities (3.15).

The characteristic feature of our generalized inequalities is that, under sufficiently mild conditions on the Hamiltonian $\mathcal{H}_N$ of the N-particle system and the bounded intensive observable J_N, they provide the upper bounds on the non-negative difference

$$0 \leqslant \Delta_n(J_N) \equiv \frac{1}{2}\langle R_n^+(J_N)R_n(J_N) + R_n(J_N)R_n^+(J_N)\rangle_{\mathcal{H}_N} - (R_n(J_N);R_n(J_N))_{\mathcal{H}_N} \qquad (3.23)$$

of equal form and equal order of magnitude (with respect to N) for all finite $n = 0, 1, 2, \ldots$, i.e., for any finite set of observables J_N, $R_1(J_N) = [\mathcal{H}_N, J_N]$, $R_2(J_N) = [\mathcal{H}_N, R_1(J_N)], \ldots$. Note that the left-hand side inequality in (3.23) is a generalization of the convexity property of the Bogoliubov-Duhamel inner product (2.18).

The required conditions are ($n = 1, 2, 3, \ldots$):

$$\begin{aligned} |\langle J_N \rangle_{\mathcal{H}_N}| &\leqslant O(1), \\ F_{2n}(J_N; J_N) &= \beta^{2n-1} \langle [R_n^+(J_N), R_{n-1}(J_N)] \rangle_{\mathcal{H}_N} \leqslant O(N^{-1}), \\ F_{2n+1}(J_N; J_N) &= \beta^{2n} \langle R_n^+(J_N) R_n(J_N) + R_n(J_N) R_n^+(J_N) \rangle_{\mathcal{H}_N} \leqslant O(1). \end{aligned} \tag{3.24}$$

They are generally satisfied for extensive Hamiltonians $\mathcal{H}_N$ with bounded interaction and bounded intensive observables J_N, which are arithmetic averages over the particles of the system of some local observables. An example will be given in the end of this section.

The above conditions may also hold in some cases when $\mathcal{H}_N$ and $R_n(J_N)$, $n = 0, 1, 2, \ldots$, contain unbounded operators. As an example in section 4.2 we will consider the Dicke model of superradiance [25], for which the proper unbounded counterpart of J_N will be found.

Under conditions (3.24), our generalized inequalities yield the following upper bounds for all finite $n = 0, 1, 2, \ldots$:

1. Generalized Harris inequality (3.7)

$$\Delta_n(J_N) \leqslant O(N^{-1}). \tag{3.25}$$

2. Generalized Plechko inequalities (3.12)

$$\Delta_n(J_N) \leqslant (J_N; J_N)^{(2k-1)/2k} O(N^{-1/2k}), \qquad (k = 1, 2, 3, \ldots), \tag{3.26}$$

which at $k = 1$ reduce to the Ginibre inequality

$$\Delta_n(J_N) \leqslant (J_N; J_N)^{1/2} O(N^{-1/2}). \tag{3.27}$$

3. Generalized Bogoliubov (Jr.)-Plechko-Repnikov inequalities (3.15)

$$\Delta_n(J_N) \leqslant (J_N; J_N)^{2k/(2k+1)} O(1), \qquad (k = 1, 2, 3, \ldots), \tag{3.28}$$

which at $k = 1$ reduce to the Bogoliubov (Jr.) inequality

$$\Delta_n(J_N) \leqslant (J_N; J_N)^{2/3} O(1). \tag{3.29}$$

Due to the relationship between the Bogoliubov-Duhamel inner product and the susceptibility of the system with respect to the external field conjugate to the observable J_N, see (2.15), we can compare the different upper bounds in the region of parameters in which the susceptibility is bounded. We see that the generalized Harris, Plechko and Ginibre inequalities yield upper bounds of the order $O(N^{-1})$, while the generalized Bogoliubov (Jr.)-Plechko-Repnikov inequalities yield upper bounds of the order $O(N^{-2k/(2k+1)})$, $k = 1, 2, 3, \ldots$.

Finally, to illustrate the validity of conditions (3.24) and the explicit form of the first generalized observables $R_n(J_N)$, we consider a simple model with separable attraction built upon bounded operators. Let the model system contain N spins and have the Hamiltonian (normalized by $k_{\mathrm{B}}T$)

$$\beta \mathcal{H}_N = -N g_x \left(J_N^x\right)^2 - N g_y \left(J_N^y\right)^2 - N \mathbf{h} \cdot \mathbf{J}_N \,, \tag{3.30}$$

where $g_x,\ g_y > 0$ are dimensionless coupling constants, $\mathbf{h} = \{h_x, h_y, h_z\}$ is the vector of the external magnetic field, $\mathbf{J}_N = \{J_N^x, J_N^y, J_N^z\}$ is the vector operator of the average spin with uniformly bounded in N components J_N^α,

$$J_N^\alpha = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^\alpha \,, \qquad \alpha = x, y, z, \tag{3.31}$$

where σ^α are the standard Pauli matrices.

By using the commutation relations for the spin operators, we obtain the observables

$$R_1(J_N^x) \equiv [\beta\mathcal{H}_N, J_N^x] = 2\mathrm{i}[g_y(J_N^y J_N^z + J_N^z J_N^y) + h_y J_N^z - h_z J_N^y], \tag{3.32}$$

and

$$\begin{aligned} R_2(J_N^x) \equiv [\beta\mathcal{H}_N, R_1(J_N^x)] \quad = \quad & 4g_y(g_y - g_x)(J_N^y J_N^y J_N^x + 2J_N^y J_N^x J_N^y + J_N^x J_N^y J_N^y) \\ & + 4g_x g_y(J_N^z J_N^z J_N^x + 2J_N^z J_N^x J_N^z + J_N^x J_N^z J_N^z) \\ & + 4(g_y - g_x)h_y(J_N^x J_N^y + J_N^y J_N^x) - 4g_x h_z(J_N^x J_N^z + J_N^z J_N^x) \\ & + 4(h_y^2 + h_z^2)J_N^x - 4h_x h_y J_N^y - 4h_x h_z J_N^z\,, \end{aligned} \tag{3.33}$$

which, by definition, have zero average values. Next,

$$\begin{aligned} F_2(J_N^x; J_N^x) \quad & \equiv \quad (R_1(J_N^x); R_1(J_N^x)) = \langle [R_1^+(J_N^x), J_N^x] \rangle \\ & = \quad \frac{4}{N}\left\{2g_y[\langle (J_N^y)^2\rangle - \langle (J_N^z)^2\rangle] + h_y\langle J_N^y\rangle + h_z\langle J_N^z\rangle\right\}, \end{aligned} \tag{3.34}$$

and

$$\begin{aligned} F_3(J_N^x; J_N^x) \quad & \equiv \quad \langle [R_1^+(J_N^x)R_1(J_N^x) + R_1(J_N^x)R_1^+(J_N^x)] \rangle \\ & = \quad \langle [g_y(J^y J^z + J_N^z J_N^y) + h_y J_N^z - h_z J_N^y]^2 \rangle. \end{aligned} \tag{3.35}$$

Rather lengthy but straightforward calculations show that

$$|F_4(J_N^x; J_N^x)| = |\langle [R_2^+(J_N^x), R_1(J_N^x)] \rangle| \leqslant O(N^{-1}). \tag{3.36}$$

One can readily extend the above results and show that for all finite n the following inequalities hold: $|\langle R_n(J_N^x)\rangle| \leqslant ||R_n(J_N^x)|| \leqslant O(1)$, $|F_{2n}(J_N^x; J_N^x)| \leqslant O(N^{-1})$, and $|F_{2n+1}(J_N^x; J_N^x)| \leqslant O(1)$. Thus, conditions (3.24) and, hence, the upper bounds (1)–(3) are fulfilled for the considered model.

4. Systems of matter interacting with Boson fields

4.1. Models and their treatment by the AHM

Here are two examples of models in solid state physics, which belong to this class: (a) The Dicke model of superradiance [25], solved exactly in [26, 27], and by the AHM in [28]. The model has been generalized to include interactions with both electromagnetic field and phonons [29, 30], and to the case of infinitely many modes of the electromagnetic field [31]. A recent review of the thermodynamic properties of the original Dicke model and its generalizations is given in [32]. (b) The Mattis-Langer model of structural instability [33], solved exactly by the AHM in [34]. A class of models, including as a special case the Dicke model, has been considered in the framework of the AHM by Bogoliubov (Jr.) and Plechko [35]. The one-dimensional case with countably infinite set of phonon modes has been solved by means of theta-function integration in [36].

The model Hamiltonian is defined on the tensor product of two Hilbert spaces, one for the subsystem describing matter (e.g., electrons in a solid, spins on a lattice), and the other for the Boson field (lattice vibrations, electromagnetic field). In the second quantization representation, the creation, $b_\mathrm{s}^\dagger$, and annihilation, b_s, operators of the Boson field modes (labeled by the subscript s) satisfy the canonical commutation relations

$$[b_\mathrm{s}, b_l^\dagger] = \delta_{s,l}, \qquad [b_\mathrm{s}, b_l] = [b_\mathrm{s}^\dagger, b_l^\dagger] = 0, \tag{4.1}$$

for all the allowed s and l. Since the Boson operators are unbounded, it is not possible to obtain easy bounds on their average values in terms of Hilbert-space norm.

Another characteristic feature of this class of models is that exact solvability by the AHM is possible when the interaction with only a finite (or growing slower than the volume V, as $V \to \infty$) number of Boson modes is taken into account. The typical model Hamiltonian has the form

$$\mathcal{H}_\Lambda = \mathcal{T}_\Lambda + \sum_{s=1}^{n} \omega_{\rm s}\, b_{\rm s}^\dagger b_{\rm s} + V^{1/2} \sum_{s=1}^{n} \lambda_{\rm s} (b_{\rm s} A_{s,\Lambda}^\dagger + b_{\rm s}^\dagger A_{s,\Lambda}). \tag{4.2}$$

Here the operators $\mathcal{T}_\Lambda = \mathcal{T}_\Lambda^\dagger$ and $A_{s,\Lambda}$, $s = 1, \ldots, n$, refer to the matter subsystem and satisfy the general conditions (2.4) and (2.6). The second term in the right-hand side of (4.2) describes a finite number of free Boson modes, $s = 1, \ldots, n$, in the space domain Λ of volume V. For the sake of simplicity, the energies $\omega_{\rm s} > 0$ and the interaction constants $\lambda_{\rm s} \in R$ are taken to be independent of the volume $|\Lambda|$. The mathematical definition of the above Hamiltonian is given in [37].

The corresponding approximating Hamiltonian depends on a set of complex numbers $\eta = (\eta_1, \ldots, \eta_n) \in \mathbf{C}^n$ and has the form, see [6, 28],

$$\mathcal{H}_\Lambda^{(0)}(\eta) = \sum_{s=1}^{n} \omega_{\rm s}\, \tilde{b}_{\rm s}^\dagger \tilde{b}_{\rm s} + \mathcal{T}_\Lambda - V \sum_{s=1}^{n} (\lambda_{\rm s}^2/\omega_{\rm s})(\eta_{\rm s} A_{s,\Lambda}^\dagger + \eta_{\rm s}^\star A_{s,\Lambda} - \eta_{\rm s}^\star \eta_{\rm s}), \tag{4.3}$$

where

$$\tilde{b}_{\rm s}^\dagger = b_{\rm s}^\dagger + V^{1/2} \frac{\lambda_{\rm s}}{\omega_{\rm s}} \eta_{\rm s}^\star\,, \qquad \tilde{b}_{\rm s} = b_{\rm s} + V^{1/2} \frac{\lambda_{\rm s}}{\omega_{\rm s}} \eta_{\rm s}\,, \tag{4.4}$$

are the creation/annihilation operators for a subsystem of free shifted bosons. The application of the Bogoliubov inequalities to the difference of the free energy densities for the model and approximating Hamiltonians yields

$$f[\mathcal{H}_\Lambda^{(0)}(\eta)] - f[\mathcal{H}_\Lambda] \geqslant 0, \tag{4.5}$$

for all $\eta \in \mathbf{C}^n$. Therefore, the best approximation is reached at $\eta = \bar{\eta}_\Lambda$, where $\bar{\eta}_\Lambda$ satisfies the absolute minimum condition

$$f[\mathcal{H}_\Lambda^{(0)}(\bar{\eta}_\Lambda)] = \min_\eta f[\mathcal{H}_\Lambda^{(0)}(\eta)]. \tag{4.6}$$

Note that the free energy density of the free bosons,

$$f\left[\sum_{s=1}^{n} \omega_{\rm s}\, b_{\rm s}^\dagger b_{\rm s}\right] = \frac{1}{\beta V} \sum_{s=1}^{n} \ln\left(1 - {\rm e}^{-\beta \omega_{\rm s}}\right), \tag{4.7}$$

is independent of the parameters $\eta = (\eta_1, \ldots, \eta_n) \in \mathbf{C}^n$ and vanishes in the thermodynamic limit as $O(V^{-1})$.

The proof of the thermodynamic equivalence of the free energy densities $f[\mathcal{H}_\Lambda^{(0)}(\bar{\eta}_\Lambda)]$ and $f[\mathcal{H}_\Lambda]$ goes again through the introduction of sources of the boson fields,

$$\begin{aligned} \mathcal{H}_\Lambda(\nu) &= \mathcal{H}_\Lambda - V^{1/2} \sum_{s=1}^{n} (\nu_{\rm s}^\star b_{\rm s} + \nu_{\rm s} b_{\rm s}^\dagger), \\ \mathcal{H}_\Lambda^{(0)}(\eta, \nu) &= \mathcal{H}_\Lambda^{(0)}(\eta) - V^{1/2} \sum_{s=1}^{n} (\nu_{\rm s}^\star b_{\rm s} + \nu_{\rm s} b_{\rm s}^\dagger), \end{aligned} \tag{4.8}$$

where $\nu = (\nu_1, \ldots, \nu_n) \in \mathbf{C}^n$.

Now, from the Bogoliubov inequalities and a subsequent use of an elementary upper bound, one obtains

$$\begin{aligned} 0 &\leqslant \min_\eta f[\mathcal{H}_\Lambda^{(0)}(\eta, \nu)] - f[\mathcal{H}_\Lambda(\nu)] \leqslant -V^{-1/2} \sum_{s=1}^{n} \lambda_{\rm s} \langle \delta b_{\rm s} \delta A_{s,\Lambda} + \delta b_{\rm s}^\dagger \delta A_{s,\Lambda} \rangle_{\mathcal{H}_\Lambda(\nu)} \\ &\leqslant V^{-1/2} \sum_{s=1}^{n} V^{-\gamma} \frac{\lambda_{\rm s}^2}{\omega_{\rm s}} \langle \delta A_{s,\Lambda}^\dagger \delta A_{s,\Lambda} \rangle_{\mathcal{H}_\Lambda(\nu)} + V^{-1/2} \sum_{s=1}^{n} V^{\gamma} \omega_{\rm s} \langle \delta b_{\rm s}^\dagger \delta b_{\rm s} \rangle_{\mathcal{H}_\Lambda(\nu)}, \end{aligned} \tag{4.9}$$

where

$$\delta A_{s,\Lambda} = A_{s,\Lambda} - \langle A_{s,\Lambda}\rangle_{\mathcal{H}_\Lambda(\nu)}, \qquad \delta b_{\mathrm{s}} = b_{\mathrm{s}} - \langle b_{\mathrm{s}}\rangle_{\mathcal{H}_\Lambda(\nu)}, \tag{4.10}$$

and $\gamma \in (0,1)$ is a free parameter.

Due to the boundedness of the operators $A_{s,\Lambda}$, $A^\dagger_{s,\Lambda}$, see conditions (2.6), the first sum in the right-hand side of the last inequality (4.9) is bounded from above by

$$V^{-1/2-\gamma} n M_1^2 \max_{\mathrm{s}} (\lambda_{\mathrm{s}}^2/\omega_{\mathrm{s}}). \tag{4.11}$$

The quadratic fluctuations of the boson fields, $\langle \delta b^\dagger_{\mathrm{s}} \delta b_{\mathrm{s}}\rangle_{\mathcal{H}_\Lambda(\nu)}$, are to be majorized by terms proportional to powers of the Bogoliubov-Duhamel inner product

$$(\delta b_{\mathrm{s}}; \delta b_{\mathrm{s}})_{\mathcal{H}_\Lambda(\nu)} = -\frac{1}{\beta}\frac{\partial^2 f[\mathcal{H}_\Lambda(\nu)]}{\partial \nu_{\mathrm{s}} \partial \nu^\star_{\mathrm{s}}}\,. \tag{4.12}$$

By using the Ginibre inequality (2.33) and choosing $\gamma = 1/3$ in (4.9), the subsequent application of the majorization technique due to Bogoliubov Jr. with the following bounds on the first derivatives ($s = 1,\dots,n$)

$$\left|\frac{\partial f[\mathcal{H}_\Lambda(\nu)]}{\partial \nu^{\#}_{\mathrm{s}}}\right| = V^{-1/2}|\langle b^{\#}_{\mathrm{s}}\rangle_{\mathcal{H}_\Lambda(\nu)}| = \omega_{\mathrm{s}}^{-1}|\lambda_{\mathrm{s}}\langle A^{\#}_{s,\Lambda}\rangle_{\mathcal{H}_\Lambda(\nu)} - \nu^{\#}_{\mathrm{s}}| \leqslant \omega_{\mathrm{s}}^{-1}(\lambda_{\mathrm{s}} M_1 + |\nu^{\#}_{\mathrm{s}}|), \tag{4.13}$$

made it possible to prove that

$$|\min_\eta f[\mathcal{H}^{(0)}_\Lambda(\eta)] - f[\mathcal{H}_\Lambda]| \leqslant \epsilon_V, \tag{4.14}$$

where $\epsilon_V = O(V^{-1/3}) \to 0$ as $V \to \infty$. Under additional conditions on the double commutators between the different $\{A^{\#}_{s,\Lambda} : s = 1,\dots,n\}$ and on the commutator of $R_1(A^{\#}_{s,\Lambda})$ with $A^{\#}_{s',\Lambda}$, the above estimate was improved up to $\epsilon_V = O(V^{-1/2})$ [7].

4.2. Application of the generalized inequalities to the Dicke model

In the remainder, by using the equality [14, 22]:

$$\beta(X; [\mathcal{H}, B])_{\mathcal{H}} = \langle [X^\dagger, B]\rangle_{\mathcal{H}}\,, \tag{4.15}$$

we shall derive a variety of explicit relationships between Bogoliubov-Duhamel inner products and usual thermal averages for different observables of the basic single-mode Dicke model in the rotating wave approximation. In the latter case, the Hamiltonian has the form (4.2) with $n = 1$,

$$T = \frac{1}{2}\epsilon\sum_{j=1}^{N}\sigma^z_j\,, \qquad A = \frac{1}{V}\sum_{j=1}^{N}\sigma^+_j\,, \qquad A^\dagger = \frac{1}{V}\sum_{j=1}^{N}\sigma^-_j\,, \tag{4.16}$$

where $\sigma^\pm_j = \frac{1}{2}(\sigma^x_j \pm \mathrm{i}\sigma^y_j)$ and σ^z_j are the Pauli matrices. From the above definitions the following commutation relations follow

$$[T, A] = \epsilon A, \qquad [A^\dagger, A] = \frac{2}{\epsilon V^2}T. \tag{4.17}$$

By direct computation we obtain

$$R_1(b) \equiv [H, b] = -(\omega b + V^{1/2}\lambda A), \tag{4.18}$$

and, since $\langle [H, b]\rangle_{\mathcal{H}} = 0$, we obtain a well known equality between average values of observables pertaining to different subsystems (boson field and matter):

$$\langle b\rangle_{\mathcal{H}} = -V^{1/2}\frac{\lambda}{\omega}\langle A\rangle_{\mathcal{H}}\,. \tag{4.19}$$

Therefore, in the case of non-vanishing polarization in the matter subsystem, $\langle A\rangle_{\mathcal{H}} \neq 0$, the average value of the boson annihilation (as well as creation) operator will behave as $\langle b\rangle_{\mathcal{H}} = O(V^{1/2})$. Hence, we deduce that the unbounded counterpart of the observable J_N in conditions (3.24) should be the normalized operator $V^{-1/2}b$. Keeping this in mind, we further calculate

$$R_2(V^{-1/2}b) \equiv [H, R_1(V^{-1/2}b)] = \omega^2 V^{-1/2}b + \lambda(\omega-\epsilon)A - \frac{2\lambda^2}{\epsilon V^{3/2}}bT, \tag{4.20}$$

and

$$\begin{aligned} F_2(V^{-1/2}b; V^{-1/2}b) &= \beta\langle [R_1(V^{-1/2}b)^\dagger, V^{-1/2}b]\rangle_{\mathcal{H}} = \frac{\beta\omega}{V}\,, && (4.21)\\ F_3(V^{-1/2}b; V^{-1/2}b) &\equiv \beta^2\langle R_1^\dagger(V^{-1/2}b)R_1(V^{-1/2}b) + R_1(V^{-1/2}b)R_1^\dagger(V^{-1/2}b)\rangle_{\mathcal{H}} \\ &= (\beta\omega)^2\left[V^{-1}\langle b^\dagger b + bb^\dagger\rangle_{\mathcal{H}} + V^{-1/2}\frac{\lambda}{\omega}\langle b^\dagger A + bA^\dagger\rangle_{\mathcal{H}} + \frac{\lambda^2}{\omega^2}\langle A^\dagger A + AA^\dagger\rangle_{\mathcal{H}}\right], && (4.22)\\ F_4(V^{-1/2}b; V^{-1/2}b) &= \beta^3\langle [R_2^\dagger(V^{-1/2}b), R_1(V^{-1/2}b)]\rangle_{\mathcal{H}} \\ &= \frac{(\beta\omega)^3}{V}\left[1 + \frac{2\lambda^2}{\epsilon\omega^2 V}\left(\frac{\epsilon}{\omega} - 2\right)\langle T\rangle_{\mathcal{H}} + \frac{2\lambda^3}{\omega^3 V^{1/2}}\langle b^\dagger A\rangle_{\mathcal{H}}\right]. && (4.23) \end{aligned}$$

The right-hand side of these expressions can be evaluated using some relationships between average values of different observables which follow from (4.15). Thus, by setting $B = b$ and $X = b$, we obtain,

$$(b; b)_{\mathcal{H}} = \frac{1}{\beta\omega} - V^{1/2}\frac{\lambda}{\omega}(b; A)_{\mathcal{H}}\,. \tag{4.24}$$

Next, from $B = b$ and $X = A$ it follows that

$$-\,(A; b)_{\mathcal{H}} = V^{1/2}\frac{\lambda}{\omega}(A; A)_{\mathcal{H}}\,. \tag{4.25}$$

Under the alternative choice $B = b^\dagger$ and $X = b^\dagger$ in (4.15), we derive

$$(b^\dagger; b^\dagger)_{\mathcal{H}} = \frac{1}{\beta\omega} - V^{1/2}\frac{\lambda}{\omega}(b^\dagger; A^\dagger)_{\mathcal{H}}\,, \tag{4.26}$$

which, due to the conjugate symmetry $(A; B) = (B^\dagger; A^\dagger)$, is equivalent to

$$(b; b)_{\mathcal{H}} = \frac{1}{\beta\omega} - V^{1/2}\frac{\lambda}{\omega}(A; b)_{\mathcal{H}}\,. \tag{4.27}$$

By comparing this equality with (4.24) we conclude that $(b; A)_{\mathcal{H}} = (A; b)_{\mathcal{H}}$. Then, taking into account (4.25) we derive the important relation

$$(b; b)_{\mathcal{H}} = \frac{1}{\beta\omega} + V\frac{\lambda^2}{\omega^2}(A; A)_{\mathcal{H}}\,, \tag{4.28}$$

which was obtained in [32] using gage invariance arguments.

Proceeding further with the evaluation of (4.22) and (4.23), we note that since the right-hand side of (4.23) is real, one must have

$$\langle b^\dagger A\rangle_{\mathcal{H}} = \langle bA^\dagger\rangle_{\mathcal{H}}\,. \tag{4.29}$$

Therefore, the application of the Schwarz inequality and the relation (4.28) yield the estimate

$$|\langle V^{-1/2}b^\dagger A\rangle_{\mathcal{H}}| = \langle V^{-1/2}bA^\dagger\rangle_{\mathcal{H}}| \leqslant \langle V^{-1}b^\dagger b\rangle_{\mathcal{H}}^{1/2}|\langle AA^\dagger\rangle_{\mathcal{H}}^{1/2}| \leqslant O(1). \tag{4.30}$$

Finally, the application of the Harris inequality (2.30) in terms of b gives

$$(b;b)_{\mathcal{H}} \leqslant \langle b^{\dagger}b\rangle_{\mathcal{H}} + \frac{1}{2} \leqslant (b;b)_{\mathcal{H}} + \frac{1}{12}\beta\omega\,, \tag{4.31}$$

which, in view of (4.28), implies $\langle b^{\dagger}b\rangle_{\mathcal{H}} = O(V)$, provided that $(A;A)_{\mathcal{H}} = O(1)$. Taking into account $||A|| = O(1)$ and $||T|| = O(V)$, we conclude that $F_2(V^{-1/2}b;V^{-1/2}b)$ and $F_4(V^{-1/2}b;V^{-1/2}b)$ are bounded from above by $O(V^{-1})$, while $|F_3(V^{-1/2}b;V^{-1/2}b)| \leqslant O(1)$.

Thus, we have proved that $V^{-1/2}b$ and $F_n(V^{-1/2}b;V^{-1/2}b)$ for $n = 2,3,4$ satisfy conditions (3.24). Therefore, bounds of the form (3.25), (3.27), and (3.28) hold true at $n = 1$ even for the unbounded operator $J_V = V^{-1/2}b$.

5. Discussion

The AHM makes it possible to rigorously obtain the exact thermodynamic properties of diverse classes of model systems in quantum statistical mechanics. Each class of models requires a certain structure of the interaction Hamiltonian and special properties of the operators in terms of which its structure is defined. Initially, the mathematical technique for derivation of bounds which prove the thermodynamic equivalence of the approximating and original Hamiltonians has been developed for systems with interaction Hamiltonians constructed with bounded operators (see section 2). Later, it was extended to the case of unbounded Bose operators (see section 4). This technique essentially exploits the possibility of estimating the correlation functions in (2.14) or (4.9) from above by expressions containing the Bogoliubov-Duhamel inner product in combination with average values of certain operators. As a rule, the latter are estimated by norm, which requires conditions (2.4)–(2.8). It is well known that this procedure is not unique [7, 8]. The distinction comes from the different inequalities used. At first, it was Bogoliubov's Jr. inequality that was used in the case of bounded operators. Latter it was realized that Ginibre's inequality (2.33) is more convenient to be used, especially in the case of interactions involving Bose operators [7], see also section 4. Moreover, it made it possible to derive a better estimate, namely $O(|\Lambda|^{-1/2})$, in both cases of bounded and unbounded operators [6–8]. However, in the latter case, two additional sufficient conditions have been imposed.

The interest that stimulates the search and use of different inequalities was prompted by the wish to improve the upper bounds on the difference of the model and approximating free energy densities and/or to enlarge the class of model systems rigorously solved by the AHM [21, 23]. In section 3, we have derived generalizations of the inequalities introduced in [21] and [23]. The novel point is that a set of new functionals $F_k(J;J)$, $k = 0,1,2,\ldots$, were defined by their spectral representation (3.1). This made it possible to obtain different upper bounds in a unified fashion.

Beyond the use in the majorization step of the AHM, our new upper bounds (3.25)–(3.29) on the difference between the Gibbs average values of a class of observables of a many-particle system and the corresponding Bogoliubov-Duhamel inner products may find wider applications. Under sufficiently mild conditions, these upper bounds have the same form and order of magnitude with respect to the number of particles (or volume) for all the quantities derived by a finite number of commutations $R_n(J)$ of an original intensive observable J with the Hamiltonian of the system $\mathcal{H}$.

In addition, we have obtained important relationship between average values of the different observables in the framework of two types of exactly solved by the AHM model systems: one with bounded separable attraction – the infinitely coordinated anisotropic Heisenberg model, and the other, the Dicke superradiance model, describing interaction of a boson field with a subsystem of matter.

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Узагальнені нерівності для внутрішнього добутку Боголюбова-Дюамеля із застосуваннями в методі апроксимуючого гамільтоніану

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Отримано нескінченні набори нерівностей, які узагальнюють всі відомі нерівності, що можуть бути використані на етапі мажорування методу апроксимуючого гамільтоніану Вони забезпечують верхні границі на різницю між квадратичними флуктуаціями інтенсивних спостережуваних N-частинкової системи і відповідного внутрішнього добутку Боголюбова-Дюамеля. Новою рисою є те, що при достатньо м'яких умовах верхні границі мають однакову форму і порядок величини по відношенню до N для всіх величин, отриманих шляхом скінченного числа перестановок початкової інтенсивої спостережуваної з гамільтоніаном. Результати ілюструються на двох типах точно розв'язуваних моделей: однієї з обмеженим сепарабельним притяганням та іншої, що містить взаємодію бозонного поля з матерією.

Ключові слова: *кореляційні функції, внутрішній добуток Боголюбова-Дюамеля, нерівності статистичної механіки, метод апроксимуючого гамільтоніану, точно розв'язувані моделі*