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A. Brooks Harris

University of Pennsylvania, harris@sas.upenn.edu

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Recommended Citation

Harris, A. (1967). Bounds for Certain Thermodynamic Averages. *Journal of Mathematical Physics*, 8 (5), 1044-1045. <http://dx.doi.org/10.1063/1.1705312>

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Bounds for Certain Thermodynamic Averages

Abstract

Upper and lower bounds for thermodynamic averages of the form $\langle \{A, A^\dagger\} \rangle$ are presented.

Disciplines

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Comparing this with Eq. (21), we see that diffusion theory gives only a discrete term and this term compares favorably with exact theory only when absorption is weak for $z < 0$. The exact result contains an additional continuous term which is expected to contribute strongly to the flux near the interface.

VII. REMARKS

Based on this and previous work, it is now certain that any half-space problems in mono-energetic transport theory with isotropic scattering can be solved exactly if the mean free path is spatially invariant. Since the kernel that results when this last

restriction is relaxed is quite complicated, it is not expected that the analytical method used above will be successful in the more general, unrestricted cross-section, problem. An analysis based on the differential form of the Boltzmann equation may be required before this problem can be done exactly. However, one may be able to approximate the solution to the more general problem by following the suggestions given in Ref. 6 on degenerate kernels. Work is now proceeding along this line. Some numerical work is also being done using the results of this paper.

⁶ L. V. Kantorovich and V. I. Krylov, *Approximate Methods of Higher Analysis* (Interscience Publishers, Inc., New York, 1958).

Bounds for Certain Thermodynamic Averages*

A. BROOKS HARRIS

Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania

(Received 12 November 1966)

Upper and lower bounds for thermodynamic averages of the form $\langle\{A, A^\dagger\}\rangle$ are presented.

THE purpose of this brief note is to present bounds for thermodynamic averages of the form $\langle\{A, A^\dagger\}\rangle$. From the lower bound we can derive a special case of the Bogoliubov¹ inequality. Our lower bound when applied to the one- and two-dimensional isotropic Heisenberg magnet² yields the same result as found by Mermin and Wagner.³ Explicitly our lower bound is

$$\langle\{A, A^\dagger\}\rangle \geq \langle[A, A^\dagger]\rangle \coth(\tfrac{1}{2}\beta\langle\omega\rangle), \quad (1)$$

where $\langle\omega\rangle$ is an average frequency computed from sum rules as described below. An upper bound for $\langle\{A, A^\dagger\}\rangle$ is given by Eq. (19) below.

The derivation of Eq. (1) is elementary. Let n label the eigenstates of $\hat{\mathcal{H}} \equiv \mathcal{H} - \mu N$, where $\mathcal{H}$ is the Hamiltonian, μ the chemical potential, and N the number operator (for simplicity we assume a homoge-

neous system), so that

$$\hat{\mathcal{H}}|n\rangle = \hat{E}_n|n\rangle. \quad (2)$$

Using a grand canonical ensemble one has

$$\langle A^\dagger A \rangle = \sum_{mn} W_m \langle m|A^\dagger|n\rangle \langle n|A|m\rangle, \quad (3)$$

where

$$W_m = e^{-\beta\hat{E}_m} / \sum_n e^{-\beta\hat{E}_n}. \quad (4)$$

Equation (3) may be manipulated to give

$$\langle A^\dagger A \rangle = \beta^{-1} \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n|A|m\rangle|^2 \frac{\beta(\hat{E}_m - \hat{E}_n)}{e^{\beta(\hat{E}_m - \hat{E}_n)} - 1}. \quad (5)$$

Define $\varphi(x) = x/(e^x - 1)$, in which case Eq. (5) is of the form

$$\langle A^\dagger A \rangle = \beta^{-1} \sum_i p(x_i) \varphi(\beta x_i), \quad (6)$$

where

$$p(x_i) = \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n|A|m\rangle|^2 \delta_{x_i, \hat{E}_m - \hat{E}_n}, \quad (7)$$

where δ_{x_i, x_j} is a Kronecker delta. From (7) one sees that $p(x)$ is nonnegative and one can easily verify that

* Supported in part by the Advanced Research Projects Agency. This paper is a contribution of the Laboratory for Research on the Structure of Matter, University of Pennsylvania.

¹ N. N. Bogoliubov, Phys. Abhandl. SU6, 1, 113, 229 (1962); see also Ref. 3.

² The proof that the spontaneous magnetization for these systems vanishes for nonzero temperature is similar to that found in Ref. 3. We obtained the same upper bounds for the low-field magnetization as in Ref. 3.

³ N. D. Mermin and H. Wagner, Phys. Rev. Letters 17, 1133 (1966).

$\varphi(x)$ is convex, i.e., $d^2\varphi/dx^2 \geq 0$. Under these conditions one can easily show that

$$\sum_i p(x_i) \varphi(\beta x_i) \geq \varphi(\beta \langle x \rangle) \sum_i p(x_i), \quad (8)$$

where

$$\langle x \rangle = \sum_i p(x_i) x_i / \sum_i p(x_i). \quad (9)$$

Applying Eq. (8) to the case of Eq. (5), we obtain

$$\langle A^\dagger A \rangle \geq \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n | A | m \rangle|^2 \frac{\langle \omega \rangle}{e^{\beta \langle \omega \rangle} - 1}, \quad (10)$$

where

$$\langle \omega \rangle = \frac{\sum_{nm} (W_n - W_m) |\langle n | A | m \rangle|^2}{\sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n | A | m \rangle|^2}. \quad (11)$$

Combining Eqs. (10) and (11) we find

$$\langle A^\dagger A \rangle \geq \langle [A, A^\dagger] \rangle / (e^{\beta \langle \omega \rangle} - 1), \quad (12)$$

from which Eq. (1) follows immediately.

It is interesting to note that Eq. (1) can be weakened to give (a) more tractable results and (b) a special case of the Bogoliubov¹ inequality. We note that $\langle \omega \rangle$ as defined by Eq. (11) may not be a convenient quantity since the denominator is not so easy to handle.⁴ However, by the Cauchy-Schwarz inequality $\langle \omega \rangle^2 \leq \langle \omega^2 \rangle$ so that the inequality (12) remains valid when $\langle \omega \rangle$ is replaced by $\langle \omega^* \rangle \equiv \langle \omega^2 \rangle / \langle \omega \rangle$ since $\langle [A, A^\dagger] \rangle$, $\langle \omega \rangle$, and $\langle \omega^* \rangle$ all have the same algebraic sign. This is easily seen by writing

$$\langle \omega \rangle = \sum_i x_i p(x_i) / \sum_i p(x_i), \quad (13a)$$

$$\langle \omega^* \rangle \equiv \frac{\langle \omega^2 \rangle}{\langle \omega \rangle} = \sum_i x_i^2 p(x_i) / \sum_i x_i p(x_i), \quad (13b)$$

$$\langle [A, A^\dagger] \rangle = \sum_i x_i p(x_i), \quad (13c)$$

and using the nonnegativity of $p(x)$. Equation (13b) can be written as

$$\langle \omega^* \rangle = \frac{\sum_{nm} (W_n - W_m)(\hat{E}_m - \hat{E}_n) |\langle n | A | m \rangle|^2}{\sum_{nm} (W_n - W_m) |\langle n | A | m \rangle|^2}, \quad (14a)$$

or simply as

$$\langle \omega^* \rangle = \frac{\langle [[A, \hat{\mathcal{H}}], A^\dagger] \rangle}{\langle [A, A^\dagger] \rangle} \quad (14b)$$

Thus a weaker but possibly more convenient inequality than (1) is

$$\langle \{A, A^\dagger\} \rangle \geq \langle [A, A^\dagger] \rangle \coth(\frac{1}{2}\beta \langle \omega^* \rangle). \quad (15)$$

⁴ The denominator in Eq. (12) is rather convenient, but a sharper use of the Cauchy-Schwarz inequality shows that this denominator can be replaced by $\sum_{nm} |W_n - W_m| |\langle n | A | m \rangle|$.

But $|\coth x| \geq |1/x|$ so that a still weaker inequality is

$$\frac{1}{2} \langle \{A, A^\dagger\} \rangle \geq kT \langle [A, A^\dagger]^2 \rangle / \langle [[A, \hat{\mathcal{H}}], A^\dagger] \rangle, \quad (16)$$

where we have used Eq. (14). The Bogoliubov inequality¹ may be written as

$$\frac{1}{2} \langle \{A, A^\dagger\} \rangle \geq kT |\langle [C, A] \rangle|^2 / \langle [[C^\dagger, \hat{\mathcal{H}}], C] \rangle, \quad (17)$$

which is identical to Eq. (16) for the special case of $C = A^\dagger$. The reason the inequality (15) gives the same upper bound for the low-field magnetization of one- and two-dimension Heisenberg magnets as Mermin and Wagner found³ using the Bogoliubov¹ inequality is that the dominant contribution to the magnetization comes from low-energy excitations in which

$$\lim_{\omega \rightarrow 0} \coth(\frac{1}{2}\beta\omega) \approx (\frac{1}{2}\beta\omega)^{-1},$$

so that nothing is lost in going from Eq. (15) to Eq. (16).

Finally an upper bound for $\langle \{A, A^\dagger\} \rangle$ is obtained as follows. We may write

$$\langle \{A, A^\dagger\} \rangle = \sum_{nm} (W_m + W_n) |\langle n | A | m \rangle|^2 \quad (18a)$$

$$= \frac{2}{\beta} \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n | A | m \rangle|^2 \times \left\{ \frac{W_n + W_m}{W_n - W_m} \right\} \frac{\beta(\hat{E}_m - \hat{E}_n)}{2}. \quad (18b)$$

But

$$\left\{ \frac{W_n + W_m}{W_n - W_m} \right\} \frac{\beta(\hat{E}_m - \hat{E}_n)}{2} = \frac{\beta(\hat{E}_m - \hat{E}_n)}{2} \coth \frac{\beta(\hat{E}_m - \hat{E}_n)}{2} \quad (19a)$$

$$\leq 1 + \frac{1}{3} (\frac{1}{2}\beta)^2 (\hat{E}_m - \hat{E}_n)^2 \quad (19b)$$

so that

$$\langle \{A, A^\dagger\} \rangle \leq \frac{2}{\beta} \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n | A | m \rangle|^2 \times \left(1 + \frac{\beta^2}{12} (\hat{E}_m - \hat{E}_n)^2 \right) \quad (20a)$$

$$\leq \frac{2}{\beta} \sum_{nm} \frac{W_n - W_m}{\hat{E}_m - \hat{E}_n} |\langle n | A | m \rangle|^2 + \frac{\beta}{6} \langle [[A, \hat{\mathcal{H}}], A^\dagger] \rangle. \quad (20b)$$

Taking $A = [B, \hat{\mathcal{H}}]$ would enable one to eliminate the energy denominators, since $\langle n | A | m \rangle = \langle n | B | m \rangle \times (\hat{E}_m - \hat{E}_n)$; however, the commutators are slightly more tedious to evaluate.

ACKNOWLEDGMENT

The author would like to thank Professor J. R. Schrieffer for calling attention to the pre-published work of Mermin and Wagner.