Susceptibility and Fluctuation

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Bounds are presented relating zero-field static isothermal magnetic susceptibilities to the mean-square fluctuations of corresponding magnetization variables. The lower bounds contain the first frequency moment of a spectral density. When this moment $\bar{\omega}$ approaches zero, the upper and lower bounds merge, and the susceptibility is determined by the mean-square fluctuation. In particular, if the susceptibility diverges at a temperature T_c, and if the expectation of the double commutator appearing in $\bar{\omega}$ is finite at and near T_c, then the fluctuation and the susceptibility diverge in the same manner, and their critical exponents will be identical.

INTRODUCTION

We present upper and lower bounds for the zero-field isothermal magnetic susceptibility and for a generalized wave-number-dependent susceptibility. These are a generalization of equations between the susceptibility and fluctuation beyond the case where magnetization operators commute with the zero-field Hamiltonian. The bounds are expressed in terms of the mean-square fluctuations in the magnetization variables and the first frequency moment of a spectral density. When this moment $\bar{\omega}$ approaches zero, the upper and lower bounds merge, and the susceptibility is determined by the mean-square fluctuation. In particular, if the susceptibility diverges at a temperature T_c, and if the expectation of the double commutator appearing in $\bar{\omega}$ is finite[1] at and near T_c, then the fluctuation and the susceptibility diverge in the same manner and their critical exponents[2] will be identical.

DEFINITIONS AND PRINCIPAL RESULTS

The zero-field isothermal magnetic susceptibility is defined by the limit equation

$$X_T = \partial\langle M\rangle_h/\partial h|_{h\to 0+}, \qquad (1)$$

where the ensemble average of the magnetization is defined by

$$\langle M\rangle_h = \mathrm{Tr}[Me^{-\beta(H_0-hM)}]/\mathrm{Tr}[e^{-\beta(H_0-hM)}], \qquad (2)$$

and H_0-hM is the Hamiltonian for the system in an external magnetic field h.

These definitions yield[3] the following formula for X_T:

$$X_T = \int_0^\beta d\lambda\langle\Delta M(\lambda)\Delta M\rangle_0, \qquad (3)$$

where

$$\Delta M = M - \langle M\rangle_0;\quad \Delta M(\lambda) = e^{\lambda H_0}\Delta M e^{-\lambda H_0};\quad \beta^{-1} = k_BT. \qquad (4)$$

The zero-field expectation value is defined for a general operator A by

$$\langle A\rangle_0 = \mathrm{Tr}(e^{-\beta H_0}A)/\mathrm{Tr}e^{-\beta H_0}. \qquad (5)$$

If M commutes with H_0, Eq. (3) shows that $\beta^{-1}X_T = \langle(\Delta M)^2\rangle_0$, the mean-square fluctuation of the magnetization.

An extension of this result to the static susceptibility for the spatial Fourier components A_k of an inhomogeneous disturbance is[4]

$$X_T(A_k,A_k^\dagger) \equiv \int_0^\beta d\lambda\langle e^{\lambda H_0}\Delta A_k e^{-\lambda H_0}\Delta A_k^\dagger\rangle_0 = X_T(A_k^\dagger,A_k), \qquad (6)$$

where the notation of Eqs. (4) and (5) has been used and $A_k^\dagger$ is the Hermitian conjugate of A_k.

Since Eq. (6) clearly reduces to Eq. (3) for the special case where A_k is the Hermitian operator M, we present our bounds for the more general quantity $X_T(A_k^\dagger,A_k)$.

In terms of the anticommutator $\{\cdots,\cdots\}$ define

$$S^{(0)} = \tfrac{1}{2}\langle\{\Delta A_k,\Delta A_k^\dagger\}\rangle_0. \qquad (7)$$

The principal results derived here are

$$(1-\exp[-\tfrac{1}{2}\beta\bar{\omega}_k])/\tfrac{1}{2}\beta\bar{\omega}_k \leqslant (\tanh\bar{y}_k)/\bar{y}_k \leqslant (\beta S^{(0)})^{-1}X_T(A_k,A_k^\dagger) \leqslant 1, \qquad (8)$$

where $\bar{\omega}_k$, the first moment of a spectral density, is defined by

$$\bar{\omega}_k = \langle[\Delta A_k,[H_0,\Delta A_k^\dagger]_-]_-\rangle_0/\langle\{\Delta A_k,\Delta A_k^\dagger\}\rangle_0 \qquad (9)$$

and is non-negative; $\bar{y}_k$ is the (positive or negative)

[1] The work of N. D. Mermin and H. Wagner, [Phys. Rev. Letters **17**, 1133 (1966)], establishes that the expectation of the relevant double commutator is bounded for the class of one-, two-, and three-dimensional, isotropic, spin-S Heisenberg models with finite-range exchange interaction [$\sum_{\mathbf{R}} R^2|J(\mathbf{R})|$ finite].

[2] We thank Professor M. E. Fisher for this statement of our results following our summary of this work at the Yeshiva University Statistical Mechanics Meeting on December 2, 1968.

[3] See, e.g., H. Falk, Phys. Rev. **165**, 602 (1968), especially Sec. III.

[4] See, e.g., H. Mori and K. Kawasaki, Progr. Theoret. Phys. (Kyoto) **27**, 529 (1962).

root of the transcendental equation

$$y_k \tanh y_k = \tfrac{1}{2}\beta\bar{\omega}_k. \tag{10}$$

Luttinger[5] and Josephson[6] have derived the upper bound in Eq. (8), and for density-density correlations in a fluid, Luttinger has also presented a weaker lower bound analogous to the weaker lower bound in Eq. (8). It is also noteworthy that Harris[7] has given an upper bound for $\langle\{A_k,A_k^\dagger\}\rangle_0$ and by rearranging terms, one obtains from it a lower bound for $\beta^{-1}X_T(A_k,A_k^\dagger)$. Harris's lower bound approaches the stronger of the lower bounds in this paper from below as $\beta\bar{\omega}_k \to 0$. For completeness, in Appendix A, we sketch a derivation of the upper bound and the weaker of the two lower bounds in Eq. (8). In Appendix B, we derive our stronger lower bound.

The bounds given in Eq. (8) provide quite general upper and lower bounds for the isothermal susceptibility at all temperatures. Of particular interest, is the critical region where the wave-number-dependent susceptibility is observed[8] to become very large for k near zero (ferromagnets) and for k near k_0 (antiferromagnets). On the other hand, the numerator in Eq. (9) has been shown[1] to be bounded for a large class of systems with finite-range interaction. Thus the ratio may be very close to zero in the critical region and the bounds may merge. Fisher[2] has pointed out that the merging of the bounds as $T \to T_c$ implies that the critical exponents for the fluctuation and the susceptibility will be identical.

The Heisenberg model provides an example for which the numerator in Eq. (9) becomes zero at $k=0$, since the total magnetization is conserved. Alternatively, the numerator can be expressed as the (zero-time) rate of change of correlation of fluctuation. The slowing down of fluctuations near the critical temperature for the Heisenberg Hamiltonian has been discussed by other workers,[4] and suggests that the numerator in Eq. (9) may become small as $T \to T_c$.

In conclusion, we mention that the technique applied by Wilcox[9] to obtain off-diagonal tensor generalizations of diagonal susceptibility bounds, would also apply to the results given here.

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[5] J. M. Luttinger, Progr. Theoret. Phys. (Kyoto) Suppl. **37**, 35 (1966).
[6] B. D. Josephson, Proc. Phys. Soc. (London) **92**, 269 (1967).
[7] A. B. Harris, J. Math. Phys. **8**, 1044 (1967), Eq. (20b).
[8] M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967); P. Heller, *ibid.* **30**, 731 (1967).
[9] R. M. Wilcox, Phys. Rev. **174**, 624 (1968).

APPENDIX A

Define the function

$$K(\lambda) \equiv \tfrac{1}{2}\langle e^{\lambda H_0}\Delta A_k e^{-\lambda H_0}\Delta A_k^\dagger\rangle_0 + \tfrac{1}{2}\langle e^{\lambda H_0}\Delta A_k^\dagger e^{-\lambda H_0}\Delta A_k\rangle_0. \tag{A1}$$

The susceptibility can then be written

$$X_T(A_k,A_k^\dagger) = \int_0^\beta d\lambda\, K(\lambda) = 2\int_0^{\beta/2} d\lambda\, K(\lambda). \tag{A2}$$

In the range of integration $0 \leqslant \lambda \leqslant \beta/2$, $K(\lambda)$ has a negative first derivative and a positive second derivative. Its maximum value is at $\lambda=0$. This last property establishes the upper bound

$$\beta^{-1}X_T(A_k,A_k^\dagger) \leqslant \tfrac{1}{2}\langle\{\Delta A_k,\Delta A_k^\dagger\}\rangle_0. \tag{A3}$$

To obtain the weaker lower bound in Eq. (8), an expression for X in terms of a spectral density is used[10]:

$$\begin{aligned} X_T(A_k,A_k^\dagger) &= \int_{-\infty}^{\infty} d\omega S_k(\omega)(1-e^{-\beta\omega})/\omega \\ &= \int_{-\infty}^{\infty} d\omega S_k(\omega)(1-e^{-\beta\omega/2})/\tfrac{1}{2}\omega. \end{aligned} \tag{A4}$$

Using eigenstates of H_0, one obtains for the spectral density

$$S_k(\omega) = \tfrac{1}{2}\sum_{ij}\delta[\omega-(E_i-E_j)](|\langle i|\Delta A_k|j\rangle|^2 + |\langle i|\Delta A_k^\dagger|j\rangle|^2)e^{-\beta E_j}/\mathrm{Tr}e^{-\beta H_0} \tag{A5}$$

and it has an integral

$$\int_{-\infty}^{\infty} d\omega\, S_k(\omega) = \tfrac{1}{2}\langle\{\Delta A_k,\Delta A_k^\dagger\}\rangle_0. \tag{A6}$$

The quantity $(1-e^{-y})/y$ is a convex, nonincreasing, non-negative function of y; the convexity yields a lower bound for an average of the function

$$\langle(1-e^{-\beta\omega/2})/\tfrac{1}{2}\beta\omega\rangle_{(k)} \equiv \left[\int_{-\infty}^{\infty} d\omega S_k(\omega)\frac{(1-e^{-\beta\omega/2})}{\tfrac{1}{2}\beta\omega}\right] \Big/ \int_{-\infty}^{\infty} d\omega' S_k(\omega') \geqslant (1-e^{-\beta\bar{\omega}_k/2})/\tfrac{1}{2}\beta\bar{\omega}_k. \tag{A7}$$

The frequency $\bar{\omega}_k$ is defined as the first frequency moment of $S_k(\omega)$

$$\begin{aligned} \bar{\omega}_k \equiv \langle\omega\rangle_{(k)} &= \int_{-\infty}^{\infty} d\omega S_k(\omega)\omega \Big/ \int_{-\infty}^{\infty} d\omega' S_k(\omega') \\ &= \langle[\Delta A_k,[H_0,\Delta A_k^\dagger]_-]_-\rangle_0/\langle\{\Delta A_k,\Delta A_k^\dagger\}\rangle_0 \\ &= d\ln K(\lambda)/d\lambda|_{\lambda=0}. \end{aligned} \tag{A8}$$

[10] W. Brenig, Z. Physik **206**, 212 (1967); his Eq. (11) is used to obtain the final equality in (A4).

The weaker lower bound in Eq. (8) then follows by use of Eqs. (A4)–(A8). The non-negative property of $\bar{\omega}_k$ may be verified by expanding the commutators in eigenstates of H_0.

APPENDIX B

Moment Problem for the Spectral Function

Given two moments of the spectral function $S(\omega)$,

$$S^{(0)}=\int_{-\infty}^{\infty} d\omega S(\omega)\,, \tag{B1}$$

$$\bar{\omega}S^{(0)}\equiv S^{(1)}=\int_{-\infty}^{\infty} d\omega\omega S(\omega)\,, \tag{B2}$$

the problem is to find the extreme values of

$$X_T=\int_{-\infty}^{\infty} d\omega S(\omega)[(1-e^{-\beta\omega})/\omega]. \tag{B3}$$

The spectral function is to be non-negative and is to satisfy the symmetry relation

$$S(-\omega)=e^{-\beta\omega}S(\omega). \tag{B4}$$

$X_T{}^t$ will be calculated for a trial spectral function [compare with the general expression Eq. (A5)]

$$S_t(\omega)=B\delta(\omega)+\sum_i A_i[\delta(\omega-x_i)+e^{\omega}\delta(\omega+x_i)]. \tag{B5}$$

The sum may contain any number of terms and energies are now given in units of k_BT. It is convenient to change the non-negative coefficients A_i to new non-negative variables a_i:

$$a_i=A_ix_i(1-e^{-x_i}). \tag{B6}$$

Then Eqs. (B1)–(B3) become

$$S^{(0)}=B+\sum_i a_i(\coth\tfrac{1}{2}x_i)/x_i\,, \tag{B7}$$

$$\bar{\omega}S^{(0)}=\sum_i a_i\,, \tag{B8}$$

$$\beta^{-1}X_T{}^t=B+2\sum_i a_ix_i^{-2}. \tag{B9}$$

With a new non-negative variable B defined as $B=B/S^{(0)}$ and positive weight factors p_i defined by

$$p_i=a_i/\sum_j a_j\,, \tag{B10}$$

Eqs. (B7)–(B9) reduce to a pair of equations

$$1=B+\bar{\omega}\sum_i p_i(\coth\tfrac{1}{2}x_i)/x_i\,, \tag{B11}$$

$$(\beta S^{(0)})^{-1}X_T{}^t=B+2\bar{\omega}\sum_i p_ix_i^{-2}. \tag{B12}$$

The problem is thus to find the distribution of p_i and x_i which extremizes Eq. (B12) with B non-negative. Equation (B12) becomes

$$(\beta S^{(0)})^{-1}X_T{}^t=1+\tfrac{1}{2}\bar{\omega}\sum_i p_ig(2/x_i). \tag{B13}$$

The function $g(z)$ is defined for positive z by

$$g(z)=z^2-z\coth(1/z)\,, \tag{B14}$$

and is a negative, monotonically decreasing function of z. Since the second derivative of $g(z)$ is non-negative, convexity theorems yield

$$(\beta S^{(0)})^{-1}X_T{}^t\geqslant 1+\tfrac{1}{2}\bar{\omega}g(2\sum_i p_i/x_i). \tag{B15}$$

Since B is non-negative, Eq. (B11) yields

$$1\geqslant\tfrac{1}{2}\bar{\omega}\sum_i p_if(2/x_i). \tag{B16}$$

The function $f(z)$ is defined for positive z by

$$f(z)=z\coth(1/z)\,, \tag{B17}$$

and is non-negative, monotonically increasing, and of positive second derivative. The convexity yields

$$1\geqslant\tfrac{1}{2}\bar{\omega}f(2\sum_i p_i/x_i). \tag{B18}$$

If a variable y_t is defined by

$$1/y_t=2\sum_i p_i/x_i\,, \tag{B19}$$

Eq. (B18) shows that y_t may be no smaller than the solution y of the equation

$$y\tanh y=\tfrac{1}{2}\bar{\omega}. \tag{B20}$$

In Eq. (B15), the function $g(1/y_t)$ can be no more negative than its value $g(1/y)$. Therefore, a lower bound for X_T is

$$X_T|_{\mathrm{lb}}=(\beta S^{(0)})\tfrac{1}{2}\bar{\omega}y^{-2}=\beta S^{(0)}(\tanh y)/y. \tag{B21}$$

This is in fact the greatest lower bound, since $X_T{}^t$ attains this value for a trial function S_t with one value of x_i (equal to y) and with B equal to zero.

The least upper bound is

$$X_T|_{\mathrm{ub}}=\beta S^{(0)}. \tag{B22}$$

This was shown to be an upper bound in Eq. (A3). $X_T{}^t$ may be made to approach it arbitrarily closely by using a trial function S_t with only one term in the i sum nonzero. The value of x_i is taken arbitrarily large; A_i is adjusted to satisfy Eq. (B2), and B approaches $S^{(0)}$.

The lower bound obtained from the work of Harris[7] corresponds to the linear expansion of Eq. (B21) at small $\bar{\omega}$.