PHYSICAL REVIEW B VOLUME 24, NUMBER 7 1 OCTOBER 1981

Fluctuation and susceptibility for the spin van der Waals model and the bounds of Falk and Bruch

I. M. Kim and M. Howard Lee*
Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602
(Received 30 March 1981)

The transverse components of the susceptibility and fluctuation for the spin van der Waals model are obtained for high- and low-temperature XY- and Ising-like regimes. The difference between the susceptibility and fluctuation, which arises because of noncommutativity, is related to certain correlation functions of S_z. In the XY-like regime, the difference vanishes since the principal long-range order is $\langle S_x \rangle$. But in the Ising-like regime, the difference persists since the principal long-range order now is $\langle S_z \rangle$. Our results are compared with the bounds of Falk and Bruch on the ratio of the susceptibility to the fluctuation. In the critical region as well as in the high-temperature region the upper and lower bounds merge. In these regions, the two correlation functions become identical in the manner indicated by Falk and Bruch. In the low-temperature region, the bounds do not merge. Here we find that in the Ising-like regime of the model the susceptibility and fluctuation are properly different, but in the XY-like regime the two functions nevertheless become identical. Thus, the susceptibility and fluctuation can evidently be the same without the bounds necessarily merging.

I. INTRODUCTION

For interacting spin models, the zero-field isothermal susceptibility χ and the variance Y in the long-range-order operator can be different. This difference arises if $[H,S_\alpha] \neq 0$, where H is the Hamiltonian and S_α is the long-range-order operator. One may explicitly obtain the difference between χ and Y by solving, for example, the susceptibililty in terms of the simpler fluctuation.

Falk and Bruch[1] obtained upper and lower bounds for the ratio χ/Y. Should the upper and lower bounds merge in some physical domain, e.g., the critical region, the result of Falk and Bruch implies that the two quantities behave in the same manner in that domain. One of us[2] demonstrated that the susceptibility and fluctuation for the nearest-neighbor three-dimensional spin-$\frac{1}{2}$ XY model have the same critical behavior in accordance with Falk and Bruch.

If the two bounds do not merge, the difference between the susceptibility and fluctuation although still bounded is not resolved. There is also the possibility that in some domain one quantity may approach the other without merging of the bounds. This possibility is not necessarily incompatible with Falk and Bruch, but we believe that the behavior of the bounds alone cannot explain it. The work of Falk and Bruch was formulated for systems with finite-range interaction. To what extent their work applies to systems with long-range interaction is somewhat unclear.

The spin van der Waals model[3–9] allows one to study some of the questions raised above. For this mean-field-like, long-range interaction model, exact expressions for the susceptibility can be given for all temperatures. Thus, one can obtain the difference between the susceptibility and fluctuation, compare the resultant ratio χ/Y with the bounds of Falk and Bruch, and explore other possibilities.

The spin van der Waals model is divided into two physical regimes. The equilibrium and nonequilibrium behavior of the model in one regime is generally quite different from the behavior in the other regime. This difference in behavior may also be reflected in the difference between the susceptibility and fluctuation, which arises because of noncommutativity. If this connection is realized, we have a means of relating the effects of noncommutativity to some physical observables and thereby seeing how noncommutativity manifests itself.

Our paper is organized as follows: In Sec. II, the susceptibility for the van der Waals model is expressed as integrals involving certain equilibrium correlation functions. In Secs. III and IV, these integrals are evaluated, respectively, in the XY- and Ising-like regimes of the van der Waals model. In Sec. V, we briefly examine the bounds of Falk and Bruch from a perspective of the van der Waals model. In Sec. VI, we discuss our results, in particular, the effects of noncommutativity.

II. FLUCTUATION AND SUSCEPTIBILITY FOR THE VAN DER WAALS MODEL

The spin van der Waals model refers to a system of spins arranged in a regular lattice, each of which is coupled to all other spins with equal strength.[3–9] The model may be defined by the following Hamiltonian:

$$H=-\frac{1}{N}\sum_{i\neq j}^{N}[J(s_i^x s_j^x+s_i^y s_j^y)+J_z s_i^z s_j^z] \quad , \tag{1}$$

where N is the total number of spins,[10] the coupling constants J and J_z are both taken to be non-negative, s_i^α denotes the α component of the spin-$\frac{1}{2}$ operator on the ith site of the lattice where $\alpha=x$, y, or z. The system will be referred to as XY-like if $J > J_z$ and as Ising-like if $J < J_z$. The general equilibrium behavior of this model is now well established.[4–8]

The fluctuation and susceptibility for this model are defined in the usual manner,[1] respectively, as

$$Y^{\alpha\alpha}=K^{\alpha\alpha}(0) \tag{2}$$

and

$$\chi^{\alpha\alpha}=\beta^{-1}\int_0^\beta d\lambda\, K^{\alpha\alpha}(\lambda) \quad , \tag{3}$$

where

$$K^{\alpha\alpha}(\lambda)=\langle e^{\lambda H}S_\alpha e^{-\lambda H}S_\alpha\rangle-\langle S_\alpha\rangle^2 \quad , \tag{4}$$

where $S_\alpha=\sum_i s_i^\alpha$, the angular brackets $\langle \cdots \rangle$ denote the canonical ensemble average.

It is convenient to denote the temperature integral in Eq. (3) by $L^{\alpha\alpha}$, i.e., $\chi^{\alpha\alpha}=L^{\alpha\alpha}-\langle S_\alpha\rangle^2$, and also to define $\Delta L^{\alpha\alpha}=L^{\alpha\alpha}-\langle S_\alpha^2\rangle$. Then, $\Delta L^{\alpha\alpha}=\chi^{\alpha\alpha}-Y^{\alpha\alpha}$. Thus, it is sufficient to consider $L^{\alpha\alpha}$ or $\Delta L^{\alpha\alpha}$ for this model in the limit $N\to\infty$. We shall limit our study to L^{xx} or ΔL^{xx} only since $L^{xx}=L^{yy}$ and $\Delta L^{zz}=0$.

The temperature integral L^{xx} may be evaluated if the time evolution of S_x is given. Dekeyser and Lee[8] have shown that

$$S_x(t)=e^{-i\omega t}[(\cos 2\omega t S_z)S_x-(\sin 2\omega t S_z)S_y] \tag{5a}$$

and

$$\langle S_x(t)S_x\rangle=e^{-i\omega t}[\langle(\cos 2\omega t S_z)S_x^2\rangle+\tfrac{1}{2}i\langle(\sin 2\omega t S_z)S_z\rangle] \quad , \tag{5b}$$

where $\omega\equiv\Delta J/N$ and $\Delta J\equiv J-J_z$. We can readily obtain the "temperature" evolution $S_x(-i\lambda)=e^{\lambda H}S_x e^{-\lambda H}$ and the "temperature" correlation function $\langle S_x(-i\lambda)S_x\rangle$, respectively, from Eqs. (5a) and (5b) by replacing t by $-i\lambda$. Hence,

$$\beta L^{xx}=\int_0^\beta d\lambda\, e^{-\lambda\omega}\langle(\cosh 2\lambda\omega S_z)S_x^2\rangle+\frac{1}{2}\int_0^\beta d\lambda\, e^{-\lambda\omega}\langle(\sinh 2\lambda\omega S_z)S_z\rangle \quad . \tag{6}$$

To evaluate the above integrals, it is necessary to first obtain the correlation functions $\langle S_z^{2n}\rangle$ and $\langle S_z^{2n}S_x^2\rangle$, where $n=1,2,3,\ldots$, in the XY- and Ising-like regimes for temperatures above and below the critical temperature.[11]

III. L^{xx} IN THE XY-LIKE REGIME

A. High temperature

For $T > T_c=J/2k$, Dekeyser and Lee[8] have obtained the following for the correlation functions:

$$\langle S_z^{2n}\rangle=\frac{2n!}{2^n n!}\langle S_z^2\rangle^n \tag{7}$$

and

$$\langle S_z^{2n}S_x^2\rangle=\langle S_z^{2n}\rangle\langle S_x^2\rangle \tag{8}$$

for $n=1,2,3,\ldots$.

Using Eqs. (7) and (8) in Eq. (6), we obtain

$$L^{xx}=\langle S_x^2\rangle F_0+\omega\langle S_z^2\rangle F_1 \quad , \tag{9}$$

where

$$F_r=\beta^{-1}\int_0^\beta d\lambda\, \lambda^r e^{\phi(\lambda)} \tag{10}$$

with

$$\phi(\lambda)=-\lambda\omega+2\lambda^2\omega^2\langle S_z^2\rangle \quad . \tag{11}$$

On the high-temperature side, F_0 and F_1 can be readily evaluated.[12] Thus to order N,

$$L^{xx}=\langle S_x^2\rangle+O(1) \quad , \tag{12}$$

where $\langle S_x^2\rangle=\frac{1}{2}N/(2-\beta J)$. Hence, to order N, $\Delta L^{xx}=0$. That is, $\chi^{xx}=Y^{xx}$ for the high-temperature XY-like van der Waals model. Our high-temperature result is exact to order N.[13]

B. Low temperature

For $T < T_c$, Dekeyser and Lee[8] have obtained the following for the correlation functions

$$\langle S_z^{2n}\rangle=\frac{2n!}{2^n n!}\langle S_z^2\rangle^n \tag{13}$$

and

$$2\langle S_z^{2n}S_x^2\rangle=\langle S_z^{2n}\rangle\langle S^2\rangle-\langle S_z^{2n+2}\rangle \tag{14}$$

for $n=1,2,3,\ldots$. Using Eqs. (13) and (14) in Eq. (6), we obtain

$$L^{xx}=\langle S_x^2\rangle F_0+\omega\langle S_z^2\rangle F_1-2\omega^2\langle S_z^2\rangle^2 F_2 \quad . \tag{15}$$

On the low-temperature side, the F's may be expressed in terms of Dawson's integral D,[14]

$$F_0=y^{-1}D(y),\quad y^2=\tfrac{1}{2}\beta^2\omega^2\langle S_z^2\rangle \quad , \tag{16a}$$

$$F_1=\tfrac{1}{2}\beta F_0 \quad , \tag{16b}$$

$$2F_2=\beta/\omega+(\tfrac{1}{2}\beta^2-\beta/\omega)F_0 \quad . \tag{16c}$$

The argument of Dawson's integral is very small if we let $N \to \infty$ while T is kept low but fixed.[10] Thus, we can replace the integral by its asymptotic form and obtain,[15]

$$\Delta L^{xx} = \tfrac{1}{2}\beta\omega\langle S_z^2\rangle - \tfrac{1}{2}(\beta\omega)^2\langle S_z^2\rangle^2 \ , \tag{17}$$

where $\langle S_z^2\rangle = \frac{1}{2}N/\beta\Delta J$. We note that $\Delta L^{xx} = O(1)$. Hence, to order N, $\chi^{xx} = Y^{xx}$ for the low-temperature XY-like van der Waals model. This result is exact to this order.

IV. L^{xx} IN THE ISING-LIKE REGIME

A. High temperature

For $T > T_c = J_z/2k$, the partition function is formally identical to that for the high-temperature XY-like. That is, Eq. (9) applies here with $\langle S_z^2\rangle = \frac{1}{2}N/(2-\beta J_z)$, which although finite in the XY-like regime can now diverge if $T \to T_c+$. The F's depend strongly on the phase factor $\phi(\lambda)$. But, to order N, we obtain the same result as in the high-temperature XY-like case.

B. Low temperature

For $T < T_c$, Dekeyser and Lee[8] have obtained the following for the correlation functions: To the leading order in N,

$$\langle S_z^{2n}\rangle = S_0^{2n} \tag{18}$$

and

$$\langle S_z^{2n} S_x^2\rangle = \langle S_z^{2n}\rangle\langle S_x^2\rangle \ , \tag{19}$$

for $n = 1, 2, 3, \ldots$, where S_0 is the long-range order, which vanishes at $T \to T_c-$ and is of order N, and $\langle S_x^2\rangle = \frac{1}{2}N/\beta\Delta J_z$, where $\Delta J_z \equiv J_z - J$, which is now finite at $T = T_c$. Using Eqs. (18) and (19) in Eq. (6), we obtain to the leading order in N,

$$L^{xx} = \langle S_x^2\rangle \sinh\beta\sigma\Delta J_z/\beta\sigma\Delta J_z + \tfrac{1}{4}N(1-\cosh\beta\sigma\Delta J_z)/\beta\Delta J_z \ , \tag{20}$$

where $S_0 = \frac{1}{2}N\sigma$ so that $\sigma = O(1)$ and $\sigma \sim (T_c - T)^{1/2}$ as $T \to T_c-$.

If $T \to T_c$, then $\Delta L^{xx} = O(\sigma)$ and $\chi^{xx} \to Y^{xx}$ to the leading order in N. But for $0 < T < T_c$, $\Delta L^{xx} = O(N)$. Thus, for the low-temperature Ising-like regime, the susceptibility and fluctuation are indeed distinguishable.[16] In Fig. 1, the susceptibility and fluctuation for the Ising-like van der Waals model are illustrated for different values of J_z/J using our high- and low-temperature results. For $T > T_c$, the susceptibility and fluctuation are the same, both following $(\beta_c J_z - \beta J)^{-1}$. For $T < T_c$, the two quantities are different as indicated, the susceptibility being the smaller of the two, excepting at T_c where both merge. Observe that the amplitudes of the susceptibility and fluctuation strongly depend on J_z/J, but the maxima occur at T_c independent of the anisotropy, already noted by Dekeyser and Lee.[8] As $J_z/J \to 1$, the amplitudes of the susceptibility and fluctuation grow, finally diverging at the isotropic limit when $T \to T_c$. The difference between the susceptibility and fluctuation becomes more pronounced as J_z/J becomes larger and also as T becomes smaller.

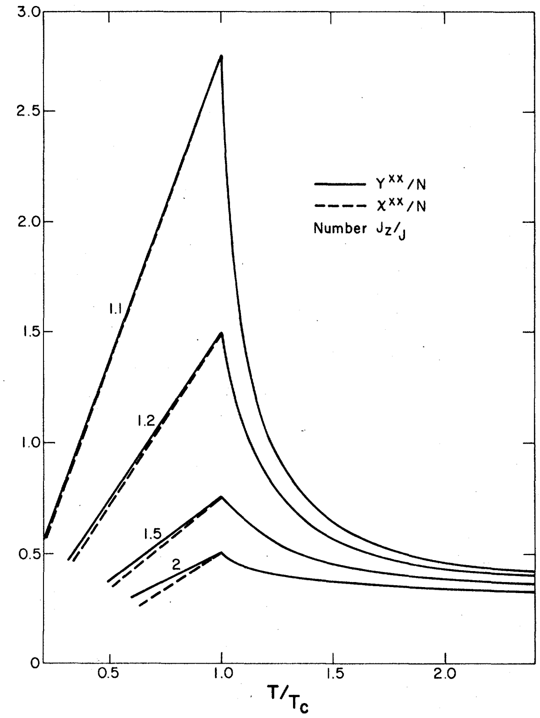

FIG. 1. Susceptibility vs fluctuation for the Ising-like van der Waals model. The susceptibility and fluctuations are shown for several different values of the anisotropy J_z/J. For $T > T_c$, where $T_c = J_z/2k$, the susceptibility and fluctuation are the same, following $(\beta_c J_z - \beta J)^{-1}$. For $T < T_c$, the susceptibility (dashed lines) and fluctuation (solid lines) are indeed different, obtained from Eq. (20).

V. BOUNDS OF FALK AND BRUCH

Falk and Bruch have given the upper and lower bounds for the ratio χ/Y in the following form

$$f_w(\bar{\omega}) \leq \chi/Y \leq 1 \ , \tag{21}$$

where

$$f_w(\bar{\omega}) = (1 - e^{-\beta\bar{\omega}/2})/\tfrac{1}{2}\beta\bar{\omega} \tag{22}$$

and $\bar{\omega} = \nu_2/2Y$, where ν_2 is the second moment (see below) and Y is the mean-square fluctuation.[17,18]

The lower bound $f_w(\bar{\omega})$ is a weaker lower bound. Falk and Bruch have found a stronger lower bound $f_s(\bar{\omega})$, satisfying $f_w(\bar{\omega}) \le f_s(\bar{\omega}) \le \chi/Y$. We shall first discuss the weaker lower bound and the possibility of its merging with the upper bound. When the weaker lower bound does *not* merge with the upper bound, it is then useful to examine the stronger lower bound to see how close or far it is from the upper bound. We shall consider the stronger lower bound at the conclusion of this section.

The above bounds (21) are flexible from the lower side only through the parameter $\bar{\omega}$. The two bounds can merge if $\bar{\omega} \to 0$. That is, $\bar{\omega} \to 0$ implies $\chi \to Y$. This possibility arises for systems with finite-range interaction if, as noted by Falk and Bruch, Y diverges as in the critical region while ν_2 remains finite.[19] (We exclude certain symmetric systems for which $\nu_2 = 0$ so that $\chi = Y$ always.) If $\bar{\omega}$ does not vanish, Eq. (21) places bounds on χ/Y. If, for example, $\frac{1}{2}\beta\bar{\omega} = 0.1$, $0.952 \le \chi/Y \le 1$. The susceptibility may nevertheless still approach the fluctuation. That is, $\chi \to Y$ does not necessarily imply $\bar{\omega} \to 0$. (In this case, the behavior of $\bar{\omega}$ seems to be insufficient to explain the behavior of the susceptibility with respect to the fluctuation.) All of these possibilities are realized in the spin van der Waals model.

We shall thus briefly examine the bounds of Falk and Bruch with respect to the van der Waals model. Falk and Bruch deduced the upper bound $\chi/Y \le 1$ based on the following three properties of $K(\lambda)$: (i) $K(\lambda) = K(\beta - \lambda)$, i.e., $K(\lambda)$ is symmetric in λ about $\lambda = \frac{1}{2}\beta$, (ii) $\min K(\lambda) = K(\frac{1}{2}\beta)$, (iii) for $0 \le \lambda \le \frac{1}{2}\beta$, $\max K(\lambda) = K(0)$. These general properties are sufficient to establish the upper bound, independently of the details of H. For the van der Waals model, these properties are satisfied in the limit $N \to \infty$ in the high- and low-temperature XY- and Ising-like regimes, and the upper bound holds precisely in accordance with Falk and Bruch.

Falk and Bruch deduced the weaker lower bound requiring only that certain sum rules are satisifed. But the lower bound, unlike the upper bound, contains model-dependent quantities Y and ν_2, the latter of which is defined as

$$\nu_2^{\alpha\alpha} = \langle [S_\alpha, [H, S_\alpha]] \rangle \quad . \tag{23}$$

The above double commutator is familiar through the f sum rule. The van der Waals model satisifes the sum rules including the f sum rule.[20] Thus the lower bound is applicable. One can readily show that for this model

$$\nu_2^{xx} = \omega(\langle S_x^2 \rangle - \langle S_z^2 \rangle) \quad , \tag{24}$$

which behaves essentially like the energy.[21] Thus, $\nu_2^{xx} = O(1)$ in the high-temperature XY- and Ising-like regimes; whereas $\nu_2^{xx} = O(N)$ in the low-temperature regimes. That is, $\bar{\omega}^{xx} = 0$ for $T \to T_c$ but $\bar{\omega}^{xx} = O(1)$ for $T < T_c$. Hence, for all high temperatures, the upper and lower bounds must necessarily merge. But for low temperatures the two bounds do not merge. In the XY-like *critical* region, $\bar{\omega}^{xx} \to 0$ in the manner of Falk and Bruch so that the two bounds merge. In the Ising-like critical region, even though Y^{xx} does not diverge, $\bar{\omega}^{xx} \to 0$ also.

TABLE I. Lower bounds for χ/Y in the XY-like regime. This table shows the values for the weaker lower bound (WLB) and stronger lower bound (SLB) as a function of T and J/J_z. In the columns for the bounds, the upper number corresponds to the WLB and the lower number to the SLB. One can determine $\bar{\omega}$ from Eq. (24) with T and J/J_z given. The range of the anisotropy J/J_z is from 1.5 to 100.

J/J_z	100		3		2		1.5	
T/T_c	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB
0.94	0.004 48	0.997 76 0.998 51	0.003 05	0.998 48 0.998 98	0.002 31	0.998 85 0.999 23	0.001 58	0.999 21 0.999 47
0.90	0.013 76	0.993 15 0.995 42	0.009 45	0.995 29 0.996 85	0.007 24	0.996 39 0.997 59	0.005 04	0.997 48 0.998 32
0.80	0.069 60	0.965 99 0.976 91	0.049 01	0.975 89 0.983 72	0.038 56	0.980 97 0.987 18	0.028 49	0.985 89 0.990 52
0.70	0.194 94	0.908 89 0.935 90	0.140 98	0.932 71 0.953 47	0.114 36	0.944 94 0.961 63	0.091 11	0.955 79 0.969 82

TABLE II. Lower bounds for X/Y in the Ising-like regime. This table shows the values for the weaker lower bound (WLB) and stronger lower bound (SLB) as a function of T and J_z/J. In the columns for the bounds, the upper number corresponds to the WLB and the lower number to the SLB. One can determine $\bar{\omega}$ from Eq. (24) with T and J_z/J given. The range of the anisotropy J_z/J is from 1.1 to 2.

J_z/J	2		1.5		1.2		1.1	
T/T_c	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB	$\frac{1}{2}\beta\bar{\omega}$	WLB SLB
0.94	0.048 49	0.976 14 0.983 89	0.021 55	0.989 39 0.992 83	0.005 30	0.997 31 0.998 20	0.001 60	0.999 20 0.999 46
0.90	0.085 20	0.958 58 0.971 76	0.037 87	0.981 30 0.987 41	0.009 47	0.995 28 0.996 84	0.002 82	0.998 59 0.999 06
0.80	0.197 14	0.907 60 0.935 20	0.087 62	0.957 44 0.970 97	0.021 90	0.989 13 0.992 71	0.006 52	0.996 75 0.997 83
0.70	0.350 34	0.843 61 0.886 17	0.155 71	0.926 04 0.948 64	0.038 93	0.980 79 0.987 06	0.011 58	0.994 23 0.996 14

According to the susceptibilities evaluated in Secs. III and IV, in the high-temperature XY- and Ising-like regimes, $\Delta L^{xx}=O(1)$ so that $X^{xx}\rightarrow Y^{xx}$, which is consistent with merging of the bounds. In the low-temperature XY-like regime, $\Delta L^{xx}=O(1)$ also so that, in spite of the bounds not merging, $X^{xx}\rightarrow Y^{xx}$. In the low-temperature Ising-like regime, $\Delta L^{xx}=O(N)$ so that $X^{xx}\neq Y^{xx}$, which, however, is entirely consistent with nonmerging of the bounds.

We shall now briefly examine the stronger lower bound,

$$f_s=\tanh\bar{y}/\bar{y}\ , \tag{25}$$

where $\bar{y}$ is the root of $y\tanh y=\frac{1}{2}\beta\bar{\omega}$. Thus the stronger lower bound f_s also depends on $\bar{\omega}$. One can determine $\bar{\omega}$ from Eq. (24) given T and the anisotropy J vs J_z. In Tables I and II, we have compared the two lower bounds at various temperatures below T_c for different values of anisotropy, J/J_z for the XY-like and J_z/J for the Ising-like. In Table I (XY-like), the anisotropy ranges from 1.5 to 100. At $T/T_c=0.94$ and $J/J_z=1.5$, both lower bounds are close to unity (the upper bound), the stronger lower bound is a little closer to the upper bound. But still it is decidedly far enough away from the upper bound. As T/T_c becomes smaller while the anisotropy remains fixed, the gap between the two lower bounds widens and also the gap between the upper and lower bounds widens. If the anisotropy becomes greater while the temperature remains fixed, the same trend is observed.

In Table II (Ising-like), the anisotropy ranges from 1.1 to 2, much smaller than in Table I. The same general trends noted for Table I are observed. The main difference is in the *change* of the values of the bounds as a function of the anisotropy. In the XY-like regime (Table I), the weaker lower bound, for example, remains reasonably close to the upper bound for a very large range of the anisotropy. In the Ising-like regime (Table II), the weaker lower bound removes from the upper bound rather more rapidly. This behavior perhaps is reflective of the fact that for the XY-like regime $X^{xx}=Y^{xx}$ but for the Ising-like regime $X^{xx}\neq Y^{xx}$.

VI. DISCUSSION

The noncommutativity of S_x with H gives rise to the possibility of defining for the van der Waals model the susceptibility X^{xx} which may be apparently different from the fluctuation Y^{xx}. The effects of the noncommutativity for this model, i.e., ΔL^{xx}, are contained essentially all in the correlation functions involving S_z [see Eq. (6)]. For high temperatures, one can show that $S_z=O(N^{1/2})$ whether the model is XY-like or Ising-like. Thus, the noncommutativity contributes only to overall corrections, all of which vanish as N^{-1}, and the susceptibility and fluctuation are identical to the leading order in N. In the low-temperature XY-like regime of this model, S_z is not the principal long-range order. Thus, the effects of the noncommutativity are again negligible and the susceptibility and fluctuation are identical. But in the low-temperature Ising-like regime, S_z is now the principal long-range order. That is, ΔL^{xx} is of the same order in N as L^{xx} itself. Hence, the susceptibility and fluctuation are indeed different quantities.

The different behavior of S_z from the XY-like regime to the Ising-like regime of the van der Waals model noted above is also reflected in the time correlation function $\langle S_x(t)S_x\rangle$. For $T > T_c$, the Ising-like time correlation function is Gaussian, but for $T < T_c$ it becomes oscillatory. The XY-like time correlation function remains Gaussian for T above and below the critical temperature.[8] The parallel behavior between the susceptibility and the time correlation function is not unexpected since the temperature evolution and the time evolution of S_x, for example, are formally similar.

Finally, our study of the susceptibility for the van der Waals model illustrates the generality of the bounds of Falk and Bruch. The applicability of the bounds on the ratio of the susceptibility to the fluctuation evidently extends to systems with long-range interaction if they satisfy certain leading sum rules. We have demonstrated via the van der Waals model that merging of the upper and lower bounds can take place outside the critical region. We have also shown that the susceptibility and fluctuation can be the same without merging of the bounds.

ACKNOWLEDGMENTS

We wish to thank Professor R. Dekeyser of the University of Leuven, Belgium for his interest in our work. This work was supported in part by the U.S. Department of Energy under Contract No. DE-AS-09-77-ER01023.

*To whom reprint requests may be addressed.

[1]H. Falk and L. W. Bruch, Phys. Rev. 180, 442 (1969).

[2]M. H. Lee, Phys. Rev. B 8, 1203 (1973).

[3]See, for example, H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford U.P., Oxford, 1971), pp. 91. Also see the references cited therein.

[4]C. Kittel and H. Shore, Phys. Rev 138, A1165 (1965).

[5]T. Niemeijer, Physica (Utrecht) 48, 467 (1970).

[6]G. Vertogen and A. S. Devries, Physica (Utrecht) 59, 634 (1972).

[7]H. Falk, Phys. Rev. B 5, 3638 (1972).

[8]R. Dekeyser and M. H. Lee, Phys. Rev. B 19, 265 (1979).

[9]D. K. Dacol, Physica (Utrecht) 100A, 496 (1980); S. Banerjee, R. Dekeyser, and M. H. Lee, J. Magn. Magn. Mater. 15–18, 427 (1980).

[10]In obtaining their solutions, e.g., the partition function, for the van der Waals model, Dekeyser and Lee (Ref. 8) require that the $N \to \infty$ limit be taken independently of all other parameters of the system and also that this limit be taken first before the limits of other parameters, e.g., $T \to T_c$. Since T_c exists only in the thermodynamic limit, this requirement is reasonable. Their requirement arises from their method of solution, which includes replacing sums by integrals, keeping terms to order N and neglecting lower order terms. Since our work is based on the results of Dekeyser and Lee, we also follow their method of solution explicitly.

[11]To the leading order of N, the phase factors in Eqs. (5) and (6) are unimportant since $\omega = O(N^{-1})$. See Ref. 10. However, the hyperbolic functions must be handled more carefully since S_z is contained in the arguments which is a function of N.

[12]For $T > T_c$ or $\beta < \beta_c$, these integrals are bounded and can be readily evaluated. Together with $\langle S_z^2\rangle = \frac{1}{2}N/(2-\beta J_z)$, which is finite at $T = T_c$, one obtains to order N, $F_0 = 1$, $F_1 = \frac{1}{2}\beta$.

[13]In the temperature integrals [see Eq. (10)], λ is bounded, i.e., $0 < \lambda < \beta \leq \beta_c$, where $\beta_c J = 2$. Hence, the correction terms always remain $O(1)$ for all values of $T \geq T_c$.

[14]M. Abramowitz and T. A. Stegun, *Handbook of Mathematical Functions*, Natl. Bur. Stand., Appl. Math. Ser. No. 55 (U.S. GPO, Washington D.C., 1970), p. 298; *Higher Transcendental Functions*, edited by A. Edélyi (McGraw-Hill, New York, 1953), Vol. II, p. 147.

[15]With $D(y) = y + O(y^3)$ for $y \to 0$, one can readily obtain to order N, $F_0 = 1$, $F_1 = \frac{1}{2}\beta$, $F_2 = \frac{1}{4}\beta^2$.

[16]Our expression (20) for L^{xx} is exact to order N, valid for $\Delta J/\hbar N^{1/2} < T < T_c$. For $T \to 0$, it is necessary to include correction terms neglected in Eq. (18). See Eq. (43a) of Ref. 8. These corrections will add other terms to our expression (20) for L^{xx}. But still we obtain $\Delta L^{xx} = O(N)$. Since our conclusion is thus unchanged, we retain here the simpler expression.

[17]A number of people have contributed to the study of the bounds referred to here. They include J. M. Luttinger, Prog. Theor. Phys. (Kyoto) Suppl. 37, 35 (1966); B. D. Josephson, Proc. Phys. Soc. London 92, 269 (1967); A. B. Harris, J. Math. Phys. 8, 1044 (1967); R. M. Wilcox, Phys. Rev. 174, 624 (1968); W. Brenig, Z. Phys. 206, 212 (1967). V. N. Plechko, *International Symposium on Selected Topics in Statistical Mechanics* (JINR, Dubna, 1978), p. 128.

[18]For more recent work on correlation inequalities, see J. Naudts and A. Verbeure, J. Math. Phys. 17, 419 (1976); G. Roepstorff, Commun. Math. Phys. 46, 253 (1976); M. Fannes and A. Verbeure, *ibid.* 57, 165 (1977); F. J. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. 18, 335 (1978); R. Martens, Physica (Utrecht) 97A, 455 (1979).

[19]N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966).

[20]P. C. Hohenberg, Phys. Rev. 158, 383 (1967) discusses systems which violate the f sum rule. See also P. W. Anderson, *ibid.* 110, 827 (1958).

[21]The energy behaves as $\langle H\rangle = -(2J/N\langle S_x^2\rangle + J_z/N\langle S_z^2\rangle)$. We note that the second moment [Eq. (24)] is the difference between $\langle S_x^2\rangle$ and $\langle S_z^2\rangle$, whereas the energy is essentially the sum. Away from the isotropic point ($J_z = J$ or $\Delta J = 0$), one term dominates over the other. Hence the energy and the moment behave similarly. Now $\langle H\rangle \sim JS^2/N$. For $T > T_c$, $\langle H\rangle = O(1)$ since $S = O(N^{1/2})$; and for $T < T_c$, $\langle H\rangle = O(N)$ since $S = O(N)$. Recall that for $T > T_c$ the specific heat for all mean-field-like models vanishes.