High-temperature longitudinal susceptibility for the $S=\frac{1}{2}$ XY model: Some numerical evidences

I. M. Kim and M. H. Lee*
Department of Physics, University of Georgia, Athens, Georgia 30602
(Received 6 November 1978)

The longitudinal component of the XY-model susceptibility is nondivergent at $T=T_c$. In an earlier paper it was shown that as $T\rightarrow T_c+$ the longitudinal susceptibility is determined essentially by nearest-neighbor correlations and it behaves as the derivative of the free energy with respect to inverse termperature. We provide here numerical evidences in support of the earlier conclusions.

The longitudinal component of the susceptibility χ^{zz},

$$\chi^{zz}=\left\langle \left[\sum_i S_i^z\right]^2\right\rangle-\left[\left\langle \sum_i S_i^z\right\rangle\right]^2 \tag{1}$$

for the $S=\frac{1}{2}$ XY model, defined by the Hamiltonian

$$H=-J\sum_{(ij)}(S_i^xS_j^x+S_i^yS_j^y) \quad , \tag{2}$$

is (unlike the transverse component) nondivergent at $T=T_c$. For $T>T_c$, it is convenient to write the longitudinal susceptibility as a sum of nearest-neighbor correlations $\tilde{\chi}^{zz}$ and all other distant-neighbor correlations Δ^{zz}, i.e.,

$$\chi^{zz}=1+\tilde{\chi}^{zz}+\Delta^{zz} \quad . \tag{3}$$

As $T\rightarrow\infty$, evidently $\chi^{zz}-1\rightarrow\tilde{\chi}^{zz}$. In a recent paper,[1] one of us showed using a somewhat involved asymptotic argument that as $T\rightarrow T_c+$, one still has $\chi^{zz}-1\rightarrow\tilde{\chi}^{zz}$. In addition, χ^{zz} behaves as $\partial F/\partial K$, where F is the free energy and $K=J/kT$. In this brief note, we provide numerical evidences for these conclusions.

Series expansions for χ^{zz} may be obtained by a method previously given[2] from which, by some modifications, series expansions for $\tilde{\chi}^{zz}$ may also be obtained.[3] The nearest-neighbor correlation function $\tilde{\chi}^{zz}$ is an important quantity in spin dynamics.[4] We list here our cubic lattice results through eight terms[5]:

(i) fcc *lattice*

$$\chi^{zz}=1-3K^2-4K^3+0.5K^4-0K^5-32.408\,333K^6 -124.416\,667K^7-354.876\,5K^8+\cdots \quad ,$$

$$\tilde{\chi}^{zz}=-3K^2-4K^3+0.5K^4+2.8K^5-21.690\,27K^6 -97.381\,78K^7-254.989\,12K^8+\cdots \quad .$$

(ii) bcc *lattice*

$$\chi^{zz}=1-2K^2+K^4-6.105\,55K^6 -14.439\,48K^8+\cdots \quad ,$$

$$\tilde{\chi}^{zz}=-2K^2+K^4-2.558\,33K^6-13.523\,80K^8+\cdots \quad .$$

(iii) sc *lattice*

$$\chi^{zz}=1-1.5K^2+1.75K^4 -3.337\,5K^6-10.697\,4K^8+\cdots \quad ,$$

$$\tilde{\chi}^{zz}=-1.5K^2+1.75K^4-2.568\,75K^6 -7.635\,34K^8+\cdots \quad .$$

In Fig. 1 we show the behavior of χ^{zz} and $1+\tilde{\chi}^{zz}$ for the cubic lattices. The critical points $K_c=0.222$, 0.344, and 0.495, respectively, for the fcc, bcc, and sc are from Betts *et al.*[6] As may be observed here, the two quantities are similar for the temperature range $T_c<T<\infty$. Also observe that each of these quantities approaches the critical point with a finite slope indicating nondivergent behavior at $K=K_c$. In Fig. 2 we compare the susceptibility with $\partial F/\partial K$, with the free energy obtained by Betts *et al.*[6] Although their amplitudes are different, the two functions appear to behave rather similarly as predicted.

We briefly discuss the general nature of our results given here. The energy and susceptibility may be each considered as a sum of certain short- and long-range correlations. For nn models such as Eq. (2), the correlations which give rise to the energy are limited to short-range types, whereas the correlations for the susceptibility are ordinarily dominated by long-range types. In terms of high-temperature series expansions one sees the difference readily. The expansion coefficients for the energy series are determined by closed graphs, but those for the susceptibility largely by open graphs.[2] The expansion coefficients for χ^{zz} for the XY model, however, are made up by

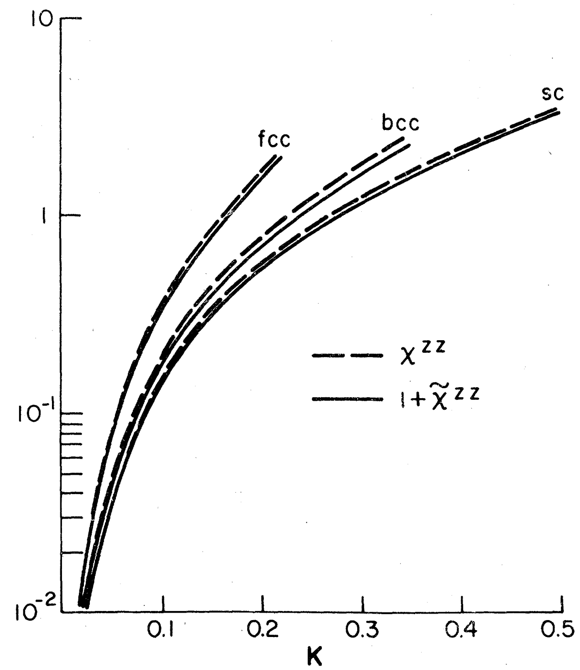

FIG. 1. Longitudinal susceptibility on cubic lattices shown as a function of $K=J/kT$. Dashed lines represent χ^{zz} and solid lines $1+\tilde{\chi}^{zz}$. The critical points are 0.220, 0.344, and 0.495, respectively, for fcc, bcc, and sc lattices (see Ref. 6).

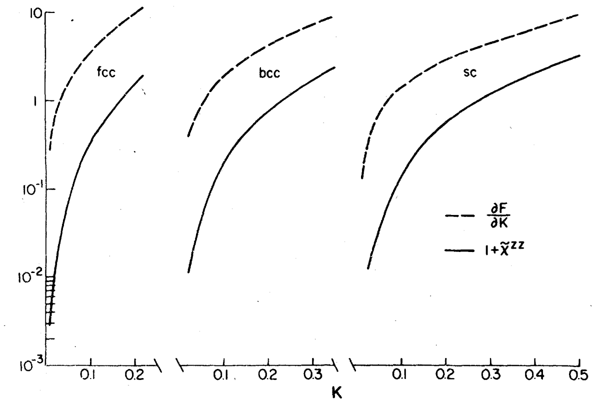

FIG. 2. Susceptibility and the derivative of the free energy shown as a function of $K=J/kT$ for cubic lattices. Solid lines represent $1+\tilde{\chi}^{zz}$ and dashed lines $\partial F/\partial K$. Although their amplitudes are different, both quantities appear to behave similarly.

closed graphs, in fact, by precisely the same graphs as those occurring in the expansion coefficients for the energy series.

To show this further, it is convenient to define an operator

$$A^{zz}=\left(\sum_i S_i^z\right)^2 . \tag{4}$$

The high-temperature expansion coefficents for χ^{zz} are of the form $\mathrm{Tr}A^{zz}H^n$, $n=1,2,\ldots,$ where H is given by Eq. (2). Now one can show that for a given n,

$$\mathrm{Tr}A^{zz}H^n=a_n\,\mathrm{Tr}H^n , \tag{5}$$

where a_n is a c number.[1] Hence the longitudinal component of the susceptibility for the XY model behaves as the energy. For the transverse components A^{xx} and A^{yy} there are no such relationships.

ACKNOWLEDGMENT

This work is supported in part by DOE ERDA under Contract No. EG-77-S-09-1023.

*To whom reprint requests may be addressed.

[1]M. H. Lee, Phys. Rev. B 12, 276 (1975).
[2]M. H. Lee, J. Math. Phys. 12, 61 (1971).
[3]Essential modifications needed are given by certain identities derived in Appendix A of Ref. 1.
[4]For example, this quantity appears as a leading term in f-sum rule. See M. H. Lee, Phys. Rev. B 8, 3290 (1973).
[5]A number of people have worked on the longitudinal component of the susceptibility: T. Obokata, I. Ono, and T. Oguchi, J. Phys. Soc. Jpn. 23, 516 (1967); K. Pirnie (unpublished); M. H. Lee, see Ref. 2; D. W. Wood and N. W. Dalton, J. Phys. C 5, 1675 (1972); J. Rogiers and R. Dekeyser, Phys. Lett. A 46, 206 (1973).
[6]D. D. Betts, C. J. Elliott, and M. H. Lee, Can. J. Phys. 48, 1566 (1970).