EVIDENCE SUPPORTING SCALING WITH A PARAMETER FOR THERMODYNAMIC FUNCTIONS AND THE PAIR CORRELATION FUNCTION *

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The first five derivatives with respect to $R \equiv J_z/J_{xy}$ of the susceptibility, specific heat, and second moment for the sc and fcc Ising models are found to be characterized by a crossover exponent $\varphi = 1.75$, supporting the predictions of scaling with respect to R for both thermodynamic functions *and* the pair correlation function.

One purpose of this work is to resolve a controversy [1,2] in the literature concerning successive derivatives of certain functions with respect to an anisotropy parameter R, where R is defined in the Hamiltonian

$$\mathcal{H}_{\text{l.anis.}} = -\sum_{\langle ij\rangle}^{xy} J_{xy}\, s_i^z s_j^z - \sum_{\langle ij\rangle}^{z} J_z\, s_i^z s_j^z$$

$$\equiv -J_{xy}\left[\sum_{\langle ij\rangle}^{xy} s_i^z s_j^z \sum_{\langle ij\rangle}^{z} + R\sum_{\langle ij\rangle}^{z} s_i^z s_j^z\right]. \tag{1}$$

This Hamiltonian describes a $S = \frac{1}{2}$ Ising system with different coupling strengths J_{xy}, J_z in different lattice directions ('lattice anisotropy') and $R \equiv J_z/J_{xy}$. The first summation is over pairs of nearest-neighbor (nn) sites whose relative displacement vector $\boldsymbol{r}_{ij}$ has no z-component, while the second summation is over all other pairs of nn sites. We treat the simple cubic (sc) and the face-centered cubic (fcc) lattice, and note that both these lattices 'cross over' to the *two*-dimensional square lattice in the limit $R \to 0$.

A second purpose of the present work is to provide the first series evidence supporting 'scaling with a parameter'. The scaling hypothesis for the pair correlation function can be extended [3] to scaling with respect to parameter R which changes the universal class of the system [in this case, from being a *two*-dimensional lattice ($R = 0$) to a three-dimensional lattice ($R \neq 0$)], i.e., there exist 4 numbers b_i such that for all positive λ,

$$C_2(\lambda^{b_\tau}\tau, \lambda^{b_H}H, \lambda^{b_r}\boldsymbol{r}, \lambda^{b_R}R) \equiv \lambda C_2(\tau, H, \boldsymbol{r}, R)\,, \tag{2}$$

from which the exponent predictions shown in the second column of table 1 follow. Here $\tau \equiv T - T_c$ ($R = 0$), H is the magnetic field ($H = 0$ in the present work), and $\boldsymbol{r}$ is the site separation vector.

A weaker statement is that only the Gibbs potential scales,

$$G(\lambda^{b_\tau}\tau, \lambda^{b_H}H, \lambda^{b_R}R) = \lambda^{b_G}G(\tau, H, R)\,. \tag{3}$$

Since

$$\int \mathrm{d}\boldsymbol{r}\; C_2(\boldsymbol{r}) = \chi_T = (\partial^2 G/\partial H^2)_T\,,$$

it follows that (2) implies (3). The converse is *not* true, and, in particular, (3) does *not* imply that

$$\mu_2 \equiv \int r^2\, C_2(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}$$

scales. Scaling also makes the predictions shown in the top line of column 2 of table 1.

The predictions of (3) are violated by previous numerical results reported in the literature [1] (cf. column 3). This previous work, based on high-temperature series, was restricted to only the sc lattice, and only the single function χ_T.

We have here analyzed general-R series for $\chi_T^{(n)}$ and $\mu_2^{(n)}$ on both the sc and fcc lattices [4], and $C_{\mathrm{H}}^{(n)}$ on the fcc using a wider variety of methods than used in refs. [1, 2] (e.g., ratio method, Park's method, Neville tables, and analysis on the series raised to different powers). We expanded all five

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Table 1

Definition of exponents	Scaling hypothesis plus $\gamma_1 = 2\gamma_0$ proof [5]	Previous numerical results (sc lattice only)	Present work (sc and fcc lattices)	
(a) Test of thermodynamic scaling with a parameter (eq. (3))			sc	fcc
$T_c(R) - T_c(0) \sim R^{1/\varphi}$	$\varphi = \gamma_0$ $[\gamma_0 = 1.75]$	$\varphi = 1.2$ [1]	$\varphi = 1.70 \pm 0.1$	
$\bar{\chi}^{(n)} \equiv \left(\frac{\partial^n \bar{\chi}}{\partial R^n}\right)_{R=0} \sim \tau^{-\gamma_n}$	$\gamma_n = \gamma_0 + n\varphi = (n+1)\gamma_0$			
	$n = 1$: 3.50	3.50[1, 2]	3.500	
	$n = 2$: 5.25	5.0 ± 0.1[1], 5.2 ± 0.1[2]	5.25 ± 0.04	5.25 ± 0.04
	$n = 3$: 7.00	6.5 ± 0.2[1], 6.9 ± 0.1[2]	7.00 ± 0.05	7.00 ± 0.04
	$n = 4$: 8.75	8.0 ± 0.3[1]	8.75 ± 0.25	8.75 ± 0.03
	$n = 5$: 10.50		$10.5 \pm^{0.50}_{1.00}$	$10.5 \pm^{0.1}_{0.2}$
$C_H^{(n)} \equiv \left(\frac{\partial^n C_H}{\partial R^n}\right)_{R=0} \sim \tau^{-\alpha_n}$	$\alpha_n = \alpha_0 + n\varphi = \alpha_0 + \gamma_0$ $[\alpha_0 = 0]$			
	$n = 2$: 3.50			3.5 ± 0.05
	$n = 4$: 7.00			7.0 ± 0.04
	$n = 6$: 10.50			10.5 ± 0.05
	$n = 8$: 14.00			14.0 ± 0.6
(b) Test of correlation function scaling with a parameter (eq. (2))				
$\mu_2^{(n)} \equiv \left(\frac{\partial^n \mu_2}{\partial R^n}\right)_{R=0} \sim \tau^{-(\gamma_0 + 2\nu_n)}$	$\gamma_0 + 2\nu_n = \gamma_0 + 2\nu_0 + n\varphi = 2\nu_0 + (n+1)\gamma_0[\nu_0 = 1]$			
	$n = 1$: 5.50		5.500	
	$n = 2$: 7.25		$7.25 \pm^{0.10}_{0.20}$	7.25 ± 0.02
	$n = 3$: 9.00		$9.0 \pm^{0.10}_{0.50}$	9.0 ± 0.1
	$n = 4$: 10.75		$10.75 \pm^{0.10}_{0.25}$	10.75 ± 0.03
	$n = 5$: 12.50		$12.85 \pm^{0.40}_{0.60}$	$12.50 \pm^{0.10}_{0.05}$

series in terms of the variable J/kT, which was found to produce slightly more regular series than the variable tanh (J/kT). Our estimate are shown in the last column. The reader will note that in all cases they do not violate the predictions of the scaling hypothesis.

That the work in ref. [1] is incorrect is also supported by the following rigorous results [5]: $\gamma_1 = 2\gamma_0$, $\gamma_2 = 3\gamma_0$ and $\gamma_3 \geqslant 4\gamma_0$.

The result $\gamma_1 = 2\gamma_0$, when combined with the scaling prediction [cf. eq. (3)] that $\gamma_1 = \gamma_0 + \varphi$, leads to the result

$$\varphi = \gamma_0 \,, \tag{4}$$

Eq. (4) was previously predicted by results based on assumed properties of multispin correlation functions [6].

In summary, if the hypothesis of scaling with a parameter is valid, then the exponents γ_n, α_n, and $2\nu_n$ differ by a constant gap index φ (e.g., $\gamma_n = \gamma_0 + n\varphi$). Moreover, $\gamma_1 = 2\gamma_0$ so that if scaling holds, then $\varphi = \gamma_0$ rigorously. We find that all these predictions are borne out by series analysis, thereby supporting the scaling hypothesis for both thermodynamic functions and the pair correlation function.

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