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An analysis of critical exponents from a renormalized Hamiltonian method

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Abstract. It is shown analytically that the critical exponents for the 3D Ising model from a renormalized Hamiltonian treatment, given by Girvin, of the thermal averages appearing in an approximate difference equation formulation, are exactly those of the spherical model ($\gamma = 2$, $\alpha = -1$). These are compared to the values computed by Girvin: $\gamma \simeq 1.78$, $\alpha \simeq 0.11$, which do not satisfy scaling. It is also noted that the behaviour $W(\lambda) \simeq W(1) + O(1-\lambda)^{1/2}$ for $\lambda \simeq 1^-$ is reproduced by the Chadi–Cohen method of computation of reciprocal lattice sums only if the criterion $q_i^2 \ll 1 - \lambda$ is met, where q_i are the smallest special points brought in at the order of approximation considered.

In a recent approximate method for the 3D Ising model phase diagram, Girvin (1978) claimed to derive the critical exponent values $\gamma \simeq 1.78$ and $\alpha \simeq 0.11$, to be compared favourably (considering the simplicity of the method) to the series expansion values $\gamma = 1.25$ and $\alpha = 0.125$. It is shown here, analytically, that this theory in fact leads to the values $\gamma = 2$ and $\alpha = -1$, which are the same as the exponents resulting from the spherical model. The method is presented by Girvin in two forms: form A, where all neighbouring sites to spin i in the renormalized Hamiltonian are assumed to be identically coupled to each other, and form B, where this assumption is not made.

The operational equations of the theory may be summarized as follows.

A. Simpler form. The renormalized Hamiltonian $\tilde{H}$, which is connected to site i and may be used to evaluate thermal averages $\langle f(\vartheta_i)\rangle$ of functions of ϑ_i only, is given by

$$\tilde{H} = \tilde{H}(\vartheta_i) = -\tilde{J}\vartheta_i^2 \tag{1}$$

where $\vartheta_i = \sum_\delta S_{i+\delta}$, $(S_j = \pm 1)$, $\tilde{J}$ is the renormalized coupling constant and the summation over δ is over nearest-neighbour lattice vectors. The original Hamiltonian is

$$H = -\tfrac{1}{2}J\sum_{i,\delta} S_i S_{i+\delta} - \sum_i h_i S_i$$

where h_i is the site-dependent magnetic field and J is the coupling constant. The other equations of the theory are

$$\langle \vartheta_i^2 \rangle_{\tilde{H}} = \langle \vartheta_i^2 \rangle_H \tag{2a}$$

$$\langle \vartheta_i^2 \rangle_H \cong (z^2/\lambda^2)(1 - 1/W(\lambda)) \tag{2b}$$

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and

$$\lambda = z\langle \tanh^2(\beta J \vartheta_i)\rangle_{\tilde{H}} / \langle \vartheta_i \tanh(\beta J \vartheta_i)\rangle_{\tilde{H}} \tag{3}$$

where

$$W(\lambda) = \frac{1}{N}\sum_q \frac{1}{1-\lambda\Gamma(q)} \tag{4}$$

is a generalization to $\lambda \neq 1$ of the usual Watson sum (Watson 1939), the subscript $\tilde{H}$ signifies that the thermal average is to be performed with the renormalized Hamiltonian $\tilde{H}$, $\Gamma(q) = J(q)/J(0)$ and where $\beta = 1/kT$. λ is *defined* by $\lambda = z\langle \tanh^2(\beta J \vartheta_i)\rangle_H / \langle \vartheta_i \tanh(\beta J \vartheta_i)\rangle_H$ but is *calculated* as in (3). ($\lambda = 1$ corresponds to the critical temperature T_c.) The calculations in (2) and (3) are simply performed using

$$\langle f(\vartheta_i)\rangle_{\tilde{H}} = \mathrm{Tr}\{e^{-\beta\tilde{H}(\vartheta_i)} f(\vartheta_i)\} / \mathrm{Tr}\{e^{-\beta\tilde{H}(\vartheta_i)}\} \tag{5}$$

together with the identity

$$\mathrm{Tr}\{g(\vartheta_i)\}/\mathrm{Tr}\{1\} = \sum_{r=0}^{z} {}^zC_r\, g(z-2r) \Big/ \sum_{r=0}^{z} {}^zC_r \tag{6}$$

where ${}^zC_r$ are the usual combinatorial coefficients. The susceptibility $\chi \sim 1/(1-\lambda)$ near T_c, as a function of $T - T_c$, gives γ through $\chi \sim (T - T_c)^{-\gamma}$. Similarly, $U_2 \equiv \langle S_i \vartheta_i\rangle / z$, which is to within a factor of $(-J/2)$ the energy per spin, is given in the theory by

$$U_2 = \frac{z}{W(\lambda)}\frac{1}{N}\sum_q \frac{\Gamma(\lambda)}{1-\lambda\Gamma(q)} \equiv \frac{z}{\lambda}\left(1 - \frac{1}{W(\lambda)}\right) \tag{7}$$

and gives α through $dU_2/dT \sim \text{constant} + (T - T_c)^{-\alpha}$ near T_c. (2) yields $\beta\tilde{J}$ as a function of λ; (3) gives βJ in terms of $\beta\tilde{J}$ and λ. Thus, one may consider $\tilde{J}$ to be a function of β and one may also eliminate $\tilde{J}$ to obtain λ as a function of T. It is evident that for the calculation of γ, it suffices to know that $W(\lambda) \sim W(1) + O(1-\lambda)^{1/2}$ (see e.g. Joyce 1972, Lax 1955, Mannari and Kageyama 1968), for (2) then gives $\beta\tilde{J} - (\beta\tilde{J})_c \sim (1-\lambda)^{1/2}$, which, combined with (3) near T_c: $1-\lambda = O(\beta\tilde{J} - (\beta\tilde{J})_c) + O(\beta J - (\beta J)_c)$, then yields $\beta J - \beta_c J \sim (1-\lambda)^{1/2}$ so that $\chi \sim 1/(1-\lambda) \sim (T - T_c)^{-2}$, i.e. $\gamma = 2$, as in the spherical model (see e.g. Amit 1984). Similarly, from (7), $U_2 \sim U_{2c} + O(1-\lambda)^{1/2} + O(1-\lambda) \sim U_{2c} + O(T - T_c) + O(T - T_c)^2$, so the specific heat, as T_c is approached from above, is $c \sim \text{constant} + O(T - T_c)$. Therefore, $\alpha = -1$ in the theory.

B. More complex form. The renormalized Hamiltonian $\tilde{H}$, which is connected to site i and may be used to evaluate thermal averages of functions of the neighbouring spins of i, is now given by

$$\tilde{H} = -\sum_{\delta_1 < \delta_2} \tilde{J}_{\delta_1\delta_2} S_{\delta_1} S_{\delta_2} \tag{8}$$

where δ_1 and δ_2 run over the nearest neighbours of i. (8) replaces (1). It involves, formally, for the SC lattice as an example, 15 ($= {}^6C_2$) $\tilde{J}_{\delta_1\delta_2}$ values (some of them being certainly

equal by symmetry). (3) still holds, but now as $\tilde{H}$ of (8) can no longer be regarded as a function of ϑ_i, (2) (still valid) is replaced by the 15 pair correlation function equations

$$\langle S_{\delta_1} S_{\delta_2} \rangle_{\tilde{H}} = \langle S_{\delta_1} S_{\delta_2} \rangle_H = \frac{1}{NW(\lambda)} \sum_q \frac{\cos(q \cdot R_{\delta_1 \delta_2})}{1 - \lambda \Gamma(q)} \tag{9}$$

where $R_{\delta_1 \delta_2}$ is the vector joining the spins δ_1 and δ_2. For the SC lattice, there are two non-equivalent pairs of nearest-neighbour sites: those separated by two lattice units and those separated by $\sqrt{2}$ lattice units; thus the 15 equations of (9) reduce to two equations for only two non-equivalent correlation functions $\langle S_{\delta_1 \delta_2} \rangle$, involving only two non-equivalent $\tilde{J}_{\delta_1 \delta_2}$. Of course, the appropriate linear combination of (9) reduces to (2). Now the behaviour of the RHS of (9) for $\lambda \simeq 1^-$ is obtained from the small-q behaviour of the summation. For small q, the cosine may be replaced by $1 + O(q^2)$ to yield

$$\langle S_{\delta_1} S_{\delta_2} \rangle_H - \langle S_{\delta_1} S_{\delta_2} \rangle_{H,c} = O(1 - \lambda)^{1/2}. \tag{10}$$

This is consistent with (2). This again leads to $\gamma = 2$ and $\alpha = -1$, in the same way as in form A.

The determination of $\gamma = 2$ for form A (though not for form B) has been checked by us computationally for the BCC lattice, using $W(\lambda)$ as given by Joyce (1972): $W(\lambda) \simeq W(1) - (2^{3/2}/\pi)(1 - \lambda)^{1/2}$ for $\lambda \simeq 1$. $\gamma = 2$ was indeed obtained. The coefficient $2^{3/2}/\pi$ in front of $(1 - \lambda)^{1/2}$ was reproduced by us by actually performing the sum as an integral using the small-q expansion of the integrand, giving confidence in (10) for form B of the method.

The result $\alpha \simeq 0.11$ of Girvin is internally consistent with his $\gamma \simeq 1.78$: $\chi \sim 1/(1-\lambda) \sim (T - T_c)^{-1.78}$, with $U_2 \sim O(1-\lambda)^{1/2}$ implies that $c \equiv dU_2/dT \sim (T - T_c)^{-0.11}$. Nevertheless, using $d = 3$ and $\eta = 0$ (note: in this method $G(q) \sim q^{-2}$ at T_c) in the scaling law $(2 - \alpha)(2 - \eta) = \gamma d$ (see e.g. Amit 1984), one sees that this law is not satisfied by Girvin's values of γ and α. ($\gamma = 1.78$ should lead to $\alpha = -0.67$.) It is satisfied by our values.

The reason that the critical exponents obtained here are the same as those for the spherical model is that (4) is the basic equation that governs the analytic properties of the system, and it is common to the spherical model and to the present model. The use of the renormalized Hamiltonian $\tilde{H}$ via (5) introduces, as demonstrated here, no further non-analytic behaviour.

To understand the discrepancy between our $\gamma = 2$, $\alpha = -1$ result and the $\gamma \simeq 1.78$, $\alpha \simeq 0.11$ result of Girvin, one must conjecture that the summations on the RHS of (9) were performed by Girvin computationally, using a method that did not sample a sufficient number of points in q-space. As an example of how this can occur, we report our attempt to compute $W(\lambda) - W(1)$ using the Chadi–Cohen technique (Chadi and Cohen 1973, Macot and Frank 1990) instead of the Joyce formula. We used $1 - \lambda$ near 10^{-8}, and the same order of approximation that gives $W(1)$ to 10-figure accuracy. The result was consistently $O(1 - \lambda)$ rather than the correct $O(1 - \lambda)^{1/2}$. It was only when we took $1 - \lambda$ near 10^{-5} that we obtained the correct result. The reason for the former, incorrect result is as follows. From the corresponding q-space integral, the correct behaviour with $1 - \lambda$ arises from the very-small-q portion of this integral. However, when $q^2 \ll 1$, $W(\lambda)$ has a summand like $1/[(1 - \lambda) + \alpha q^2]$ where α is $O(1)$. Thus, non-analytic behaviour can only appear if the special-point approximations are carried far enough so as to bring in q values satisfying the criterion $q^2 \ll 1 - \lambda$. The smaller the values of $1 - \lambda$ chosen, the higher the order of approximation (and hence, exponentially, the amount of computer time) needed.

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