Rigorous Inequalities for the Spin-Relaxation Function in the Kinetic Ising Model

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Rigorous lower bounds are established for the spin-relaxation function in kinetic Ising models. A recently published estimate, based on Monte Carlo calculations, that the spin autocorrelation time is proportional to $|T-T_c|^{-1}$ in two dimensions, near the critical temperature T_c, is shown to be incorrect because it violates these inequalities.

One of the simplest models exhibiting nontrivial time-dependent behavior near a second-order critical point is the kinetic Ising model, first introduced by Glauber[1] in 1963 and later extended by other authors to various cases. As a result of the purely relaxational nature of the dynamics of this kind of model, it has been possible to prove a number of useful rigorous inequalities concerning the dynamic behavior of the system.[2–6] In the present note, we present some extensions of these results, which may be helpful in understanding the behavior of the kinetic Ising model near its critical point.

The kinetic Ising model is a system of "spins," interacting with a heat bath that gives rise to spontaneous flips of spins.[7] The state of the system at some instant of time is described by the values of the N spin variables s_i $(i=1,\ldots,N)$ with $s_i=\pm 1$. In an infinitesimal time interval dt, the system may make a transition from a state $\{s_1,\ldots, s_j,\ldots, s_N\}$ to another state $\{s_1,\ldots, -s_j,\ldots, s_N\}$ which differs from the first only by having a single flipped spin on site j. The probability of making such a transition is proportional to dt, and may be written $w_j(s_1,\ldots,s_N)\,dt$. Let $P(s_1,\ldots,s_N;t)$ be the probability of finding the system in the state $\{s_1,\ldots,s_N\}$ at time t. Then P evolves in time according to the master equation

$$\begin{aligned}\frac{dP(s_1,\ldots,s_N;t)}{dt} &= -\sum_j w_j(s_1,\ldots,s_j,\ldots,s_N)\\ &\quad\times P(s_1,\ldots,s_j,\ldots,s_N;t)\\ &\quad+\sum_j w_j(s_1,\ldots,-s_j,\ldots,s_N)\\ &\quad\times P(s_1,\ldots,-s_j,\ldots,s_N;t).\end{aligned} \tag{1}$$

The law of detailed balance requires that

$$\frac{w_j(s_1,\ldots,s_{j-1},1,s_{j+1},\ldots,s_N)}{w_j(s_1,\ldots,s_{j-1},-1,s_{j+1},\ldots,s_N)}=e^{-2E_j/T}, \tag{2}$$

where T is the temperature, and $-2E_j$ is the energy difference between the two states:

$$-2E_j=E(s_1,\ldots,1,\ldots,s_N)-E(s_1,\ldots,-1,\ldots,s_N). \tag{3}$$

If the energy $E\{s\}$ is given by a nearest-neighbor Ising Hamiltonian, then E_j depends only on the orientations of the spins adjacent to the site j.

The relation (2) assures that the thermal equilibrium distribution, $P\{s\}\propto e^{-E\{s\}/T}$, is a steady-state solution of (1). This relation does not completely determine the transition rates w_j, however, and a number of choices are possible. In Refs. 1 and 4–8, for example, the transition rates were chosen to be

$$w_j=\tfrac{1}{2}\gamma_0[1-s_j\tanh(E_j/T)], \tag{4}$$

where γ_0 is a constant. In the Monte Carlo work of Schneider *et al.*,[9] however, it was more convenient to use

$$\begin{aligned} w_j&=\gamma_0, &&\text{if } s_jE_j\leqslant 0,\\ &=\gamma_0 e^{-2s_jE_j/T}, &&\text{if } s_jE_j\geqslant 0.\end{aligned} \tag{5}$$

Our conclusions apply equally well to these two cases.

The kinetic Ising model discussed by Kawasaki[2] differs from the above, however, in that transitions involve the interchange of a *pair* of spins in his model, thus conserving the total magnetization. We shall discuss this case at the end.

Let f be any function of the spin variables $\{s_i\}$ and let $C_f(t)$ denote the time-dependent autocorrelation function of f, in thermal equilibrium,

$$C_f(t)\equiv\langle f^*(0)f(t)\rangle. \tag{6}$$

The master equation described by Eqs. (1)–(3) is purely relaxational, in the sense that all the eigenvalues of the "transition matrix" are real.[3] For any such system, the correlation function C_f has a spectral representation of the form

$$C_f(t)=\int_0^\infty \alpha_f(\nu)e^{-\nu|t|}\,d\nu, \tag{7a}$$

with

$$\alpha_f(\nu)\geqslant 0 \quad\text{for all } \nu \tag{7b}$$

(see, for example, Sec. 4 of Ref. 7). A representation such as (7) is *not* possible for more general dynamic systems, such as those describable by a Hamiltonian, where oscillations may take place. A number of useful inequalities follow immediately from this representation. For example, we have

$$C_f(t) > 0 \quad \text{for all } t, \tag{8}$$

$$\frac{dC_f}{dt} < 0 \quad \text{for all } t > 0. \tag{9}$$

Let us define the "characteristic time" τ_f and the "initial relaxation rate" ν_f for the variable f, according to

$$\tau_f \equiv \int_0^\infty \tilde{C}_f(t)\,dt/\tilde{C}_f(0)$$

$$= \int_{0^+}^\infty \alpha_f(\nu)\nu^{-1}\,d\nu/\tilde{C}_f(0), \tag{10}$$

$$\nu_f = -dC_f/dt|_{t=0^+}/\tilde{C}_f(0)$$

$$= \int_0^\infty \alpha_f(\nu)\nu\,d\nu/\tilde{C}_f(0), \tag{11}$$

where

$$\tilde{C}_f(t) = C_f(t) - C_f(\infty) = \int_{0^+}^\infty \alpha_f(\nu)e^{-\nu t}\,d\nu. \tag{12}$$

The quantity $C_f(\infty)$ is nonzero if α_f contains a δ-function contribution at $\nu=0$, which occurs when the equilibrium expectation value $\langle f\rangle$ is nonzero.

By applying the Schwarz inequality to Eqs. (10)–(12), one derives the relation

$$\tau_f \geq \nu_f^{-1}. \tag{13}$$

One also may show that

$$\frac{d^2}{dt^2}\ln C_f(t) \geq 0 \quad \text{for all } t \neq 0, \tag{14}$$

and thus

$$-\frac{d}{dt}\ln C_f(t) \leq \nu_f \quad \text{for all } t > 0, \tag{15}$$

$$C_f(t) \geq C_f(0)e^{-\nu_f|t|} \quad \text{for all } t. \tag{16}$$

[Similar relations hold for the function $\tilde{C}_f(t)$.]

Consider the case where f is $s(\vec{q})$, the spin density at wave vector $\vec{q}$:

$$s(\vec{q}) = N^{-1/2}\sum_i e^{i\vec{q}\cdot\vec{r}_i}s_i. \tag{17}$$

Then for the equal-time correlation function we have

$$\tilde{C}_{s(\vec{q})}(0) = T\chi(\vec{q}), \tag{18}$$

where $\chi(\vec{q})$ is the static susceptibility describing the linear response of the system to an applied magnetic field of wave vector $\vec{q}$. Abe[7] has shown that

$$\frac{d}{dt}\langle s_i(0)s_j(t)\rangle\,|_{t=0^+} = -R\delta_{ij}, \tag{19}$$

where

$$R = 2\langle w_j(s_1,\ldots,s_N)\rangle. \tag{20}$$

For transition probabilities given by (4) or (5), it is easily seen that R is a finite, continuous, positive function of T, and in fact $R(T_c)$ has been evaluated exactly for a number of two-dimensional lattices.[4,7] It follows that for any $\vec{q}$,

$$T\chi(\vec{q})\nu_{s(\vec{q})} = -\frac{d}{dt}\langle s^*(\vec{q},0)s(\vec{q},t)\rangle|_{t=0^+} = R, \tag{21}$$

$$\tau_{s(\vec{q})} \geq T\chi(\vec{q})/R. \tag{22}$$

For $q=0$, $N^{1/2}s(\vec{q})$ is just the total magnetization M, so that (22) is just the inequality proved by Abe and Hitano for the relaxation rate of the uniform magnetization,

$$\tau_M \geq T\chi(\vec{q}=0)/R. \tag{23}$$

If τ_M and χ exhibit power-law divergences near T_c,

$$\tau_M \sim |T-T_c|^{-\Delta}, \quad \chi(q=0) \sim |T-T_c|^{-\gamma}, \tag{24}$$

then (23) implies

$$\Delta \geq \gamma. \tag{25}$$

Let us next consider the case where f is the spin variable on a single site i. The single-spin autocorrelation time $\tau_A \equiv \tau_{s_i}$ is of particular interest because it is directly proportional to the linewidth for nuclear magnetic resonance, under appropriate circumstances.[10] Note that

$$\tilde{C}_{s_i}(0) = 1 - N^{-2}\langle M\rangle^2, \tag{26}$$

so that

$$\nu_{s_i} = R/(1 - N^{-2}\langle M\rangle^2) \tag{27}$$

is a continuous function of temperature. Consequently, the direct application of (13) does not imply any divergence for the single-spin autocorrelation time τ_A.

A more interesting result is obtained if one uses the relation

$$\tilde{C}_{s_i}(t) = \int\frac{d\vec{q}}{(2\pi)^d}\,\tilde{C}_{s(\vec{q})}(t), \tag{28}$$

where the integration is over the Brillouin zone, and d is the dimensionality of the lattice. From (10), (18), (26) and (13), we have

$$\tau_A\left(1 - \frac{\langle M\rangle^2}{N^2}\right) = \int\frac{d\vec{q}}{(2\pi)^d}\,T\chi(\vec{q})\tau_{s(\vec{q})} \tag{29a}$$

$$\geq \frac{T^2}{R}\int\frac{d\vec{q}}{(2\pi)^d}[\chi(\vec{q})]^2. \tag{29b}$$

Let us define the "reciprocal correlation length" κ as the largest value of $|q|$ such that

$$\chi(\vec{q}\,') \geq \tfrac{1}{2}\chi(q=0) \quad \text{for all } |q'| < |q|. \tag{30}$$

(This definition differs slightly from the more usual definition of κ, as will be discussed below.) If we assume that near T_c

$$\tau_A \sim |T - T_c|^{-\Delta_A}, \quad \kappa \sim |T - T_c|^{\nu}, \tag{31}$$

we find[11]

$$\Delta_A \geq 2\gamma - d\nu . \tag{32}$$

For the three-dimensional Ising model, it is believed that $\gamma \approx 1.25$, $\nu \approx 0.64$. Inequalities (25) and (32) thus become

$$\Delta \gtrsim 1.25 , \tag{33}$$

$$\Delta_A \gtrsim 0.58 . \tag{34}$$

For the two-dimensional Ising model, it is known that $\gamma = \frac{7}{4}$, $\nu = 1$. Inequalities (25) and (32) then give

$$\Delta \geq 1.75 , \tag{35}$$

$$\Delta_A \geq 1.5 . \tag{36}$$

In Ref. 9, Schneider *et al.* have extracted values of $\Delta \approx 1.75$, $\Delta_A \approx 1$ from their Monte Carlo calculations of a two-dimensional kinetic Ising model. The quoted value for Δ_A violates (36), and clearly is in error. In a more recent preprint,[12] Stoll *et al.* have carefully reanalyzed their Monte Carlo calculations, taking into account the inequalities derived in the present paper. In this new analysis, the values of the exponents have been revised to

$$\Delta = 1.90 \pm 0.10, \quad \Delta_A = 1.60 \pm 0.10 ,$$

which is consistent with inequalities (35) and (36), and with the dynamic scaling equation (38). The value of Δ may be compared with the estimate from high-temperature series expansions, $\Delta = 2.0 \pm 0.05$, given in Refs. 6 and 8. The value of Δ_A quoted in Ref. 9 is thus identified as an "effective" exponent, valid in a region not too near T_c. Stoll *et al.* have also obtained exponents for the energy-energy and energy-spin correlation functions, and have shown these to be consistent with rigorous inequalities derived by Schneider[13] and by Suzuki.[5]

It should be noted that the autocorrelation time τ_A is very much longer, near T_c, than would be predicted from the initial decay rate ν_{s_i} of the autocorrelation function. Thus in obtaining τ_A from calculated forms of the autocorrelation function $C_{s_i}(t)$, one must be careful to integrate for sufficiently large values of t. A useful check on calculated forms of $C_{s_i}(t)$, for finite times t, may be had by combining (28) with (16) and (21), employing an appropriate calculated form for $\chi(\vec{q})$. Similar checks have indeed been employed by Stoll *et al.* in the recent work referred to above.[12]

The inequality (29) may also be applied directly to check calculated values of τ_A at any temperature. For this purpose it is useful to note that the integral on the right-hand side of (29) may be written

$$T^2 \int \frac{d\vec{q}}{(2\pi)^d} [\chi(\vec{q})]^2 = \sum_j (\langle s_i s_j \rangle - N^{-2}\langle M \rangle^2)^2 . \tag{37}$$

In calculations based on high-temperature series expansions, or on Monte Carlo calculations, it is usually easier to calculate correlation functions in real space than in Fourier space.

Some additional remarks may help clarify the relationship of the present observations to previous work.

According to the "conventional" (Van Hove) theory of critical slowing down, expression (25) should hold as an equality, $\Delta = \gamma$. Evidence based on Wilson-type expansion methods,[14] as well as the earlier high-temperature series calculations,[6,8] suggests that in fact Δ is greater than γ.

The dynamic scaling hypothesis[15] predicts

$$\Delta_A = \Delta + \gamma - d\nu . \tag{38}$$

This is, of course, consistent with the inequalities (25) and (32), but is not in any way required by these inequalities.

The model considered by Kawasaki in Ref. 2 differs from the present model in that transitions conserve the total magnetization M, as was mentioned above. Since Kawasaki's model also comes from a master equation with a Hermitian transition matrix,[3] the general relations (7)–(16) apply in his case, as he noted in Ref. 2. Instead of Eqs. (21) and (22) however, Kawasaki has

$$-\frac{d}{dt} \langle s^*(\vec{q}, 0) s(\vec{q}, t) \rangle_{t=0^+} = r q^2 , \tag{39}$$

$$\tau_{s(q)} \geq T\chi(q)/q^2 r , \tag{40}$$

where r is a continuous function of $\vec{q}$ and T, whose value remains finite and positive at $\vec{q} = 0$, and $T = T_c$. In two dimensions, it is seen from Eq. (29a) that the single-spin autocorrelation time τ_A must be infinite at any temperature T, for Kawasaki's model. In three dimensions τ_A will exist for any T other than T_c, and the divergence of τ_A near T_c must satisfy

$$\Delta_A \geq 2\gamma - \nu . \tag{41}$$

The same results apply to the first of the two models considered by Kadanoff and Swift.[3]

Finally, we comment on the definition of the reciprocal correlation length κ [Eq. (30)] used in the present paper. A number of different definitions are commonly employed for κ.[16] For example, κ is frequently defined to be the rate of exponential decay of the spin-spin correlation function at large separations of the two spins. A second common choice is to define κ^{-2} as the ratio of the second and zeroth spatial moments of the correlation function. If *static scaling* holds, these definitions differ from each other and from the present definition only by a factor of order unity, so that the exponent ν is the same for all definitions. The static scaling laws are known to hold in two dimensions, and in fact there is no evidence in any system for breakdown of the weak form of static scaling required here. If one wishes nevertheless to entertain the possibility of more than one exponent ν in, say, the three-dimensional Ising system, then of course one must consider that inequalities (32) and (41) may hold for some definitions of ν but not others.

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