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Non-equilibrium dynamics of the one-dimensional Glauber model

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Abstract: We study the relaxation of the one-dimensional Glauber model towards equilibrium at finite temperature, taking averages over all possible initial configurations. Let $C(q,t)$ denote the spatial Fourier transform of the equal-time two-point correlation function $\langle\sigma_0\sigma_n\rangle_t$. It can be written as the Laplace transform of a relaxation spectrum $\rho_q(\omega)$. The latter turns out to contain a non-integrable singularity at a q-dependent frequency $\omega = \theta(q)$. The singularity originates from the self-term in the equations of motion and has important consequences. E.g., it produces the dominating finite-size correction to $C(q,t)$. As a consequence, we are able to formulate a finite-size scaling theory in the limit of zero temperature, long times and small wave vectors.

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1. Introduction

Most problems in the field of non-equilibrium statistical mechanics appear to be rather unaccessible for theoretical analysis. The present paper deals with the simple looking question how a system in thermodynamical equilibrium at an initial temperature T_0 is relaxing in time when it is suddenly cooled towards a second order phase transition temperature T_c. Exact calculations on this problem are possible for the one-dimensional Ising model with Glauber dynamics, altough in this case the transition occurs at $T_c = 0$. In particular, scaling of the non-equilibrium equal-time correlation function $C(q,t)$ has been described recently by Bray[BA]. These results are reproduced here starting from an exact expression for $C(q,t)$ instead of an approximate one.

As a technical tool we introduce the relaxation spectrum $\rho_q(\omega)$ which is in fact the non-equilibrium analogue of the frequency-dependent structure function (which itself is the Fourier transform with respect to space and time of the two-point correlation function). In systems in equilibrium the frequency-dependent structure function cannot be negative. Here, the relaxation spectrum will be shown to be positive for small ω and negative for large ω, both regions being separated by a non-integrable singularity. In order to clarify the important rôle of this singularity we show that it determines the leading order finite size corrections to scaling.

According to Pandit et al.[PF], dynamical finite-size scaling theory cannot be applied in the one-dimensional Ising model because the gap in the hamiltonian vanishes when the temperature tends to zero, even if the system is still finite. The corresponding slowly relaxing mode can be identified to be the uniform magnetisation. If however averages are taken over all possible initial configurations then by symmetry the average magnetisation will remain zero at all times and the slowly relaxing mode is absent. It is then feasible and meaningful to calculate the finite-size corrections to the equal-time pair correlation function. The interest of doing so is that the one-dimensional Ising model offers the unique opportunity of exact calculations.

2. Model

A *configuration* η of the system with size N is a map from $\{0, 1, \cdots, N-1\}$ into $\{-1, 1\}$. The *spin variables* $\sigma_0, \sigma_1, \cdots \sigma_{N-1}$ are defined by $\sigma_n(\eta) = \eta(n)$.

The time evolution of the kinetic Ising model is described by the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\eta; t) = \sum_{n=0}^{N-1} \left[c_n(\eta^n) P(\eta^n; t) - c_n(\eta) P(\eta; t) \right] \tag{2.1}$$

where η^n is defined by $\eta^n(n) = -\eta(n)$, and $\eta^n(m) = \eta(m)$ otherwise, and where $c_n(\eta)$ is the *rate* with which the sign of $\eta(n)$ changes. In the Glauber model these transition rates are given by

$$c_n = \frac{1}{2} \left[1 - \frac{\gamma}{2} \sigma_n (\sigma_{n-1} + \sigma_{n+1}) \right] \tag{2.2}$$

(periodic boundary conditions are used in case of finite N). The parameter γ is related to the inverse of the temperature T in such a way that $\gamma \to 1$ when $T \to 0$ ($\gamma = \tanh(2J/k_B T)$ where $J > 0$ is the interaction strength of the Ising model and k_B is Boltzmann's constant).

The non-equilibrium equal-time two-point correlation function is the expectation $\langle \sigma_0 \sigma_n \rangle_t$ of the product of the two spin variables σ_0 and σ_n with respect to the distribution of configurations at time t. It satisfies the equations of motion:

$$\frac{\partial}{\partial t} \langle \sigma_0 \sigma_n \rangle_t = -2\langle \sigma_0 \sigma_n \rangle_t + \gamma \left(\langle \sigma_0 \sigma_{n-1} \rangle_t + \langle \sigma_0 \sigma_{n+1} \rangle_t \right), \qquad (n \neq 0) \tag{2.3}$$

Introduce the Fourier transformed correlation function

$$C(q,t) = \sum_{n=0}^{N-1} e^{iqn} \langle \sigma_0 \sigma_n \rangle_t \tag{2.4}$$

Then (2.3) becomes (using periodic boundary conditions)

$$\frac{\partial}{\partial t} C(q,t) = -\theta(q) C(q,t) + \frac{1}{N} \sum_{q^*} \theta(q^*) C(q^*,t) \tag{2.5}$$

with $\theta(q) = 2(1 - \gamma \cos(q))$.

3. Infinite system

The equations of motion (2.5) can be solved by taking the Laplace transform $\tilde{C}(q,z)$ of $C(q,t)$. One obtains in the limit $N \to \infty$

$$\tilde{C}(q,z) = \frac{\sqrt{z^2 + 4z + 4(1-\gamma^2)}}{z(z + \theta(q))} \tag{3.1}$$

((16) of ref. [BA] coincides with (3.1) for $z \to 0$, $q \to 0$).

By inverse Laplace transform of $\tilde{C}(q,z)$ one obtains $C(q,t)$. It is however easier to make the *ansatz* that $\tilde{C}(q,z)$ is the Stieltjes transform of a relaxation spectrum $\rho_q(\omega)$

$$\tilde{C}(q,z) = \frac{1}{z} C(q,\infty) + \int_0^\infty \mathrm{d}\omega \ \rho_q(\omega) \frac{1}{z + \omega} \tag{3.2}$$

with

$$C(q,\infty) = \frac{2\sqrt{1-\gamma^2}}{\theta(q)} \tag{3.3}$$

and then to calculate the inverse Stieltjes transform

$$\rho_q(\omega) = -\frac{1}{\pi} \mathrm{Im} \left[\tilde{C}(q, -\omega + i0) - \frac{C(q,\infty)}{-\omega + i0} \right], \qquad \omega > 0 \tag{3.4}$$

One obtains

$$\rho_q(\omega) = \frac{1}{\pi} \frac{\sqrt{4\gamma^2 - (\omega-2)^2}}{\omega\,[\theta(q) - \omega]} \quad \text{if} \quad 2(1-\gamma) \le \omega \le 2(1+\gamma) \qquad (3.5)$$
$$= 0 \quad \text{otherwise}$$

See fig. 1. Note that $\rho_q(\omega)$ contains a non-integrable singularity at $\omega = \theta(q)$. Now $C(q,t)$ is obtained as the Laplace transform of $\rho_q(\omega)$:

$$C(q,t) = C(q,\infty) + \mathbf{P}\int_0^\infty \rho_q(\omega) e^{-\omega t}\,\mathrm{d}\omega \qquad (3.6)$$

The symbol $\mathbf{P}$ indicates that the principal value has to be taken when integrating through the singularity. By a change of integration variable one obtains

$$C(q,t) = C(q,\infty) + \frac{1}{\pi}\mathbf{P}\int_0^\pi \frac{X_t(q^*,q)}{q-q^*}\,\mathrm{d}q^* \qquad (3.7)$$

with

$$X_t(q^*,q) = \frac{4\gamma^2 - (\theta(q^*)-2)^2}{\theta(q^*)}\; e^{-\theta(q^*)t}\; \frac{q-q^*}{\theta(q)-\theta(q^*)} \qquad (3.8)$$

Because $\rho_q(\omega) \ge 0$ for small ω one has always for long times that $C(q,t) > C(q,\infty)$. In fact, there exists a time-dependent wave vector $q_0(t)$ which tends to zero as $t \to \infty$ in such a way that $C(q,t) > C(q,\infty)$ if and only if $q > q_0(t)$. For small $q \neq 0$ this implies that $C(q,t)$ will first rise and cross the equilibrium value $C(q,\infty)$ and then, for long times, will converge by decreasing. See fig. 2.

4. Finite-size corrections

Now we calculate $C(q,t)$ for a finite ring with N spins. Then, by comparison with the result for the infinite system, we can understand the origin of the singularity in $\rho_q(\omega)$. In addition, finite-size corrections can be calculated.

We use the method of Reiss[RH]. It was introduced to generalise Glauber's method[GR] to the case of temperature varying with time. Here we assume an initial configuration corresponding to infinite temperature, and evolution of the system with Glauber dynamics at fixed temperature. The result of the calculations is

$$\langle\sigma_0\sigma_n\rangle_t = \frac{2\gamma}{N} \sum_{m\ \mathrm{odd},=1}^{N-1} \sin(\pi\frac{mn}{N})\sin(\pi\frac{m}{N})\frac{1-e^{-\theta(q_m)t}}{\theta(q_m)} \qquad (4.1)$$

with $q_m \equiv \pi m/N$. After Fourier-transformation one obtains

$$C_N(q_{2n},t) = C_N(q_{2n},\infty) + \frac{2}{N}\sum_{m\ \mathrm{odd},=1}^{N-1} \frac{X_t(q_m,q_{2n})}{q_{2n}-q_m} \qquad (4.2)$$

where X_t has been defined in (3.8). Hence a near-singularity is already present in the finite system and obviously, (4.2) converges to (3.7) as $n \to \infty$, $N \to \infty$ in such a way that $q = q_{2n} \equiv 2\pi n/N$ remains constant.

Note that the longest relaxation time is $1/\theta(\pi/N)$ which becomes $1/4\sin^2(\pi/2N)$ at zero temperature ($\gamma = 1$). Hence, in contrast to the situation of ref. [PF], in the finite system the gap in the spectrum of the generator of the time evolution does not vanish in the limit of zero temperature (see the introduction).

At this point we need a trick to calculate the difference between $C(q,t)$ and $C_N(q,t)$ to first order in $1/N$. The essence is that the function $q^* \to X_t(q^*, q)$ is analytic also in the point $q^* = q$. In fact, from the definition (3.8) follows

$$X_t(q,q) = \frac{\sqrt{4\gamma^2 - (\theta(q) - 2)^2}}{\theta(q)} \; e^{-\theta(q)t} \tag{4.3}$$

For convenience we take N even. The integral in (3.7) can be split into two parts, one containing the singularity, the other containing the complicated but regular contribution. The latter integral can be approximated by a sum.

$$\begin{aligned}
&C(q,t) - C(q,\infty) \\
&= X_t(q,q)\frac{1}{\pi}\mathbf{P}\int_0^\pi \frac{1}{q - q^*}\, dq^* + \frac{1}{\pi}\int_0^\pi \frac{X_t(q^*,q) - X_t(q,q)}{q - q^*}\, dq^* \\
&= -X_t(q,q)\frac{1}{\pi}\ln\frac{\pi - q}{q} + \frac{2}{N}\sum_{m \text{ odd},=1}^{N-1} \frac{X_t(q_m,q) - X_t(q,q)}{q - q_m} + \mathrm{O}\left(N^{-2}\right) \\
&= C_N(q,t) - C_N(q,\infty) + \frac{1}{N}X_t(q,q)\left[\frac{1}{q} - \frac{1}{\pi - q}\right] + \mathrm{O}\left(N^{-2}\right)
\end{aligned} \tag{4.4}$$

In the last line we used that

$$\frac{2}{N}\sum_{m \text{ odd},=1}^{N-1} \frac{1}{q_{2n} - q_m} = -\frac{1}{\pi}\ln\frac{\pi - q}{q} + \frac{1}{N}\left[\frac{1}{\pi - q} - \frac{1}{q}\right] + \mathrm{O}\left(N^{-2}\right) \tag{4.5}$$

The second term in the r.h.s. of (2.5) is sometimes called the *self*-contribution, because it arises from the fact that (2.3) is not valid for $n = 0$ (note that $N^{-1}\sum_q \theta(q)C(q,t) = 2 - \gamma\langle\sigma_0\sigma_1\rangle_t - \gamma\langle\sigma_0\sigma_{N-1}\rangle_t$). If one omits the self-term in (2.5) then $C(q,t)$ relaxes in a pure exponential way with relaxation time $1/\theta(q)$. Hence the structure of the relaxation spectrum $\rho_q(\omega)$ originates fully from this self-contribution. In this light it is not unexpected that the leading-order correction term to $C(q,t)$ relaxes as $\exp(-\theta(q)t)$, as follows from (4.3) and (4.4).

Finally, note that the finite-size analogue of (3.1) is

$$\tilde{C}_N(q,z) = \tilde{C}(q,z)\frac{1 - K(z)^N}{1 + K(z)^N} \tag{4.6}$$

with

$$K(z) = \frac{1}{2\gamma}\left(2 + z - \sqrt{z^2 + 4z + 4(1-\gamma)^2}\right) \tag{4.7}$$

5. Finite-size scaling

Introduce the scaling variables

$$a = 2(1-\gamma)t \qquad \text{and} \qquad b = 2\gamma(1-\cos(q))t \tag{5.1}$$

Note that the thermal correlation length ξ is approximately equal to $1/\sqrt{2(1-\gamma)}$. Hence the choice of the scaling variable a implies a dynamic exponent $z = 2$. By a change of integration variable, (3.6) becomes, in the limit of $t \to \infty$, $q \to 0$, and $\gamma \to 1$,

$$C(q,t) = C(q,\infty) + \sqrt{t}\; g_0(a,b) + \cdots \tag{5.2}$$

with the scaling function g_0 given by

$$g_0(a,b) = 2e^{-a}\pi^{-1}\mathbf{P}\int_0^\infty \mathrm{d}y\; e^{-y}\frac{\sqrt{y}}{(y+a)(b-y)} \tag{5.3}$$

Note that g_0 can be rewritten as

$$g_0(a,b) = -\frac{2\sqrt{a}}{a+b} + \frac{2}{a+b}\frac{1}{\sqrt{\pi}}\int_0^1 \mathrm{d}y\frac{1}{\sqrt{y}}\;\left\{a\; e^{-ay} + b\; e^{-a-b(1-y)}\right\} \tag{5.4}$$

and hence coincides with the scaling function proposed by Bray[BA].

The relaxation spectrum corresponding with (5.2), (5.3) is

$$\begin{aligned} \rho_q(\omega) &= \frac{2}{\pi}\frac{\sqrt{\omega-\omega_0}}{\omega(k^2+\omega_0-\omega)} \qquad && \text{if } \omega \geq \omega_0 \\ &= 0 \qquad \text{if } \omega \leq \omega_0 && \end{aligned} \tag{5.5}$$

with the gap frequency $\omega_0 = 2(1-\gamma) \simeq \xi^{-2}$ and the scaled wave vector k such that $k^2 = 2\gamma(1-\cos q) \simeq q^2$. In fact, (5.5) can be obtained immediately from (3.5) by assuming that ω and ω_0 are small.

In finite-size scaling[BM] the extra scaling variable that one expects is t/N^2 (note that $z = 2$). Let

$$c = \sqrt{t}/N \tag{5.6}$$

¿From (4.4) and (5.2) follows in the limit of $t \to \infty$, $q \to 0$, and $\gamma \to 1$

$$C_N(q,t) - C_N(q,\infty) = \sqrt{t}\left[g_0(a,b) + c\; g_1(a,b) + \mathrm{O}(c^2)\right] + \cdots \tag{5.7}$$

with

$$g_1(a,b) = 2\frac{e^{-(a+b)}}{a+b} \tag{5.8}$$

This result is compatible with the existence of a scaling function g such that

$$C_N(q,t) - C_N(q,\infty) = \sqrt{t}\ g(a,b,c) + \cdots \tag{5.9}$$

The leading order correction to the relaxation spectrum (5.5) is a Dirac-delta function at the frequency $\omega_0 + k^2$

$$\frac{2}{\omega N}\delta(\omega - \omega_0 - k^2) \tag{5.10}$$

with k and ω as in (5.5).

6. Epilogue

We expect some of our formulas to be more generally valid. However, already a modest generalisation like replacing the Glauber dynamics by some other dynamics satisfying detailed balance with respect to the Ising Hamiltonian makes the present approach very hard, if not impossible. Indeed, in general the equations of motion (2.3) are not closed but involve products of more than 2 spin variables. Hence it is not clear how to obtain (3.1) in closed form. Therefore, more abstract methods will be needed.

References

[BM] see e.g. M.N. Barber, *Finite-size Scaling,* in: Phase Transitions and Critical Phenomena, Vol. 8, ed. C. Domb and J.L. Lebowitz (Academic Press, 1983), p. 145 — 266.

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Figure Captions

Fig. 1: Spectral density $\rho_q(\omega)$ as a function of ω for $\gamma = 0.9$ and $\theta(q) = 0.4$ (see 3.5).

Fig. 2: $C(q,t)$ as a function of q for $t = 0.2, 1.0, 5.0$ and $\gamma = 0.8$ obtained by numerical integration of (3.7); the dashed line is the $t = \infty$ result.