Large Fluctuations of Local Magnetizations

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Large spatial-fluctuations of local magnetizations in the Ising chain are studied from the rigorous treatment of the fluctuation spectrum and the generalized spatial correlations. It is shown that at low temperatures the functions relevant to the large fluctuations satisfy scaling laws near a certain characteristic value q_* of the intensive variable q relevant to the present approach.

1. Introduction

Consider a magnetic system with the Hamiltonian

$$H_N(h) = H_N(0) - h \sum_{i=1}^{N} S_i, \tag{1.1}$$

where $H_N(0)$, N being the number of spins, is the Hamiltonian without magnetic field, S_i is a certain component of the i-site spin varibable and h is the applied scalar magnetic field. The Gibbs free energy $g(\beta,h)$ per spin for the inverse temperature β is given by

$$Z_N(\beta,h) = \mathrm{Tr}e^{-\beta H_N(h)} \sim e^{-\beta g(\beta,h)} \tag{1.2}$$

for large N provided that the interaction range is finite. The magnetization $m^0(h)$ and the susceptibility $\chi^0(h)$ per spin are given as

$$m^0(h) = -g_1(\beta,h), \quad \chi^0(h) = \frac{\partial m^0(h)}{\partial h} = -g_2(\beta,h), \tag{1.3}$$

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where $g_l(\beta,h) = \partial^l g(\beta,h) / \partial h^l$, $(l=1,2)$.

The fact that the relative fluctuation strength of the total magnetization is small $(=O(1/\sqrt{N}))$ for a large N does not imply that fluctuation of local magnetizations are small. In fact slightly above a magnetic critical point, the strong spatial correlation causes the development of magnetic domain structures highly correlated. This yields a large deviation of the average magnetization over the domain from that for the whole system. The present paper deals with such large fluctuations of local magnetizations for the Ising chain.

2. Large fluctuations of local magnetizations

Let us take a one semi-macroscopic magnetic region composed of n spins. The average local magnetization over the region,

$$m_n = \frac{1}{n} \sum_{j=1}^{N} S_j, \tag{2.1}$$

approaches the ensemble average, i.e., $m_\infty = m^0(0)$ as $n \to \infty$. For a large but finite n, m_n is a fluctuating quantity and its probability distribution $\rho_n(m)$ is given by

$$\rho_n(m) \equiv \langle \delta(m_n - m) \rangle, \tag{2.2}$$

where $\langle \cdots \rangle = \mathrm{Tr} \cdots e^{-\beta H_N(0)} / Z_N(\beta, 0)$. *The extensivity of* nm_n suggests that the generating function

$$M_q(n) \equiv \langle e^{qnm_n} \rangle = \int_{-\infty}^{\infty} \rho_n(m') e^{qnm'} dm', \tag{2.3}$$

takes the form [1,2]

$$M_q(n) \sim e^{\phi(q) n}, \tag{2.4}$$

for large n as long as the interaction range is finite. The expression (2.4) is consistent with the asymptotic behavior

$$\rho_n(m) \sim \sqrt{n} e^{-\sigma(m)n}. \tag{2.5}$$

The *fluctuation spectrum* [1,2] $\sigma(m)$ is thus identical to the decay rate of the fluctuation m as n increased. Evaluating (2.3) with the saddle point method yields

$$\phi(q) = -\min_{m'} [\sigma(m') - qm'], \tag{2.6}$$

($\phi''(q)>0$, $\sigma''(m)>0$) . In Ref. [3] the same approach was applied to the analysis of large fluctuations of 2d Ising spin patterns near the critical point.

On the other hand, the generating function $M_q(n)$ asymptotically takes the form $M_q(n) \sim Z_{N-n}(\beta,0)\, Z_n(\beta,q/\beta)/Z_N(\beta,0)$ for $N \to \infty$ *and* $n \to \infty$, since the contribution of the interface can be neglected in comparison with the bulk contribution. One obtains

$$\phi(q) = -\beta\{g(\beta, \frac{q}{\beta}) - g(\beta,0)\}, \tag{2.7}$$

or equivalently

$$g(\beta,h) - g(\beta,0) = -\frac{1}{\beta}\phi(\beta h). \tag{2.8}$$

This argrees with the expression of the characteristic function for the whole system [1]. We define

$$m(q) \equiv \phi'(q), \quad \chi(q) \equiv \frac{dm(q)}{dq} \equiv \phi''(q). \tag{2.9}$$

The magnetization $m^0(h)$ and the susceptibility $\chi^0(h)$ are thus obtained as $m^0(h) = m(\beta h)$ and $\chi^0(h) = \beta\chi(\beta h)$.

Since the function $\phi(q)$ characterizes the fluctuation statistics of local magnetizations without magnetic field, r.h.s of(2.8) describes the properties of the whole system under the magnetic fields $h=0$ and $h=k_B T_q$.

It is possible to find and the magnetic-field dependence of the total magnetization interms of fluctuations of local magnetizations without magnetic field. Namely by observing $m^0(h)$ as a function of external field h, the numerical integration of (2.7) yields $\phi(q) = \beta \int_0^{q/B} m^0(h')\, dh'$, provided that $m^0(h)$ is a unique function of h. Thus the observation of the relationship between the applied external field and the *total magnetization*, enables us to determine the fluctuation spectrum relevant to the *local fluctuation-characteristic* without external field. On the contrary once $\phi(q)$ is observed, the free-energy difference for the corresponding magnetic field is obtained (Eq. (2.8)) .

Turn to spatial correlations. We introduce generalized spatial power spectra of fluctuations without magnetic field by [4]

$$I_q(\boldsymbol{k}) \equiv \lim_{n\to\infty} \frac{< I_n\{\boldsymbol{k}\}\, \delta\ (m_n - m(q)) >}{\rho_n(q)} \quad , \tag{2.10}$$

with

$$I_n\{\boldsymbol{k}\} \equiv \frac{1}{n} \mid \sum_{j=1}^{N} (S_j - m(q)) e^{-ikr_j} \mid^2, \tag{2.11}$$

where r_j the position vector of the j-th spin site. This describes the spatial correlation over the region whose magnetization per spin is $m(q)$ [3]. Equation (2.10) is rewritten as

$$I_q(\boldsymbol{k}) = \lim_{n\to\infty} \frac{< I_n\{\boldsymbol{k}\}\, e^{qnm_n} >}{M_q(n)} \ , \tag{2.12}$$

since the space region where the spatial power specturm is taken is chosen to be more larger than any correlation length. This leads to the equality

$$I_q(\boldsymbol{k}) = \mathrm{I}\ (\boldsymbol{k};\ \frac{q}{\beta}\ ), \tag{2.13}$$

where $I\ (\boldsymbol{k};h) = \lim_{n\to\infty} \mathrm{Tr}e^{-\beta H_n(h)}\ I_n\{\boldsymbol{k}\} / Z_n(\beta, h)$ is the ordinary power spectrum under the magnetic field h. The inverse Fourier transform of $I_q(\boldsymbol{k})$ yields the order-q double point correlation function $C_q(\boldsymbol{R})$, R being the relative vector between those points.

The observation of the ordinary power spectrum $I(\boldsymbol{k};h)$ thus immediately yields the order-q power spectrum $I_q(\boldsymbol{k})$ for $q = \beta h$ describing the spatial correlation over the region whose magnetization per site is $m(q)$. Inversely, if $I_q(\boldsymbol{k})$ is known, one gets the ordinary power spectrum $I(\boldsymbol{k};h = k_B T_q)$.

3. Ising chain

The Hamiltonian of the Ising chain is given by

$$H_N(h) = -J \sum_{j=1}^{N} S_j S_{j+1} + h \sum_{j=1}^{N} S_j , \tag{3.1}$$

($S_{N+1}=S_1$, $S_j=\pm 1$). In terms of the well-known expressin of the partition function [5]

$$Z_N(h) = [\upsilon_+(h)]^N + [\upsilon_-(h)]^N . \tag{3.2}$$

with

$$\upsilon_\pm(h) = \mathrm{e}^K \cosh(\beta h) \pm \sqrt{\mathrm{e}^{2K} \sinh^2(\beta h) + \mathrm{e}^{-2K}} , \tag{3.3}$$

($K=\beta J$), the free energy is obtained as $g(\beta, h) = -k_B T \log \nu_+(h)$. This yields

$$\phi(q) = \log \left[\frac{\mathrm{e}^K \cosh(q) + \sqrt{\mathrm{e}^{2K} \sinh^2(q) + \mathrm{e}^{-2K}}}{\mathrm{e}^K + \mathrm{e}^{-K}} \right] , \tag{3.4}$$

$$m(q) = \frac{\mathrm{e}^K \sinh(q)}{\sqrt{\mathrm{e}^{2K} \sinh^2(q) + \mathrm{e}^{-2K}}} , \tag{3.5}$$

$$\chi(q) = \frac{\mathrm{e}^{-K} \cosh(q)}{[\mathrm{e}^{2K} \sinh^2(q) + \mathrm{e}^{-2K}]^{3/2}} \tag{3.6}$$

$$\sigma(m) = m \log \left[\frac{m}{\sqrt{1-m^2}} \right] \mathrm{e}^{-2K} + \sqrt{1 + \frac{m^2}{1-m^2} \mathrm{e}^{-4K}} \tag{3.7}$$

$$-\log \left[\mathrm{e}^K \sqrt{1 + \frac{m^2}{1-m^2} \mathrm{e}^{-4K}} + \frac{\mathrm{e}^{-K}}{\sqrt{1-m^2}} + \log(\mathrm{e}^K + \mathrm{e}^{-K}) \right]$$

Furthermore the order-q double point correlation function is obtained as

$$C_q(R) = C_q(0)\ (\mathrm{sgn}\ (J))^R \mathrm{e}^{-R/\xi_q}, \tag{3.8}$$

($R = 0,1,2,\cdots\cdots$), with the variance

$$C_q(0) = \frac{\mathrm{e}^{-2K}}{\mathrm{e}^{2K}\sinh^2(q) + \mathrm{e}^{-2K}}, \tag{3.9}$$

and the correlation length ξ_q

$$\xi_q = \{2\log\ [\frac{\mathrm{e}^K\cosh(q) + \mathrm{e}^{2K}\sinh^2(q) + \mathrm{e}^{-2K}}{\sqrt{|\mathrm{e}^{2K} - \mathrm{e}^{-2K}|}}]\}^{-1} \tag{3.10}$$

Consider two limits, $T \to \infty$ and $T \to 0$. For the high temperature limit, the trivial results $\phi(q) = \log\ [\cosh(q)]$ and $\xi_q \to 0$ are obtained, which simply implies there is no spatial correlation among spins. For the low temperature limit, scaling laws for re levant functions hold as follows.

A. Ferromagnetic coupling (J>0)

By putting $\kappa = \mathrm{e}^{-2K}$, the scaling law for thermodynamic functions is obtained as

$$\begin{aligned} &\phi(q) = \kappa\ (\sqrt{1+\frac{q^2}{\kappa^2}} - 1), \qquad m(q) = \frac{q}{\kappa} \Big/ \sqrt{1+\frac{q^2}{\kappa^2}} \\ &\chi(q) = \kappa^{-1}\ (1 - \frac{q^2}{\kappa^2})^{-3/2}, \qquad \sigma(m) = \kappa\ (1 - \sqrt{1-m^2}) \end{aligned} \tag{3.11}$$

The correlation function satisfies

$$C_q(0) = (1 + \frac{q^2}{\kappa^2})^{-1}, \quad \xi_q = \frac{\kappa^{-1}}{2\sqrt{1+\frac{q^2}{\kappa^2}}} \tag{3.12}$$

See Fig. 1.

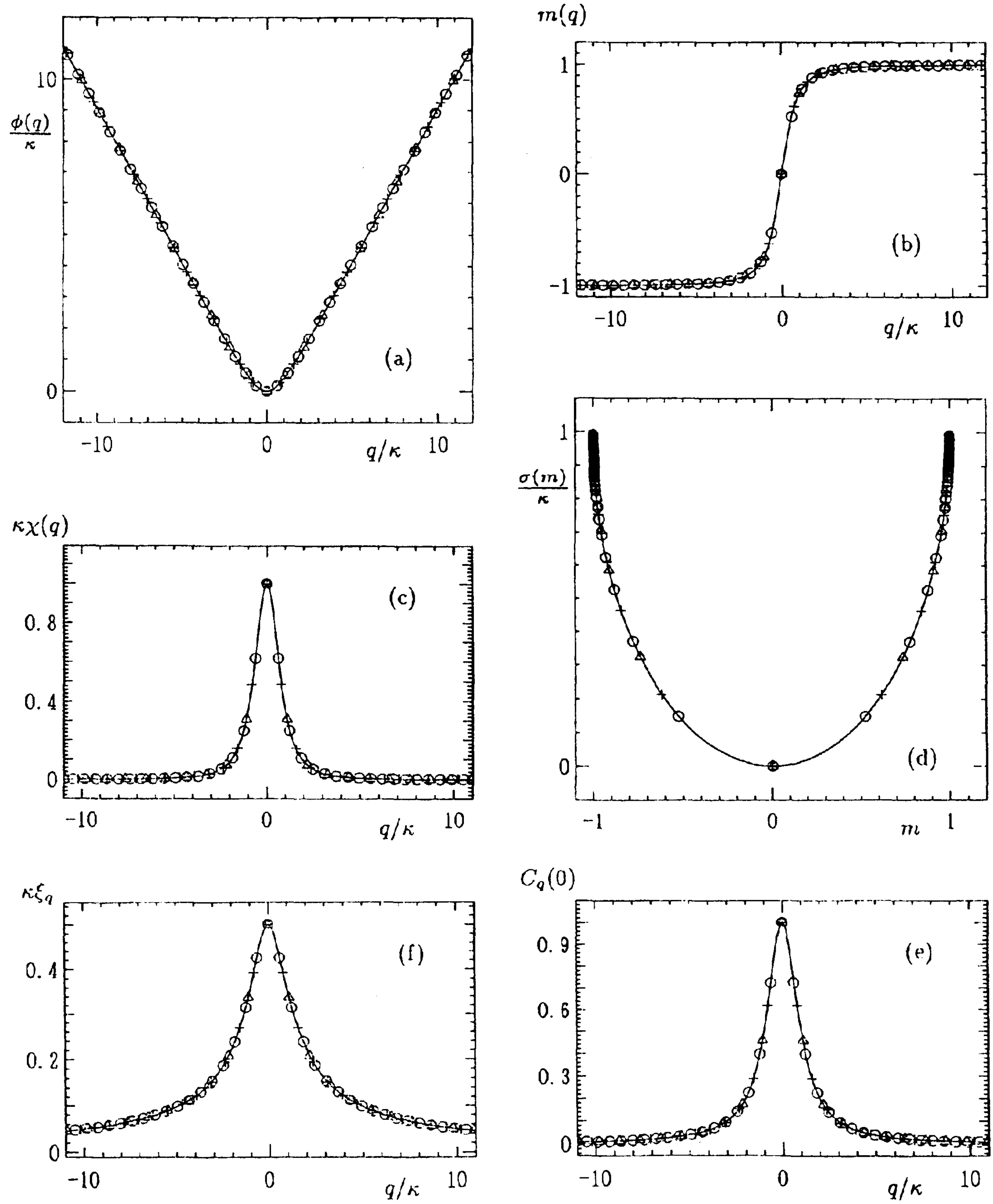

Fig. 1 . Scaling laws of thermodynamic functions (a−d) and order-q double point correlation functions (e,f) for ferromagnetic Ising chain at low temperatures. Symbols correspond to k_BT/J=0.15(○), 0.3(+) and 0.5(△). The solid lines are the analytic results in (3.11) and (3.12). For small T scaling relations hold.

B. Antiferromagnetic coupling (J<0)

In this case, there occur two types of scaling behaviors. First let q be kept finite. For a low temperature limit ($K \to -\infty$), putting $\kappa \equiv e^{2K}$, we get

$$\phi(q) = 2\kappa \sinh^2\left(\frac{q}{2}\right), \quad m(q) = \kappa \sinh(q)$$

$$\chi(q) = \kappa \cosh(q), \tag{3.13}$$

$$\sigma(m) = \kappa \left\{ \frac{m}{\kappa} \log\left(\frac{m}{\kappa} + \sqrt{1+\frac{m^2}{\kappa^2}}\right) + 1 - \sqrt{1+\frac{m^2}{\kappa^2}} \right\}$$

The correlation function is obtained as

$$C_q(0) = 1, \qquad \xi_q = \frac{\mathrm{sech}(q)}{2\kappa}. \tag{3.14}$$

See Fig. 2.

The second is seen for large $|q|$ values. Define the characteristic value q_* via $q_* = \sinh^{-1}(e^{-2K}) = \log(e^{-2K} + \sqrt{1+e^{-4K}}) \simeq 2|K| + \log 2$. Consider the case near $q = |q_*|$. After slight calculations Eqs. (3.4−6) reduce to

$$\phi(q) = \log\left[e^{\varepsilon q - q_*} + \sqrt{1+e^{2(\varepsilon q - q_*)}}\right]. \tag{3.15}$$

$$m(q) = \frac{\varepsilon e^{\varepsilon q - q_*}}{\sqrt{1+e^{2(\varepsilon q - q_*)}}}, \tag{3.16}$$

$$\chi(q) = \frac{e^{\varepsilon q - q_*}}{[1+e^{2(\varepsilon q - q_*)}]^{3/2}}, \tag{3.17}$$

near $q = \varepsilon q_*$, ($\varepsilon = \pm$). Accordingly the fluctuation spectrum takes the form

$$\sigma(m) = q_*|m| + |m|\log|m| \tag{3.18}$$
$$- \frac{1}{2}(1+|m|)\log(1+|m|) + \frac{1}{2}(1-|m|)\log(1-|m|).$$

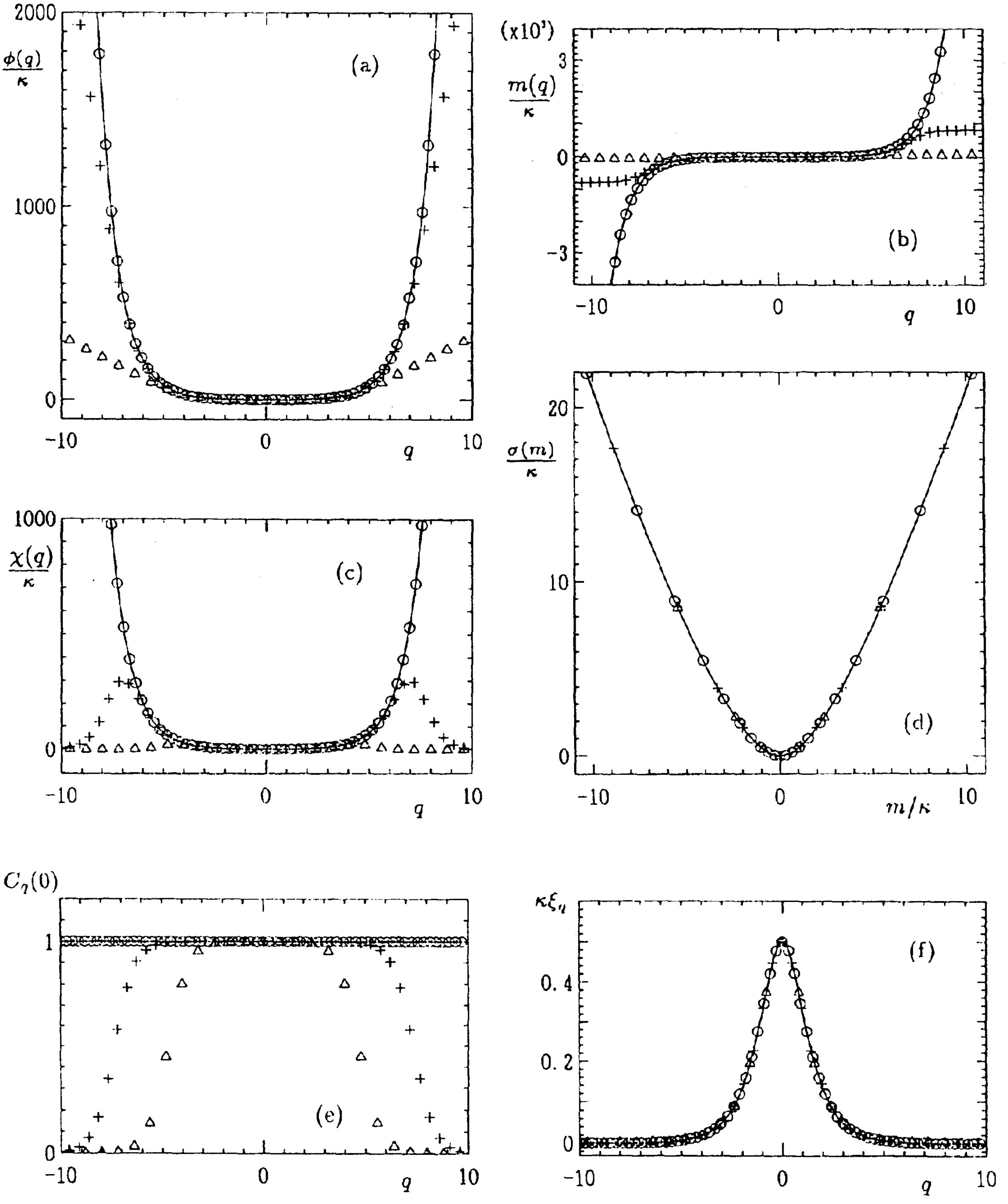

Fig. 2. Scaling laws of thermodynamic functions (a-d) and order-q double point correlation functions (e,f) for antiferromagnetic Ising chain at low temperatures. Symbols correspond to $k_B T/J$=0.15(○), 0.3(+) and 0.5(△). The solid lines are the analytic results in (3.13) and (3.14). For small T scaling relations hold.

See Fig. 3.

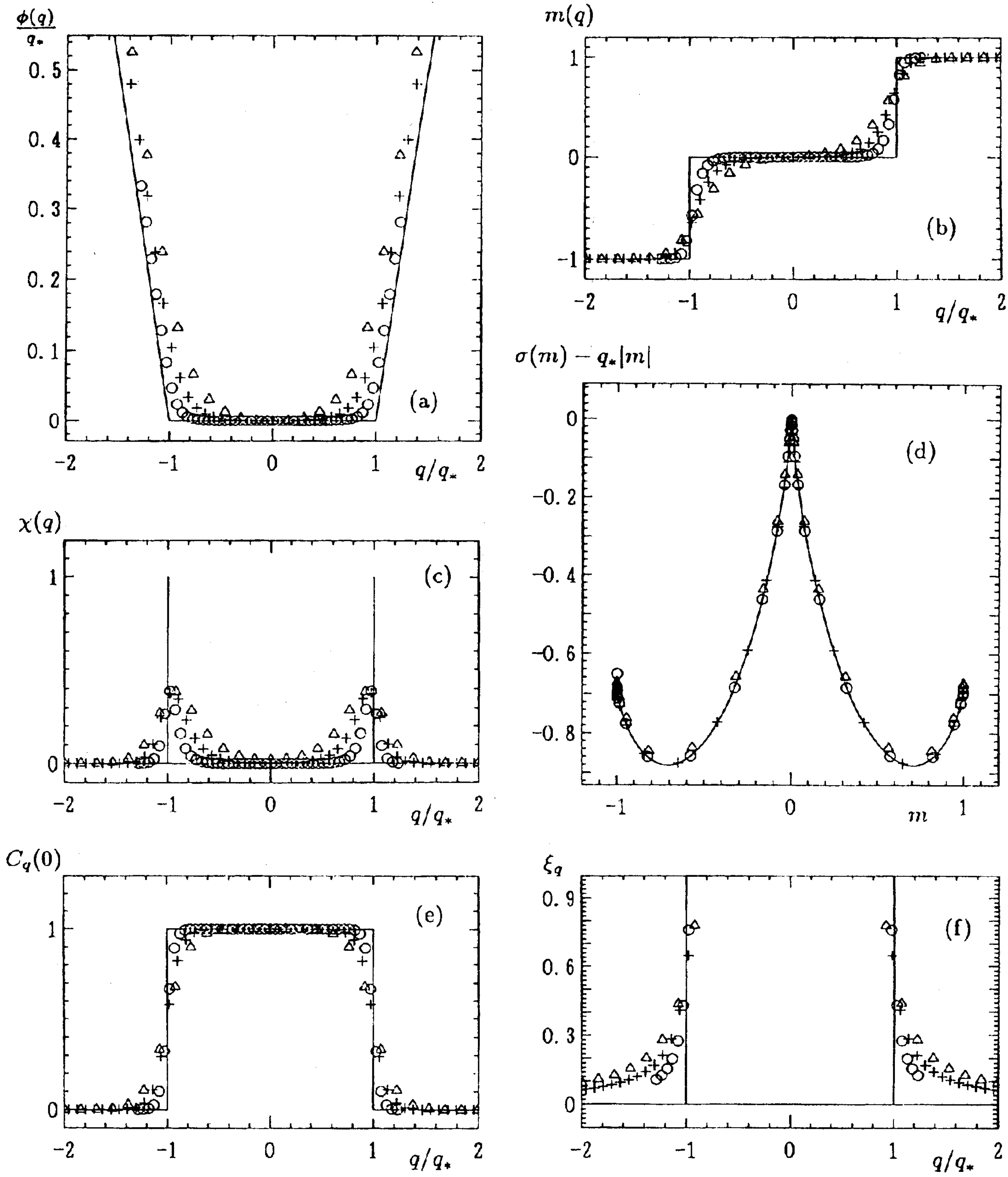

Fig. 3. Scaling laws of thermodynamic functions (a–d) and order-q double point correlation functions (e,f) for antiferromagnetic Ising chain at low temperatures. This is valid for q of the order q_*,($q_* \simeq 2\,|\,\mathrm{K}\,|\, + \log 2$). Symbols are for k_BT/J=0.15(○), 0.3(+) and 0.5(△). The solid lines are the analytic results in (3.15–3.20).

Furthermore one finds

$$C_q(0) = [1+e^{2(\varepsilon q - q_*)}]^{-1}, \tag{3.19}$$

$$\xi_q = \{2\log[e^{\varepsilon q - q_*} + \sqrt{1+e^{2(\varepsilon q - q_*)}}]\}^{-1}, \tag{3.20}$$

near $q=\varepsilon q_*$, (Fig.3b).

4. Concluding remarks

A few decades ago van Kampen [9], Kubo-Matsuo-Kitahara [10] and Suzuki [11] discussed the fluctuation of macrovariables using the system size expansion (the Ω expansion). Assuming that the master equation for the macrovariable α_Ω can be expanded in the power series of $1/\sqrt{\Omega}$, they tried to find the asymptotic master equation valid for a large system size. The final master equation always takes the linear Fokker-Planck equation. This is a straightforward result of the central limit theorem which is valid only for small fluctuations from the average in the thermodynamic limit. Their studies inform us that although the extensivity relation that the probability distribution for α_Ω depends onthe system size as exp $[-\Omega\Psi(\alpha)]$, $(\Psi(\alpha)=0(1))$, holds, one *can not* expand the fluctuation in the power series of $1/\sqrt{\Omega}$ as long as a large deviation from the ensemble average is concerned.

Large deviations from the Gaussian of fluctuations in the thermodynamic system are thus small and hard to be observed. However if one observes local fluctuations of thermodynamic system he can detect large fluctuations.

In the present paper with the above fundamental motivation we discussed the overall (small and large) fluctuaions of local magnetizations without magnetic field. Due to the statistical independence of sub-"thermodynamic" regions in the thermodynamic system, the characteristic function $\phi(q)$ relevant to the overall statistics of local magnetizations are determined by those of the whole system under corresponding magnetic field, (Eqs. (2.7) and (2.13)). Namely the quantities $m(q)$, $\chi(q)$ etc describing large local fluctuations of magnetizations of the system without magnetic field are uniquely determined by the averages under the magnetic field k_BTq. This is due to the fact that large fluctuations can be simply generated by applying the external field. This is the key point for the observation of large fluctuations of the system without external field.

Based on the above fundamental remarks we discussed the overall fluctuation characteristics of 1d Ising with the well-known rigorous result for the free energy and the spatial correlation function. In the low temperature limit the relevant statistical quantities of the ferromagnetic Ising model have an anomaly at $q=0$,i.e. at zero external field. On the other hand the fluctuations of the antiferromagnetic Ising model in the low temperature limit are enhanced for certain large $|q|$ values, i.e. for corresponding large external fields. Near such "phase transition points" [12] statistical quantities satisfy the scaling laws.

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Appendix A —Relation between the fluctuation spectrum and the entropy—

In this appendix the explicit interrelation between the fluctuation spectrum and the entropy where there is no coexistence of several phases is derived. Let $g(T,h)$ and $s(u,m)$ be respectively the Gibbs free energy and the entropy per spin, where the entropy is chosen to be a function of the internal energy u and the magnetization m. As is well known the steepest descent method in the thermodynamic limit yields

$$g(T,h) = -\max_{u',m'} [T_s(u', m') - u' + hm'] . \tag{A.1}$$

The solutions of

$$T \frac{\partial s(u,m^0)}{\partial u} = 1, \quad T \frac{\partial s(u,m^0)}{\partial m^0} = -h, \tag{A.2}$$

yield the internal energy $u(T,h)$ and the magnetization $m^0(T,h)$. Equation (A.1) is rewritten as

$$g(T,h) = u(T,h) - hm^0(T,h) - Ts(u(T,h), m^0(T,h)). \tag{A.3}$$

The characteristic function and the fluctuation spectrum are respectively obtained as

$$\phi(q)=-\beta\{u(T,\frac{q}{\beta})-\frac{q}{\beta}m^0(T,\frac{q}{\beta})-Ts(u(T,\frac{q}{\beta})),m^0(T,\frac{q}{\beta}))\quad (A.4)$$

$$-u(T,0)+Ts(u(T,0),m^0(T,0))\},$$

$$\sigma(m(q))=qm-\phi(q)=qm+\frac{1}{k_BT}\{g(T,k_BT_q)-g(T,0)\}$$

$$=\frac{1}{k_B}\{s(u(T,0),m^0(T,0))-s(u(T,k_BT_q),m^0(T,k_BT_q))\quad (A.5)$$

$$+\frac{1}{T}[u(T,k_BT_q)-u(T,0)]\}.$$

Since

$$m=\frac{\partial\phi(q)}{\partial q}=-\frac{\partial g(T,h)}{\partial h}\Big|_{h=k_BT_q}=m^0(T,k_BT_q),\quad (A.6)$$

the insertion of the solution $k_BTq=A(T,m)$ of (A.6) into (A.5) yields the interrelation between the entropy and the fluctuation spectrum for local magnetizations as

$$\sigma(m)=\frac{1}{k_B}\{s(u(T,0),m^0(T,0))-s(u(T,A(T,m)),m)\quad (A.7)$$

$$+\frac{1}{T}[u(T,A(T,m))-u(T,0)]\}.$$

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