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# Distribution of Yang-Lee Zeros of the $\pm J$ Ising Model

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A numerical technique to find out the distribution of the zeros of the partition function in the complex field plane is presented for the Ising model with arbitrary nearest-neighbor interactions. We apply it to the symmetric $\pm J$ model in two and three dimensions and obtain the distribution of the zeros of the effective partition function whose zeros in the complex field plane determine the analytical properties of the configuration-averaged free energy. Making use of the results, we discuss some problems of the short-range spin glass model including the existence of the Griffiths singularity and the AT line.

## §1. Introduction

The mean field theory of spin glasses has succeeded in providing a unified picture on the low temperature phase of the Edwards-Anderson model.[1] Active current interest of researchers in this field is in the applicability of the mean field predictions to finite-dimensional systems. The existence of a finite spin glass transition temperature in the three-dimensional $\pm J$ Ising model is strongly supported by Monte Carlo simulations[2,3] and high-temperature expansions.[4] Less well established are the properties of the spin glass phase and the dynamical aspects of the phase transition. The mean field theory predicts an infinite number of pure states in the spin glass phase with ultrametric structure in the space of these states.[1] The validity of this picture in three-dimensional systems has been challenged by several authors who argue the spin glass phase is much more simple in the finite-dimensional world.[5-7] If this is true, the de Almeida-Thouless[8] (AT) line as an equilibrium transition line is probably absent in three dimensions. Theoretical investigation of dynamics of spin glasses has been carried out by Randeria *et al.*[9] using a cluster model and by Ogielski[10] in his extensive Monte Carlo simulations. Of particular interest among the results of these authors is an anomalous decay of the autocorrelation function $q(t)$ above the spin glass transition temperature $T_g$. Ogielski finds a stretched exponential decay of $q(t)$ in the temperature range $T_g < T < T_c$ where $T_c$ denotes the transition point of the corresponding non-random system. This strange behavior of a dynamical variable in the presumed paramagnetic phase reminds us of the Griffiths singularity in the diluted ferromagnet[11] (in fact Randeria *et al.*[9] called this phase a Griffiths phase).

Investigation on both of the above problems (existence of the AT line and dynamics) is still in a primitive stage, in our opinion, and needs additional points of view. We have thus followed the approach of Yang and Lee[12,13] who could shed light on the phase transition by investigating the distribution of zeros (Yang-Lee zeros) of the partition function in the complex fugacity plane. They applied their basic theorem to the ferromagnetic Ising model in the complex field plane. This approach finds its natural significance in the $\pm J$ Ising model because, first, the Griffiths singularity is closely related to the Yang-Lee zeros[11] and, second, the field dependence of the free energy determines the existence of the AT line.

It is not possible to apply straightforwardly the theory of Yang and Lee to the random system of our interest. We could nevertheless define an effective partition function whose zeros in the complex field plane determine the analytical properties of the configuration-averaged free energy. We have also developed a novel numerical technique to find out the distribution of the Yang-Lee zeros. From the resulting graphical representation of the zero-distribution, we have extracted suggestions on the problems explained above.

In §2, basic ideas of our numerical investigation are explained. Results are given in §3 and physical implications are discussed there. A brief summary is found in §4.

## §2. Numerical Evaluation of the Yang-Lee Zeros

Let us first explain our method of calculating the location of Yang-Lee zeros of the finite Ising model on a two- or three-dimensional lattice with cylindrical boundary conditions (free in one direction and periodic in the others). The Hamiltonian is given as

$$\mathcal{H}=-\sum_{(i,j)} J_{ij}S_iS_j-H\sum_i S_i \quad (S_i=\pm 1), \qquad (2.1)$$

and the partition function is defined by

$$Z=\sum_{\{S_i=\pm 1\}} \exp(-\beta\mathcal{H}). \qquad (2.2)$$

In the present method of calculation it is not necessary to assume translation invariance of the system. The interaction $J_{ij}$ is fixed to an arbitrary value at each bond. The range of interaction extends only to nearest neighbors so that the numerical transfer-matrix[14] method can be applied to the system. For the Ising model (2.1), it is possible to rewrite the partition function (2.2) as

$$Z(y, T)=y^{-N/2}\sum_{l=0}^{N} a_l(T)y^l, \qquad (2.3)$$

where $y\equiv\exp(2\beta H)$ and $N$ is the number of sites. Making use of the linearity of the right hand side of eq. (2.3) in $a_l(T)$'s, we can obtain the values of these coefficients at a fixed temperature in the following manner. The first step is to evaluate the partition function at $N+1$ different field values $H_1, H_2, \cdots, H_{N+1}$, which are complex in general, using the numerical transfer-matrix method.[14] Next, we solve the linear equations of $N+1$ independent variables $(a_0, a_1, \cdots, a_N)$

$$y_i^{-N/2}\sum_{l=0}^{N} a_l y_i^l=Z(y_i, T) \quad (i=1, \cdots, N+1), \qquad (2.4)$$

where $y_i=\exp(2\beta H_i)$ $(i=1,\cdots, N+1)$. Using the results $a_0, a_1,\cdots, a_N$, we can finally obtain the location of $N$ zeros of the partition function (2.3) by solving the algebraic equation

$$\sum_{l=0}^{N} a_l(T)y^l=0. \qquad (2.5)$$

There are a few simplifications due to the symmetry of the Ising system. Since the partition function is an even function of $H$, the following relations hold for the coefficients:

$$a_l(T)=a_{N-l}(T) \quad (l=0,\cdots, N). \qquad (2.6)$$

Equation (2.6) implies that the partition function can be regarded as a function of $x\equiv(y+y^{-1})$:

$$Z(x, T)=\sum_{l=0}^{N/2} b_l(T)x^l. \qquad (2.7)$$

Then the number of independent variables in the linear equations (2.4) reduces to $N/2+1$ (we assume that $N$ is an even number). An additional simplification comes from the realness of coefficients $b_l(T)$'s, from which we have

$$Z^*(x, T)=Z(x^*, T). \qquad (2.8)$$

Thus we have to evaluate the partition function at about $N/4$ field-values in the complex $x$-plane.

We have checked efficiency of this method in the Ising ferromagnet ($J_{ij}=1$ for all $(i, j)$ pairs of nearest neighbor) on the square lattice. For this model, it has been proven by Lee and Yang[13] that all zeros lie on the unit circle in the complex $y$-plane. Our calculations were carried out for the size up to $10\times 10$, and all zeros obtained were confirmed to be located on the unit circle. The largest possible system size $N$ (or the smallest possible temperature $T$) is determined by the rounding errors in practical applications of the present method. Accuracy deteriorates with the system size increase or with the temperature decrease, since the ratio (in absolute value) of the largest and the smallest coefficients $a_0(T)/a_{N/2}(T)$ (or $b_0(T)/b_{N/2}(T)$) rapidly increases, say, in proportion to $\exp(c\beta N)$ with $c$ a constant.

We have applied the present method to the $\pm J$ Ising model on the square and the simple cubic lattices. The Hamiltonian is given in eq. (2.1) with the nearest neighbor interaction $J_{ij}$

randomly distributed independently at each bond with the probability

$$P(J_{ij})=\frac{1}{2}\{\delta(J_{ij}-J)+\delta(J_{ij}+J)\}. \tag{2.9}$$

The free energy of such a quenched random system is defined by

$$F=-k_{\mathrm{B}}T[\ln Z\{J_{ij}\}]_{\mathrm{c}}. \tag{2.10}$$

Here $Z\{J_{ij}\}$ is the partition function for a particular bond configuration $\{J_{ij}\}$ and $[\cdots]_{\mathrm{c}}$ denotes the average over the bond configuration:

$$[\ln Z\{J_{ij}\}]_{\mathrm{c}}\equiv\int\prod_{(i,j)}\mathrm{d}J_{ij}P(J_{ij})\cdot\ln Z\{J_{ij}\}. \tag{2.11}$$

In the case of the distribution (2.9), all bond configurations have the same probability $2^{-N_{\mathrm{b}}}$, where $N_{\mathrm{b}}$ is the number of bonds. Thus the free energy of the present system is written as

$$F=-k_{\mathrm{B}}T2^{-N_{\mathrm{b}}}\sum_{\{J_{ij}\}}\ln Z\{J_{ij}\}, \tag{2.12}$$

where the summation is taken over all possible bond configurations. From eq. (2.12), we may define the effective partition function as

$$Z=C\prod_{\{J_{ij}\}}Z\{J_{ij}\}, \tag{2.13}$$

where $C$ is a constant independent of $H$ and $T$. The singularity of the free energy is determined by zeros of this effective partition function. The distribution of the Yang-Lee zeros of the effective partition function is constructed by a superposition of zeros of each $Z\{J_{ij}\}$.

The sizes of the system we have investigated are $4\times4$, $6\times6$ and $6\times8$ for the square lattice, and $3\times3\times2$, $3\times3\times4$ and $3\times4\times4$ for the simple cubic lattice. The last digits in the above list represent the system sizes in the direction of the free boundary. As mentioned before, the problem of rounding errors limits the system size to relatively small values. (Difficulties occur mainly in solving the algebraic equation (2.5), for which we used the finite bit method.[15]) In fact it was necessary to use complex numbers with quadruple precision in our FORTRAN statements in order to achieve satisfactory reliability at low temperatures. Since the total number of the possible bond configurations is very large (about $2.7\times10^{8}$ for the $4\times4$ lattice and about $5.4\times10^{39}$ for the $3\times4\times4$ lattice), it is not possible to calculate all zeros of the effective partition function (2.13). We approximate the distribution of the Yang-Lee zeros by taking a sufficient number of samples.

## §3. Results and Discussion

We measure the temperature in units of $J/k_{\mathrm{B}}$ and the field in units of $J$, hereafter. In Fig. 1 we show a typical example of the distribution of the Yang-Lee zeros of the $\pm J$ model ($T=0.75$, $3\times4\times4$ lattice) obtained by randomly choosing 210 samples of bond configurations. One should note that the distribution is plotted in the complex $2\beta H$ $(=\ln y)$ plane instead of the $y$-plane. The unit circle in the $y$-plane corresponds to the imaginary axis in this $2\beta H$-plane. The whole real axis (the positive part as well as the negative part)

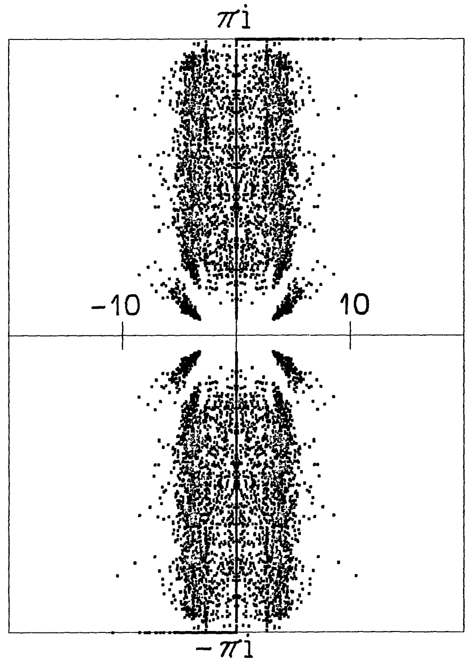


Fig. 1. A typical example calculated by the present method. The distribution of the Yang-Lee zeros of the $\pm J$ model on the lattice $3\times4\times4$ at $T=0.75$ obtained by randomly choosing 210 samples of bond configurations is plotted on the complex $2\beta H$-plane. Each point corresponds to one obtained zero. The symmetries $H\leftrightarrow-H$ and $H\leftrightarrow H^{*}$ can be clearly seen in this plane.

represents physically sensible field values in contrast to the case of the $y$-plane (where only real and positive $y$ is experimentally accessible).

In the following figures we plot the distributions of the Yang-Lee zeros only in the upper half plane, Im $H \geq 0$, because of the symmetry $H \leftrightarrow H^*$. The results on the square lattice are shown in Fig. 2 for temperatures $T=5.0$, 2.5, 2.0, 1.5, 1.0 and 0.5 from top to bottom. The results on the simple cubic lattice are given in Fig. 3 for temperatures $T=10.0$, 5.0, 4.0, 2.0, 1.0 and 0.75. The number of samples of each diagram is listed in the figure captions.

It is useful to make a note here on the size dependence of the Yang-Lee edge[16,17] at a fixed temperature, in order to discuss the singularities of the free energy of the present random system. In the ferromagnetic Ising system the Yang-Lee edge is defined as the location of nearest zero to the real axis, which always lies on the imaginary axis in the $2\beta H$-plane. In the temperature region where the free energy is not singular as a function of real $H$, the edge remains away from the real axis independent of the system size. On the contrary in the temperature range where the free-energy singularity occurs, the edge approaches the real axis as $N \to \infty$. In the random system, we call the locations of nearest zeros to the real axis the edges even if these do not lie on the imaginary axis.

Let us first analyze the data on the two-dimensional model (Fig. 2). At high temperatures ($T=5.0$ and 2.5), the location of the edge is roughly independent of the system size. Since the free energy is not singular as a function of real $H$ in this temperature range, one does not expect that the zero-distribution touches upon the real axis as is consistent with the above observation. On the other hand, if the temperature is lower than the non-random critical value ($T_c \simeq 2.27$), the edge is seen to slowly approach the origin ($H=0$) with the increase of the system size. One may be able to attribute this tendency to the existence of the Griffiths singularity in this $\pm J$ Ising system.[9,10] However we would rather avoid to draw a definite conclusion on this problem because statistical fluctuations originating in the finite sample number may mask the asymptotic behavior as $N \to \infty$. In the lowest-temperature case ($T=0.5$), there appears a mustache-like wing in the distribution (Figs. 2(l) and 2(r)). As the system size increases from $4 \times 4$ to $6 \times 8$, the edge of this wing (i.e. the nearest point to the real axis in the wing) approaches the origin $H=0$ with an approximately constant angle measured from the real $H$ axis. This tendency also is not incompatible with a Griffiths singularity at $H=0$ for $T < T_c$.

The data on the three-dimensional system suffer from statistical fluctuations as in the two-dimensional case. If one is allowed to neglect isolated zeros in Figs. 3(i) and 3(o), since these may not yield finite contributions in the thermodynamic limit, one could interpret the approach of the edge to the origin (as a function of $N$) when $T < T_c$ ($\simeq 4.51$) as an indication of a Griffiths singularity. However, our view is that statistical uncertainties are larger than the scale of the subtle motion of the edge. Below the accepted spin glass transition temperature ($T_g \simeq 1.18$),[2-4,10] a wing of distribution develops (Figs. 3(k), 3(l), 3(q) and 3(r)). As in the two-dimensional case, the edge of this wing approaches the origin at a constant angle from the real axis as the system size increases. Therefore, if the edge reaches the real axis in the limit $N \to \infty$ at $T < T_g$, it will be only at the origin, not at other locations of the real axis. This observation implies that in the spin glass phase the free energy as a function of the real field $H$ is singular, if it is at all, only at $H=0$. The absence of the AT-line in three dimensions as claimed by Fisher and Huse[5] is consistent with the above behavior of the edge of the wing: If there is the AT line in the $H$-$T$ phase diagram, the free energy should be singular at $H_c(T) \neq 0$ for $T < T_g$.

## §4. Summary

A numerical technique to find out the distribution of the Yang-Lee zeros in the complex field plane is presented for the Ising model with arbitrary nearest-neighbor interactions. The technique has its basis on the numerical transfer-matrix method evaluated in a complex external field. We apply the method to the symmetric $\pm J$ model and obtain zeros of the effective partition function which determine the analytical properties of the configuration-averaged free energy. By

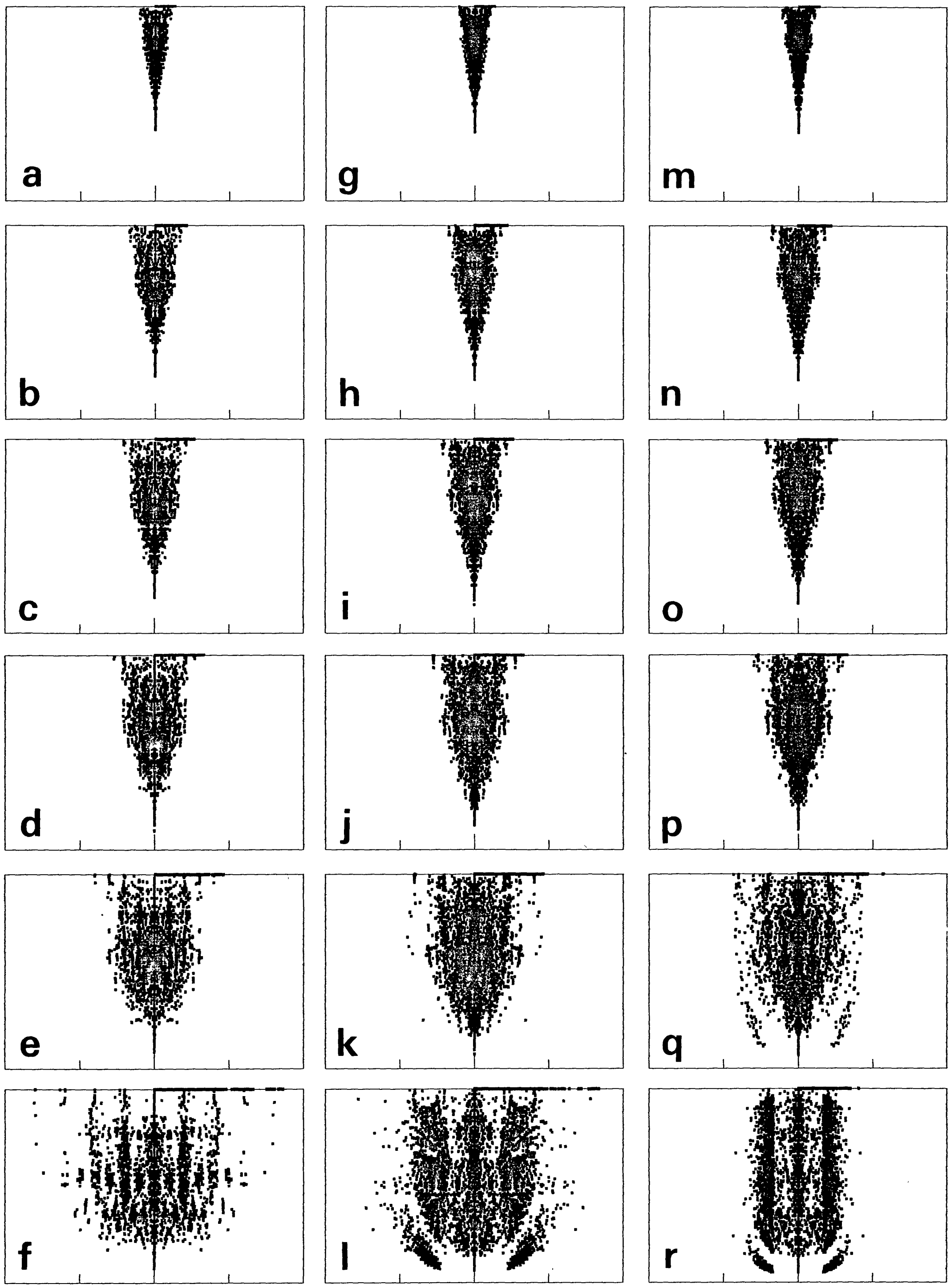


Fig. 2. The results on the square lattice. All zeros are plotted only in the upper half plane, Im $H \geq 0$, because of the symmetry $H \leftrightarrow H^*$. The scale of each diagram is the same as that of Fig. 1. The system sizes are $4 \times 4$, $6 \times 6$ and $6 \times 8$ from left to right. The temperatures are $T=5.0$, 2.5, 2.0, 1.5, 1.0 and 0.5 from top to bottom. The numbers of samples are (a) 160, (b) 250, (c) 320, (d) 420, (e) 600, (f) 1200, (g) 72, (h) 112, (i) 150, (j) 185, (k) 300, (l) 368, (m) 55, (n) 85, (o) 110, (p) 140, (q) 177, (r) 206.

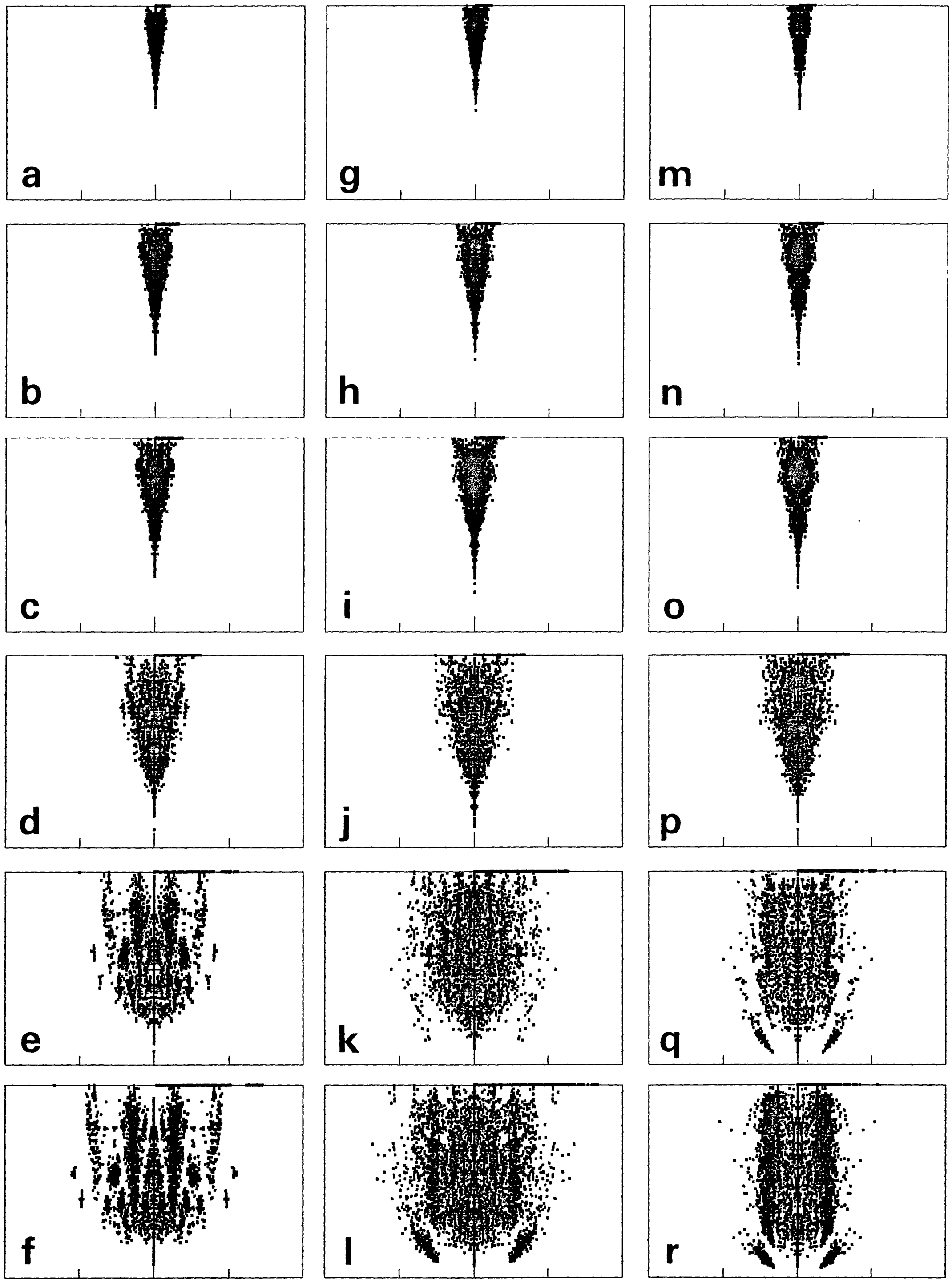


Fig. 3. The results on the simple cubic lattice. The scale of each diagram is the same as that of Fig. 1. The system sizes are $3\times3\times2$, $3\times3\times4$ and $3\times4\times4$ from left to right. The temperatures are $T=10.0$, 5.0, 4.0, 2.0, 1.0 and 0.75 from top to bottom. The numbers of samples are (a) 120, (b) 160, (c) 200, (d) 280, (e) 600, (f) 1100, (g) 60, (h) 80, (i) 100, (j) 140, (k) 277, (l) 374, (m) 40, (n) 60, (o) 70, (p) 100, (q) 133, (r) 210.

making use of these results, some problems of the short-range spin glass model are discussed. In two and three dimensions we observe the tendency which may be interpreted as indicating the existence of the Griffiths singularity. However statistical uncertainties are too large to give a definite conclusion. In three dimensions we observe the tendency consistent with the absence of the AT line.

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