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Statics and Dynamics of a Two-Dimensional Ising Spin-Glass Model

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The temperature and field dependence of spatial correlations and relaxation times are investigated in detail by Monte Carlo simulations for a two-dimensional Ising spin-glass model. There is no transition, but, in zero field, barrier heights and correlation range increase smoothly at low temperatures. This increase does not seem to be fast enough to explain experiments. In a field, barrier heights and the correlation length tend to a finite limit as $T \to 0$. Points in the h-T plane with constant relaxation time satisfy $T(h)-T(0) \propto h^{2/3}$ at moderately low temperatures.

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There are several calculations[1] on spin-glass models with short-range interactions which predict a lower critical dimension (LCD) of 4. Consequently there should be no spin-glass transition in three dimensions and the infinite-range Sherrington-Kirkpatrick[2] (SK) model, which does have a transition, should be inappropriate for explaining experiments. It is therefore surprising that the following experimental results are reasonably well described by the SK model: (a) There is a dramatic increase[3,4] in the nonlinear susceptibility, χ_{nl}, in the same region of temperature, T, as the cusp in the linear susceptibility. χ_{nl} diverges in the SK model but remains finite if there is no transition. (b) There is evidence[5,6] for a "transition line" in the h-T plane (h is a uniform field), similar to the Almeida-Thouless[7] line for the SK model. Even the power-law variation $T_c(h) - T_c(0) \propto h^{2/3}$, for small h, predicted by Almeida and Thouless, seems to be found experimentally. (c) For certain materials at least, the temperature of the susceptibility peak varies very little with frequency,[8] as is natural in the phase-transition hypothesis. However, a much larger variation is predicted by the alternative picture of "gradual freezing."[9]

These results suggest that either the prediction of an LCD equal to 4 is wrong or correlation lengths, and relaxation times, while not strictly diverging, increase considerably over a narrow temperature range as a result of cooperative effects between the spins. In order to decide which of these two alternatives is correct one needs to know *quantitatively* the range of correlations in space and time as functions of h and T. While the spatial extent of correlations with $h=0$ has been discussed,[1,10] albeit on somewhat small lattices, virtually[11] no precise results on relaxation times have been given, and little is known about the effect of a magnetic field. Here I start to fill in this important gap by reporting results of detailed Monte Carlo studies of the Edwards-Anderson model with Ising spins on fairly large square lattices of size $N=L\times L$, where $L=68$ and 128. The Hamiltonian is given by

$$H = -\sum_{\langle ij\rangle} J_{ij} S_i S_j - h\sum_i S_i, \qquad (1)$$

where $S_i = \pm 1$, $i=1,\ldots N$, and J_{ij} is a nearest-neighbor interaction taking values ± 1 with equal probability. Averages over several samples (typically 20–60) were made. The calculations were performed on the distributed array processor, which can perform 4096 similar operations in parallel. It is, to my knowledge, substantially faster for this problem than any other multipurpose computer, a fliptime of 0.2 μsec/spin being readily obtained (with $h=0$). Details of the computations and results in three dimensions will be published separately. If the LCD is 4 there should not be a qualitative difference between two and three dimensions.

My main conclusions are the following:

(i) No transition is found in the temperature range studied. Very low temperatures are inaccessible because equilibrium cannot be established within the available computer time. Although I cannot completely rule out a transition at a low but finite temperature, this seems unlikely, and the present results are quite consistent with Morgenstern and Binder's (MB) prediction that, for $h=0$, the spin-glass susceptibility, χ_{SG}, defined in Eq. (4) below, and the corresponding correlation length ξ, have a power-law divergence as $T\to 0$. The present results appear to rule out Fernandez's claim of a transition of $T\simeq 1$. For $h=0$, $\chi_{SG}\propto\chi_{nl}$ and, although the extrapolation of the present results to low T gives a large χ_{nl}, the increase does not appear to be as rapid as that seen experimentally.[3]

(ii) When $h=0$ χ_{SG} saturates to a finite value as $T\to 0$.

(iii) Results analogous to (i) and (ii) are obtained also for dynamics. An "average relaxation time," τ, and corresponding "characteristic energy barrier" ΔE ($=T\ln\tau$) are evaluated. For $h=0$ I find $\Delta E\propto T^{-1}$, whereas in a field ΔE saturates to a finite value as $T\to 0$. The T^{-1} variation of ΔE gives a more rapid increase in relaxation time with decreasing temperature than a simple Arrhenius law ($\Delta E=$const) but does not seem sufficiently rapid to explain the almost frequency-independent freezing temperatures found in Ref. 8. From (i)–(iii) it seems clear that the growth in ΔE at low T is associated with the increase in ξ (and hence χ_{SG}).

(iv) Lines of constant τ in the h-T plane are plotted and, for the lowest temperatures studied, do seem to vary the same way as the Almeida-Thouless line, i.e., $T(h)-T(0)\propto h^{2/3}$, although the exponent is not determined with great precision. These results seem quite similar to the experiments of Bontemps, Rajchenbach, and Orbach.[6]

Next I describe quantities that are calculated. Information on dynamics is conveniently extracted from the usual autocorrelation function

$$q(t)=N^{-1}\sum_{i=1}^{N}\langle S_i(t_0)S_i(t_0+t)\rangle_J, \qquad (2)$$

where t_0 is the equilibration time and $\langle\cdots\rangle_J$ indicates an average over samples. t_0 is estimated by observing the time, τ_0, that $q(t)$ takes to reach its equilibrium value, and ensuring that $t_0\geqslant\tau_0$. This sets a lower limit on the temperature range. For $t\to\infty$, $q(t)\to q=\langle\langle S_i\rangle_T^2\rangle_J$, where $\langle\cdots\rangle_T$ is a statistical-mechanics average. For this model $q=0$ if $h=0$. From $q(t)$, we define τ by[11]

$$\tau=(1-q)^{-1}\int_0^\infty[q(t)-q]dt. \qquad (3)$$

The decay of $q(t)$ is certainly not exponential (at low T it is close to logarithmic) and if we represent the decay by a spectrum of relaxation times $P(\hat\tau)$ so that

$$q(t)=q+(1-q)\int_0^\infty P(\hat\tau)\exp(-t/\hat\tau)d\hat\tau$$

then $\tau=\int_0^\infty\hat\tau P(\hat\tau)d\hat\tau$ is the *average* relaxation time.

Information on the spatial range of correlations is obtained from

$$\chi_{SG}(t)=N^{-1}\sum_{i,j=1}^{N}\langle S_i(t_0)S_j(t_0)S_i(t_0+t)S_j(t_0+t)\rangle_J-q^2$$

which, for sufficiently long times (in practice $t>t_0$) becomes χ_{SG}, where

$$\chi_{SG}=N^{-1}\sum_{i,j=1}^{N}\langle\langle S_iS_j\rangle_T^2\rangle_J-q^2. \qquad (4)$$

For $h=0$, $\chi_{SG}=3T^3\chi_{nl}$, the nonlinear susceptibility. Since $S_i=\pm1$ the number of spins correlated with a given spin, denoted by ΔN, is given by $\chi_{SG}-1$ where I have chosen to subtract the $i=j$ terms in Eq. (4). As χ_{SG} grows so does ΔN and hence so does the correlation length. For $h=0$ the latter has also been directly evaluated by calculating correlations between *lines* of spins. Defining, in an obvious notation,

$$\Gamma(n)=N^{-1}\sum_{i_y=1}^{L}\sum_{i_x,j_x=1}^{L}\langle\langle S_{i_x,i_y}S_{j_x,i_y+n}\rangle_T^2\rangle_J, \qquad (5)$$

I always found $\Gamma(n)\propto\exp(-n/\xi)$ from which the correlation length ξ can be extracted.

I now present my results. Data for $\chi_{SG}^{1/2}$ and ξ with $h=0$ are given in the inset to Fig. 1 down to $T=1.0$ for 64^2 and 128^2 lattices. No dependence on system size was found as expected because $\xi\ll L$. These results rule out the transition at $T=1.0$ proposed by Fernandez.[10] When ξ is large one expects that $\chi_{SG}\propto\xi^2$ and MB have claimed that $\xi\propto T^{-2}$ and $\chi_{SG}\propto T^{-4}$. The present results

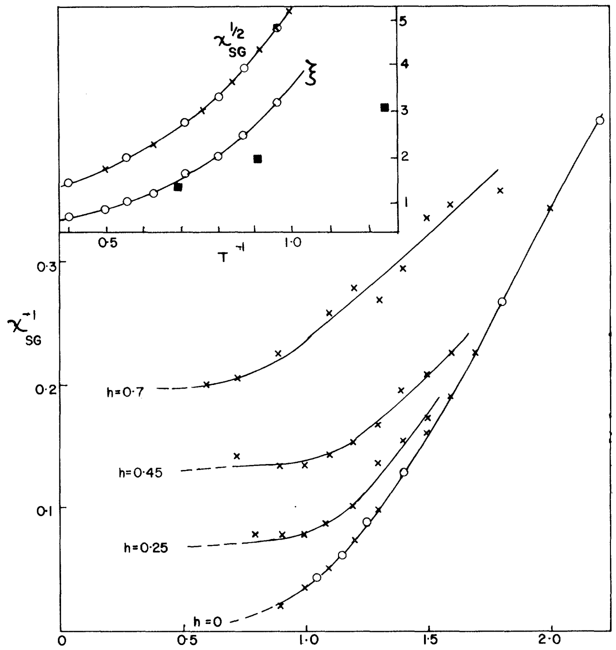

FIG. 1. Inset: $\chi_{SG}^{1/2}$ and ξ for $h = 0$ as a function of T^{-1} for 64^2 (circles) and 128^2 (crosses) lattices. Data for ξ from Morgenstern and Binder are indicated by squares. The main figure shows χ_{SG}^{-1} against T for several different values of h; again circles denote a 64^2 lattice and crosses a 128^2 lattice. The curves are guides to the eye.

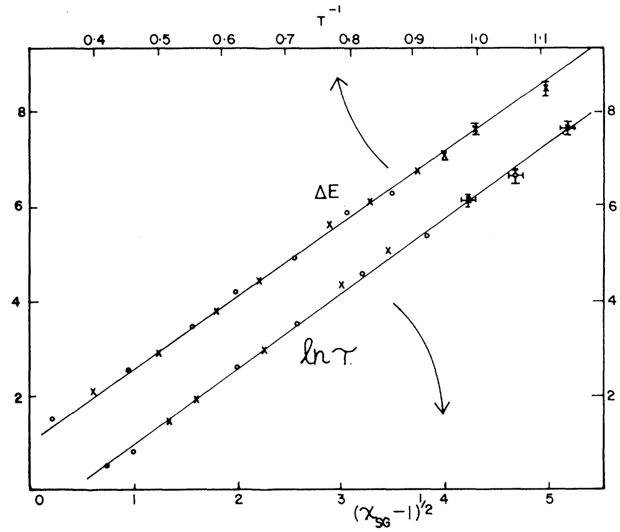

FIG. 2. Plot of ΔE against T^{-1} and $\ln\tau$ $(= \Delta E/T)$ against $(\chi_{SG} - 1)^{1/2}$ for 64^2 (circles) and 128^2 (crosses) lattices. The lines are guides to the eye.

show $\chi_{SG}^{1/2}$ and ξ increasing faster than T^{-1} and are quite consistent with MB's prediction of T^{-2} but I cannot go to low enough T to determine the power law accurately. Note that MB's results, indicated by the squares, seem to underestimate ξ, perhaps because of the smaller sizes used in their calculations (up to 18^2). Assuming T^{-4} variation for χ_{SG} below $T=1$, then at $T=0.58$ (the significance of which is explained below) one has $\chi_{SG} \simeq 300$, which can be compared with the results of Omari, Prejean, and Souletie[3] for 1% CuMn that $\chi_{nl} = \chi_{SG}/3T^3 \simeq 500$ at $T=12.5$ K and $\chi_{nl} \simeq 3500$ at $T=11.15$ K. The rate of increase observed experimentally is much faster than T^{-7} at these temperatures.

Data for χ_{SG} in a field are also given in Fig. 1 and suggest very strongly that χ_{SG} saturates to a finite value as $T \to 0$ when $h \neq 0$.

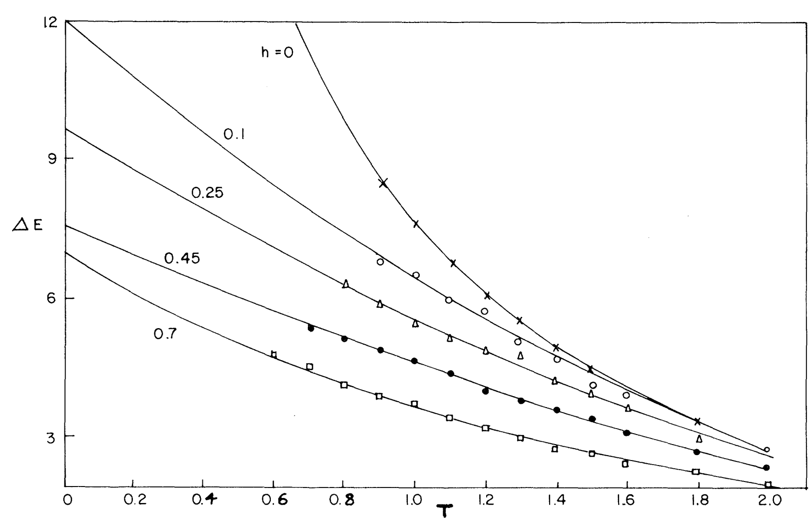

FIG. 3. ΔE against T for $h = 0$ (crosses), 0.1 (open circles), 0.25 (triangles), 0.45 (closed circles), and 0.7 (squares) for 128^2 lattices. The lines are least-squares fits by the form $\Delta E = a + b/(c+T)$.

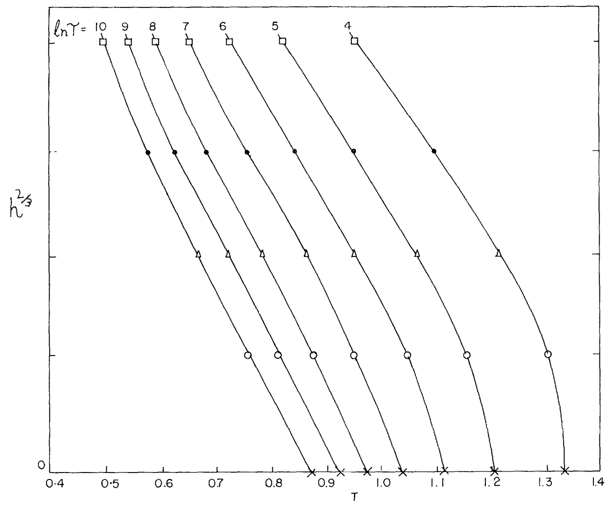

FIG. 4. The points are where $\ln\tau$ has a certain value for the given field and are determined from the fits of Fig. 3. The lines are a guide to the eye and the numbers at the top of each line give the corresponding values of $\ln\tau$.

In Fig. 2 ΔE ($= T\ln\tau$) for $h=0$ has been plotted against T^{-1} and the good straight-line fit indicates a divergence of the barrier heights as $T\to 0$. No evidence of Vogel-Fulcher[12] behavior is observed. Also given is a plot of $\ln\tau$ against $\Delta N^{1/2}$, where $\Delta N = \chi_{SG} - 1$ is the number of spins correlated with a given spin. Again a good straight-line fit is obtained. If we take literally the extrapolations in Fig. 2 then $\chi_{SG} \propto (\Delta E/T)^2 \sim T^{-4}$ in precise agreement with MB. Morgenstern[13] has argued that $\Delta E(T)$ saturates to a finite value (of about 15) at $T=0$. This cannot be ruled out by the results of Fig. 2.

Mulder, van Duyneveldt, and Mydosh[8] find that the freezing temperature, T_f, varies with frequency ν according to $d\ln T_f/d\ln\nu \simeq \frac{1}{500}$ for several metallic spin-glass alloys in the range $\nu = 1-10^3$ Hz. If we assume a microscopic time $\tau_{micr} = 10^{-11}$ sec and equate $(\nu\tau_{micr})^{-1}$ with an average dimensionless relaxation time at the freezing temperature, then the freezing temperature for $\nu = 10$ Hz, say, corresponds, in the simulation, to the temperature where $\tau = 10^{10}$. Extrapolation of the data for $\ln\tau$ using the fit in Fig. 3 gives $T=0.58$ at which $|d\ln T/d\ln\tau| = \frac{1}{50}$, smaller than the Arrhenius law (ΔE constant), where $|d\ln T/d\ln\tau| = (\ln\tau)^{-1} = \frac{1}{23}$, but much larger than the value of $\sim\frac{1}{500}$ from experiment. It remains to be seen whether a more rapid increase in $\ln\tau$ occurs in three-dimensional models.

Figure 3 shows ΔE for several fields. The lines are least-squares fits by the form $\Delta E = a + b/(c + T)$. Apparently ΔE (like χ_{SG}) tends to a finite value as $T\to 0$ in a field. From the least-squares fits one can obtain the temperature where $\ln\tau$ has a prescribed value. These temperatures are plotted in Fig. 4 against $h^{2/3}$ for several values of $\ln\tau$ and at lower temperatures the data are consistent with $T(h) - T(0) \propto h^{2/3}$ for fixed $\ln\tau$, but the exponent is not accurately determined.[14] This is rather similar to the results of Bontemps, Rajchenbach, and Orbach[6] on $Eu_{0.4}Sr_{0.6}S$ who find different "transition lines" depending on meassuring time.

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Possible Direct Observation of Phasons in Potassium

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The nonlinear response expected in a potassium point-contact device has been calculated with inclusion of the electron-phason interaction of Overhauser. With use of the theory of Kulik *et al.*, to describe the point contact, a peak is found at low energy (at approximately 0.3 meV). This peak agrees well in energy, shape, and magnitude with an unexplained peak in the point-contact data of Jansen *et al.* A rather strong temperature dependence of the position, shape, and magnitude of this peak has also been found in the present calculations.

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Recently point-contact spectroscopic results have been reported by Jansen *et al.* for metallic potassium,[1] in which peaks occur in the second derivative of voltage with respect to current at energies (e times the voltage) corresponding to the peaks in the phonon density of states.[2] These peaks arise in the range of 4 to 10 meV. In addition there is a small experimental peak at the very small energy of approximately 0.3 meV. This is at much too small an energy to be due to phonons. Overhauser[3] has suggested that this small-energy peak arises from the scattering of the conduction electrons by phasons in the potassium.[4] This is just the energy at which the peak in the phason density of states occurs according to the analysis of low-temperature electrical resistivity by Bishop and Overhauser.[5]

If phasons (and the corresponding charge-density wave) do exist in potassium, one of the best ways of seeing them would be through point-contact spectroscopy. The electron-phason interaction leads primarily to large-angle scattering of the electrons. The nonlinear characteristic of the point contact is produced mainly by large-angle scattering. Thus electron-phason scattering should be enhanced compared to say electron-defect scattering (or other low-energy scattering mechanisms) in point-contact spectroscopy unlike the situation, for example, in ordinary low-temperature resistivity.

We report here the results of calculations which show that there is quantitative agreement (with essentially no adjustable parameters) between Overhauser's theory of phasons in potassium,[4,5] and the experimental point-contact results,[1] both with regard to the shape of the low-energy peak and its magnitude.

A charge-density wave (CDW) is characterized by a modulation of the electronic charge density

$$\rho(r)=\rho_0[1+p\cos(\vec{Q}\cdot\vec{r}+\varphi)], \qquad (1)$$

where ρ_0 is the electron charge density in the absence of the CDW, and p, $\vec{Q}$, and φ are the amplitude, wave vector, and phase, respectively, of the CDW. Accompanying the CDW is a distortion of the lattice with low-frequency collective modes called phasons.[4] The conduction electrons in the metal can scatter with the emission or absorption of a phason similar to the effect of the electron-phonon interaction. Thus the electron-phason interaction should contribute to the electrical resistivity of any metal in which CDW's occur. However, because of the very low energy of the phasons, this contribution should be observable only at very low temperatures. Bishop and Overhauser[5] have analyzed low-temperature electrical resistivity data on potassium in terms of electron-phason scattering and have determined the parameters of the theory from the data.

Amarasekara and Keesom[6] have measured the specific heat of K at very low temperatures (down to 0.4 K), and they found at their lowest temperatures a contribution to the specific heat in addition to that expected from the electrons and phonons. They further found that this additional low-temperature specific heat can be fitted by the phasons of Overhauser[4] with essentially the same parameters as determined by Bishop and Over-

