Monte Carlo simulations of a disordered, three-dimensional system of Josephson junctions

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Using a Monte Carlo technique we study properties of a disordered three-dimensional system of Josephson junctions. We focus on the anisotropy of the critical magnetic field and on relaxation processes in a zero-field-cooled sample.

Results of many measurements on samples of new high-T_c superconductors have been interpreted as a manifestation of a superconducting glassy state.[1-6] The main features were metastable magnetization in zero-field cooled samples,[2-5] existence of a "quasi"-de Almeida-Thouless line separating reversible and irreversible trajectories on a phase diagram,[2,4,6] and a logarithmic time decay of remanent magnetization.[5] Bednorz, Takashige, and Müller[1] suggested that below T_c superconducting clusters coupled by Josephson junctions may be formed inside a ceramic sample. Similar systems have been previously investigated as models of granular superconductivity,[7-12] and the role of frustration and disorder has been discussed.

More recent simulations[13] of two-dimensional, weakly disordered arrays of Josephson junctions confirmed that such a model may account for many experimental results—in particular a quasi-de Almeida-Thouless line has been reproduced. It was further argued that due to a very short coherence length and many twinning boundaries, Josephson junctions may exist inside the physical grains.[13-14] Indications of the glassy behavior of single crystals have indeed been found,[6,15,16] although some results were interpreted within a standard theory of a flux creep in type-II superconductors.[6,16] On the other hand, evidence of Josephson junctions formed on the boundaries of physical grains has also been reported.[17] Although Cu-O planes play a crucial role for the high-T_c superconductivity, this phenomenon is of three-dimensional character.[18,19] It was then suggested[13,14] that inside a physical grain Josephson junctions form a system of weakly coupled two-dimensional array. Within such a model observed critical-current anisotropies were qualitatively explained.

In this paper we investigate properties of the three-dimensional, disordered system of Josephson junctions. Our system consists of evenly spaced arrays coupled by "vertical" links. We mainly focus on metastable effects and on the anisotropy of magnetic properties. Since our system reveals many features similar to type-II superconductors we investigate anisotropy of the critical field H_{c1}. Our aim is more to study general properties of a disordered, three-dimensional system than to make detailed comparisons with experimental data; therefore, values of some parameters were chosen for numerical convenience.

We consider a system of N superconducting grains coupled via a nonsuperconducting host. Such system is described by the Hamiltonian[20,21]

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}) \tag{1}$$

with

$$A_{ij} = 2\pi/\Phi_0 \int_i^j \mathbf{A} d\boldsymbol{l} , \tag{2}$$

where ϕ_i is the phase of the order parameter in the ith grain, $\Phi_0 = hc/2e$ is the magnetic flux quantum, $\mathbf{A}$ is the vector potential and the integral in (2) is taken along a straight line. In principle $\mathbf{A}$ should include fields due to the superconducting currents within the system. This would lead to a complicated self-consistent problem. For simplicity we take into account only external field $\mathbf{H}$ and use a symmetric gauge

$$\mathbf{A}(\mathbf{r}) = \tfrac{1}{2} \mathbf{H} \times \mathbf{r} . \tag{3}$$

The sum in (1) runs over all linked pairs of grains. We assumed all J_{ij} to be equal and neglected its dependence on temperature and magnetic field.

We investigated a three-dimensional generalization of a system studied by Ebner and Stroud.[10] Our system consists of superconducting grains distributed randomly over ten evenly spaced planes parallel to the xy plane with distance d between two adjacent planes. The cluster is generated as follows. We randomly choose coordinates (x,y) of a grain and a plane number. This grain is added to the system when its distance to all other grains on the same plane is bigger than a_r and is discarded otherwise. We assume that tunneling junction exists between two grains in the same plane if their distance is less than $2a_r$. Grains in two adjacent planes are coupled if their projections on the xy plane are not further apart than a_p. All "loose ends," i.e., strings of coupled grains which do not form closed loops are removed.[10]

The ratio a_p/a_r controls the number of links between planes, while d/a_r affects geometrical anisotropy of the system. In the following all lengths are in the units of a_r.

In order to obtain thermodynamic properties of the system we treat phases ϕ_i as classical variables within a canonical ensemble and use standard Monte Carlo (MC) algorithm to compute thermal averages. We are mainly interested in magnetization which we define as an average magnetic moment per grain, with magnetic moment μ given by

$$\mu = \frac{\pi J}{2\Phi_0} \sum_{\langle i,j \rangle} \sin(\phi_i - \phi_j - A_{ij})(\mathbf{x}_i - \mathbf{x}_j) \times (\mathbf{x}_i + \mathbf{x}_j) , \qquad (4)$$

where $\mathbf{x}_i$ is a position of a grain i.

All presented results are for a system of 381 grains. (Systems of similar size were discussed in Refs. 9, 10, and 13.) Since we deal with a relatively small, strongly disordered system, results should be averaged over different systems of the same size. Instead, we compared results for two such systems to check that all features we are going to discuss are in both cases equivalent.

To investigate properties of a field-cooled system we applied the following procedure. For a given H at temperature $T=4$ (in J/k units which are used throughout this paper) random values of ϕ_i are chosen. At each T, the system evolves for 20 000 MC steps (in one MC step all ϕ_i are changed one by one) before temperature is lowered. Last, 15 000 steps are used to compute thermal averages. After subsequent coolings through $T=2$, 1, and 0.5 to $T=0.25$ the whole system is reheated to $T=4$ and cooled again. Figure 1 shows magnetization as a function of temperature and magnetic field. Each point was obtained as an average of three subsequent coolings. Components parallel to the external field are shown for (a) H along the z axis, i.e., perpendicular to the planes, and for (b) H along the x axis for the system with $a_p=0.3$ and $d=3$.

In small magnetic fields and for $T<2$ magnetization decreases with increasing field unless a critical value $H=H_{c1}$ is reached when first flux quantum penetrates into the system. Values of H_{c1} for H perpendicular ($H_{c1}^{\perp}$) and parallel ($H_{c1}^{\parallel}$) to the planes are different with $H_{c1}^{\perp} > H_{c1}^{\parallel}$. Three factors in our model may be responsible for this anisotropy: distribution of grains, number of vertical links, and distance d between planes. To check for the role of the latter we repeated calculations assuming $d=1$. Results are shown in Fig. 1(c) for magnetic field along the x axis (for H perpendicular to the planes results are not changed with d since $\mathbf{A}$ is then orthogonal to the z axis). Critical magnetic field increased, and for $d=1$ $H_{c1}^{\perp} < H_{c1}^{\parallel}$ which agrees with scaling arguments applied to the Hamiltonian (1). It is also visible that at low temperatures and in small fields magnetization is proportional to the field. The point at which deviation from linearity occurs depends on temperature. At $T \geq 2$ magnetic field has no effect on the magnetic moment which indicates that transition temperature is between $T=1$ and $T=2$, in agreement with Ref. 9.

To simulate properties of zero-field-cooled samples we modified our procedure to imitate (in a very simplified way) experimental conditions. We put $T=0$, and for each value of magnetic field simulation starts with all ϕ_i

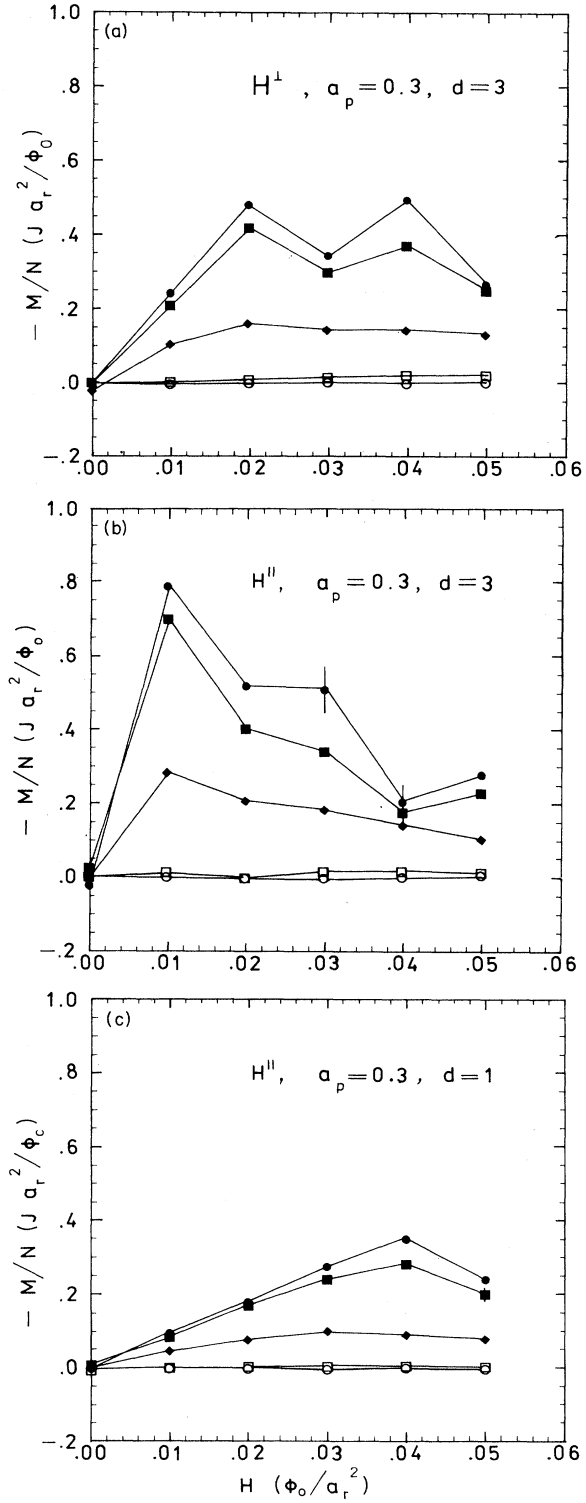

FIG. 1. Magnetization (per grain) parallel to the applied field of a field-cooled system is shown for cases (a), (b), and (c) corresponding to three sets of cluster parameters and field directions with respect to the cluster planes indicated in figure. Symbols correspond to the temperature in units of J/k_B: $T=0.25$, full circles; $T=0.5$, full squares; $T=1.0$, full diamonds; $T=2.0$, open squares; $T=4.0$, open circles. Lines are drawn only as a guide to the eye.

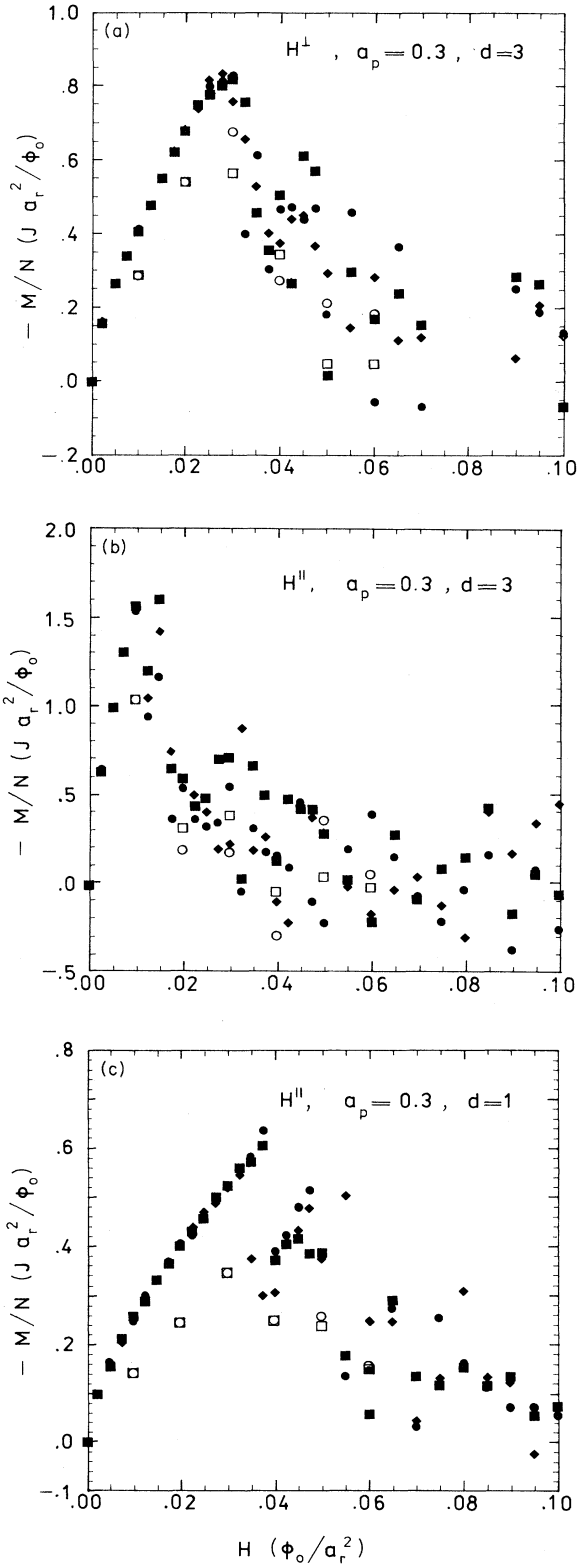

FIG. 2. Magnetization (per grain) parallel to the applied field of a zero-field-cooled system calculated in five independent MC runs for each of three cluster/field direction cases (a), (b), and (c), defined as in Fig. 1. Full (open) symbols are the results of 3000 (20000) MC steps runs.

equal (system in its $H=0$ ground state). After 2500 (Fig. 2, filled symbols) and 19500 (Fig. 2, open symbols) MC steps we take "snapshots" of our system and use next 500 MC steps to calculate averages. The whole procedure is then repeated three times and two times for shorter and longer MC runs, respectively. Parts (a) and (b) of this figure correspond to the case $d=3$ and field parallel to the z and x axis, respectively, while part (c) depicts $d=1$ case for H along the x axis. When we compare filled and open symbols in Fig. 2 it is evident that after 3000 MC steps the system has not yet reached its equilibrium state. Nevertheless, independent "experiments" give practically identical results for small magnetic fields. Only when H is close to H_{c1} results of independent runs start to differ. This effect shows up in the results of shorter as well as longer MC runs although magnetization values corresponding to the reproducible parts of the plots are

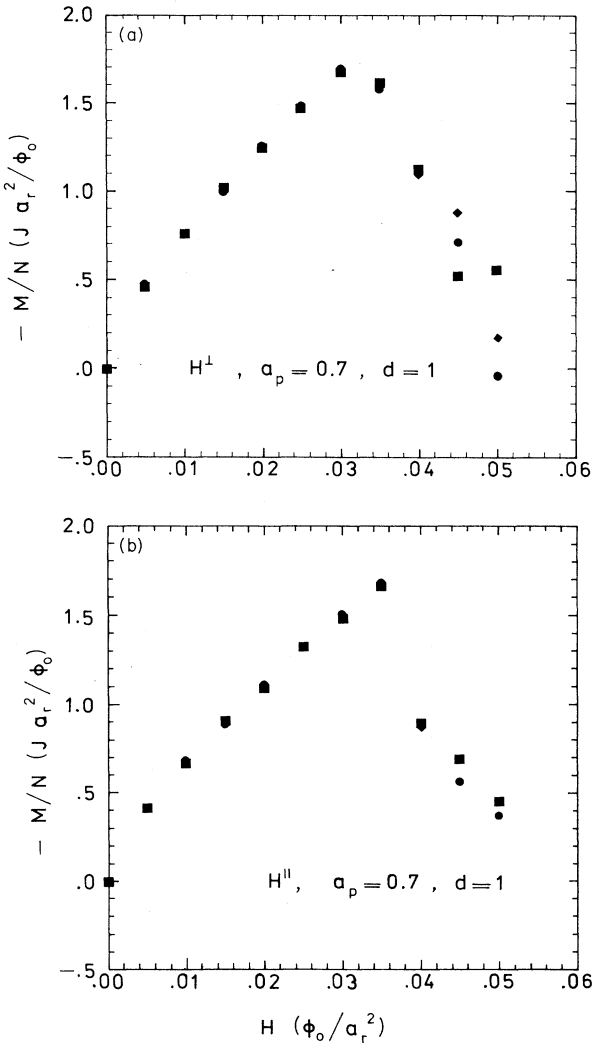

FIG. 3. The same as in Fig. 2 calculated for the cluster with the number of vertical links increased more than two times. Results of 3 (2) independent 3000 MC steps runs are shown for field perpendicular (a) [parallel (b)] to the cluster planes.

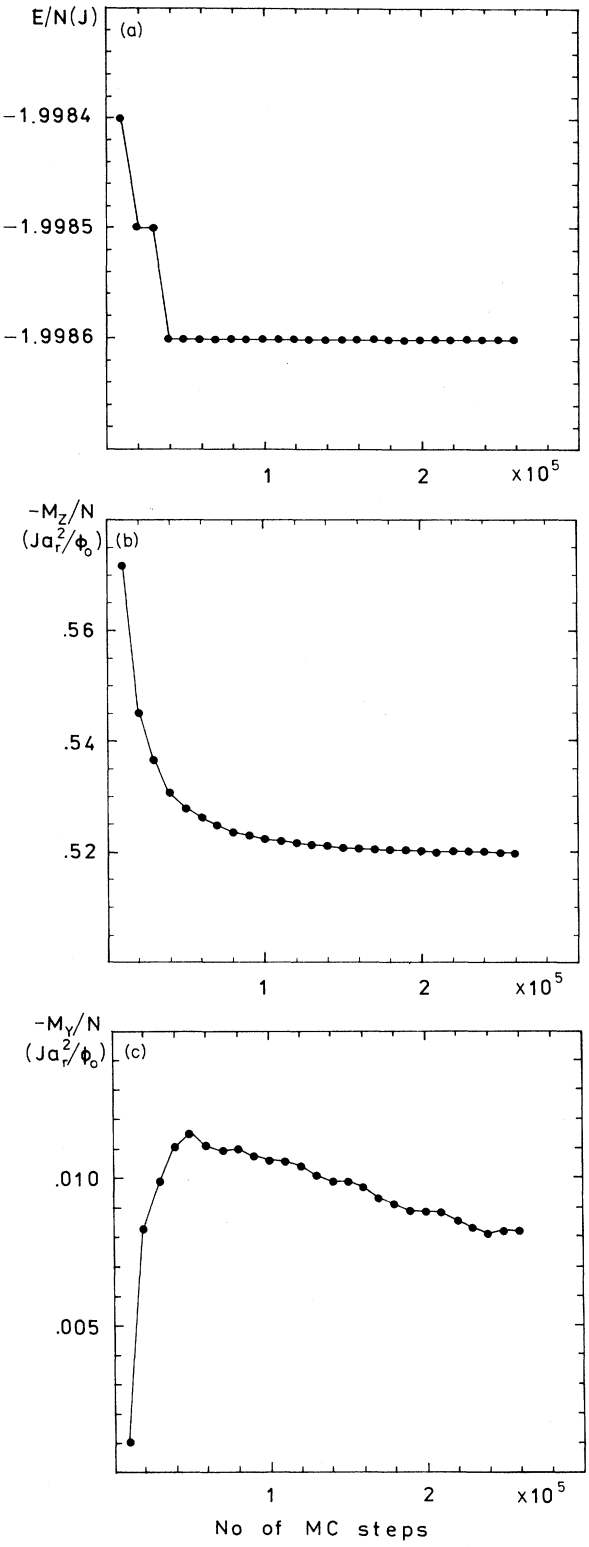

FIG. 4. Equilibration of (a) energy, (b) magnetization component M_z parallel to the field, and (c) magnetization component M_y perpendicular to the field. The parameters are $H_\perp = 0.02\Phi_0/a_r^2$, $a_p = 0.3$, $d = 1$, and $T = 0$.

different. This means that for not too large magnetic fields, relaxation of the system, though very slow, always goes through nearly the same sequence of states. With the field increasing above H_{c1} the number of energetically equivalent equilibration paths drastically increases resulting in a nonreproducible relaxation. Within the accuracy of our simulation, critical magnetic fields are the same for field-cooled and zero-field-cooled samples.

To check for the dependence of magnetic anisotropy on the "topology" of the system we repeated calculations analogous to those reported in Fig. 2 but with $a_p = 0.7$ ($d = 1$). The results for two field directions in Figs. 3(a) and 3(b) should be compared with Figs. 2(a) and 2(c), respectively (different d values in case a are irrelevant since the field is perpendicular to the cluster planes). The change in a_p more than doubled the number of vertical links but has not affected critical field values (Fig. 3). It seems that the anisotropy of the critical field is not sensitive to the number of links between planes unless they are very scarce ($a_p \approx 0$) and the system becomes two dimensional.

Results discussed so far indicate that the investigated system is strongly frustrated with very slow relaxation. It is then interesting to see how such a relaxation process develops in time. We have performed the simulation of 260000 MC steps and calculated energy and magnetization every 10000 steps (the last 500 steps of each subsequent 10000 MC steps were used in the summation procedure). We chose $a_p = 0.3$, $d = 1$, magnetic field along the z axis with $H = 0.02$, a value slightly lower than H_{c1} in this case. After 40000 MC steps energy was practically at its final value [Fig. 4(a)] and in subsequent 220000 steps changed less than 2.5×10^{-3}%. Relaxation of magnetization was considerably slower with the component μ_z parallel to the field changing at the same time by 2% [Fig. 4(b)]. Still slower was the equilibration of magnetization components perpendicular to the field and, e.g., μ_y changed by more than 20% during the last 220000 steps [Fig. 4(c)]. Although Monte Carlo evolution differs from the true dynamics of a system we believe that main qualitative features are in both cases similar.[13]

In summary, results of our Monte Carlo simulations indicate that critical magnetic field anisotropy of the three-dimensional layered system of Josephson junctions depends strongly on the distance between layers and is not affected when the number of vertical links is changed unless it becomes very small. Relaxation of a zero-field-cooled sample is fully reproducible if the field does not exceed its critical value H_{c1}. However, even for fields lower than H_{c1} we found the relaxation process to be very slow with magnetization components perpendicular to the external field evolving an order of magnitude slower than the one parallel to the field.

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