THE VORTEX GLASS

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Abstract

The recently proposed state of a disordered type-II superconductor in a magnetic field, the "vortex glass", is discussed and compared with the "spin glass" transition in magnetic systems. We discuss the results of Monte Carlo simulations on a model that seems to have the necessary ingredients to describe this state, in two, three and four dimensions. The technique involves computing the free energy cost to twist the direction of the phase of the condensate and analyze the results by finite-size scaling. The results show clearly that the model has different behavior in the different dimensions: $d = 4$ clearly has a finite transition temperature; T_c, $d = 3$ is close to the marginal dimension (though T_c is probably also finite); and $d = 2$ only has a transition at $T = 0$. The results are compared with experiments. Recent ideas on obtaining transport properties, such as current-voltage characteristics, from Monte Carlo simulations are also discussed. It is shown that the fluctuation-dissipation theorem and the Kubo formula, familiar from continuous-time Hamiltonian dynamics, are also valid for discrete-time stochastic Monte Carlo dynamics.

To appear in the proceedings of the Ray Orbach Inauguration Symposium, published by World Scientific.

1 Introduction

I am honored to participate in the symposium to commemorate Ray Orbach's inauguration as Chancellor of UC Riverside. I am particularly pleased to talk on a topic which incorporates two of his main interests, spin glasses and superconductivity.

Since I had a background in magnetic phase transitions, I decided to work in the area of frustrated systems called "spin glasses" [1]. At that time, my knowledge of superconductivity was very rudimentary since it didn't seem strongly related to the things that I was working on. Nonetheless, it turns out that there *is* a connection between spin glasses and superconductivity. In a magnetic field, a superconductor experiences frustration, and, in most samples of high-T_c materials, there is significant disorder. Thus, the two necessary conditions for spin glass behavior, randomness and frustration, [1] *are* found in superconductors. Because of this, Matthew Fisher [2] proposed that bulk, disordered type-II superconductors in a magnetic field go into a new state, the "vortex glass" which is analogous to the spin glass state in magnetic systems. Properties of the vortex glass were subsequently worked out in detail by Fisher, in collaboration with Daniel Fisher and David Huse [3]. For conventional low temperature superconductors, fluctuation effects are very small and mean field theories (such as the BCS theory and Ginzburg-Landau theory) work extremely well so vortex glass behavior would probably not be observable. However, high-T_c superconductors have not only a much higher T_c but also a much greater range of temperature where critical fluctuations are observable [3]. Consequently, it was argued [3], the vortex glass phase should be observable in high T_c compounds, and this turned out to be the case [4]. The question of whether or not the vortex glass phase exists is not an entirely academic issue because only in this phase is the resistance really zero in the limit of vanishing current [3] (for a disordered material in a field greater than H_{c_1}).

The question of whether the vortex glass actually occurs has therefore aroused a lot of interest. One expects that fluctuation effects destroy the state if the dimension of space, d, is less than a critical dimension, d_l. The question can therefore be rephrased in terms of the value of the lower critical dimension. Numerical results presented here show that there is definitely a transition in $d = 4$ (not very relevant for experiments, it must be admitted, but this example does provide a striking illustration of the method of finite-size-scaling used in the analysis), while in $d = 2$ there is only a transition at $T = 0$. The most physically relevant case of $d = 3$ is less clear. It does appear that T_c is finite, though d_l is probably quite close to 3, and the possibility that $d_l = 3$ exactly cannot be ruled out.

In section 2, I discuss the spin glass phase transition and go on, in section 3, to consider a model which should describe the spin glass (vortex glass) transition in disordered superconductors. The finite-size scaling techniques, needed to extract results for the thermodynamic limit from the small samples used in the Monte Carlo simulations, are discussed in section 4. The results are presented in section 5, while section 6 comments on the computation of transport properties by Monte Carlo simulations. The conclusions are summarized in section 7. In the appendix, we show that familiar results from linear-response theory for continuous-time Hamiltonian dynamics, such as the fluctuation-dissipation theorem and the Kubo formula, are also valid for discrete-time, stochastic Monte Carlo dynamics. This is useful when computing transport properties by Monte Carlo simulations.

2 The Phase Transition

In this section I will discuss the spin glass transition in magnetic systems. In the following section these ideas will be applied to superconductivity and a simple model for the vortex glass transition described.

Spin glasses are magnetic systems which are disordered and frustrated [1]. No conventional type of long range order, such as ferromagnetism or antiferromagnetism can arise, but a sharp transition to a new type of "ordered" state can occur. To see how this can arise, it is helpful to consider first the simpler case of ferromagnetism. At a second order ferromagnetic transition, there is a correlation length, ξ_F, (the distance over which spins are correlated) which diverges at the transition temperature, T_c. To a good approximation we have

$$\langle S_i S_j \rangle \sim \exp(-R_{ij}/\xi_F) \quad . \tag{1}$$

Here R_{ij} is the distance between lattice points i and j. We assume, for simplicity, Ising spins, $S_i = \pm 1$, but this is not essential. As the transition temperature is approached, ξ_F diverges with a power of the reduced temperature, $t \equiv (T - T_c)/T_c$, *i.e.*

$$\xi_F \sim t^{-\nu} \quad . \tag{2}$$

The ferromagnetic susceptibility, χ_F, also diverges, *i.e.*

$$\chi_F \equiv \frac{1}{k_B T} \sum_J \langle S_i S_j \rangle \sim t^{-\gamma} \quad . \tag{3}$$

In a spin glass there is no net tendency towards ferromagnetism or antiferromagnetism so ξ_F stays short range. Nonetheless, if one looks at a pair of spins a given relative distance apart, they will have substantial correlation, but some pairs will be ferromagnetically correlated and others will have an antiferromagnetic correlation, so the *average* will be close to zero. This cancellation coming from random signs will not occur if we square the correlation function, so we define the spin-glass correlation length, ξ_{SG} by

$$[\langle S_i S_j \rangle^2]_{\rm av} \sim \exp(-R_{ij}/\xi_{SG}) \sim t^{-\gamma} \quad , \tag{4}$$

where $[\cdots]_{\rm av}$ denotes an average over different realizations of the disorder. This is more convenient theoretically than the equivalent procedure of considering a single set of interactions and averaging over all pairs of spins a given distance apart. Just as with ferromagnets, there is a corresponding susceptibility, known as the spin-glass or Edwards-Anderson susceptibility, obtained by summing the squared correlation function over all distances, *i.e.*

$$\chi_{SG} \equiv \sum_j [\langle S_i S_j \rangle^2]_{\rm av} \quad . \tag{5}$$

A spin glass transition is characterized by the divergence of ξ_{SG} and χ_{SG} as the temperature is lowered, *i.e.*

$$\begin{aligned} \xi_{SG} &\sim t^{-\nu} \quad , \\ \chi_{SG} &\sim t^{-\gamma} \quad , \end{aligned} \tag{6}$$

without a divergence of ξ_F or χ_F.

In magnetic systems, the divergence of χ_{SG}, can be directly measured, because χ_{SG} diverges in the same way [1] as the non-linear susceptibility, χ_{nl}, defined as the coefficient of h^3 (where h is the magnetic field) in the expansion of the magnetization, m, *i.e.*

$$m = \chi_F h - \chi_{nl} h^3 + \cdots \quad . \tag{7}$$

The divergence of χ_{nl} has been measured in a variety of spin glass systems and provides strong evidence for a spin glass transition at finite temperature. However, in superconductors, neither χ_F nor χ_{nl} can be measured because it is not possible to couple to the overall phase of the pair condensate. Superconductors do, of course, have striking electrical transport properties, and evidence for a superconducting state comes from [3] a study of current-voltage, (I-V), characteristics. Note, however, that unlike the magnetic measurements of a spin glass, the I-V characteristics of a superconductor do not directly determine the *nature* of the superconducting state, *i.e.* the transitions to the Meissner state, the vortex lattice and the vortex glass all show *qualitatively* the same I-V characteristics.

3 Models and Symmetries

Since fluctuation effects play a much more important role in high temperature superconductors than in conventional superconducting materials, there has been a great deal of effort [3] to understand the behavior of type II superconductors in a magnetic field, including the effects of disorder, when one goes beyond the mean field picture of BCS or Ginzburg–Landau theories. One new aspect of this work is the vortex glass state [2, 5], in which the off diagonal long range order of the pair condensate has a phase which is random in space but frozen in time, much like the order parameter in a spin glass discussed above. This can arise because the Abrikosov flux lattice, which forms in pure samples, is destroyed by disorder in less than 4 dimensions [6] beyond a certain length scale, l_{dis}. The phase of the condensate does not then form a regular periodic pattern on scales larger than l_{dis}, but, according to the vortex glass hypothesis, the system undergoes a transition into a spin glass–like state in which the phase is frozen in time. At the transition, the vortex glass correlation length, ξ diverges. A number of experiments [4] have found evidence for such a transition in the I-V characteristics of Y-B-Cu-O samples. Only if there is a vortex glass phase does the resistance really vanish [3] for $H > H_{c_1}$. Otherwise, the resistance is, in principle, finite because clusters of vortices on scale ξ can move by thermal activation over barriers, a process known as "flux creep" [7]. These effects are observable [8] in high–T_c compounds since they have much larger fluctuations than conventional materials.

The model that is generally studied in numerical work, known as the "gauge glass", has the following Hamiltonian:

$$\mathcal{H} = - \sum_{<i,j>} \cos(\phi_i - \phi_j - A_{ij}) \quad . \tag{8}$$

The phase, ϕ_i, is defined on each site of a regular lattice, square for two dimensions, simple cubic for $d = 3$ and simple hypercubic for $d = 4$, with $N = L^d$ sites. Periodic boundary conditions are imposed. The sum is over all nearest neighbor pairs on the lattice. The effects of the magnetic field and disorder are represented by the quenched vector potentials, A_{ij}, which we take to be independent random variables with a uniform distribution between 0 and 2π. This model seems to be the simplest model with the correct ingredients of randomness, frustration and order parameter symmetry. It plays the same role for the vortex glass, as the Edwards-Anderson [9] model played for spin glasses. The gauge glass model is expected to describe the physics on scales longer than l_{dis} and does not, therefore, describe the details of pinning of individual flux line by defects. The model ignores screening, and therefore corresponds to an extreme type II limit in which $\kappa = \lambda/\xi \to \infty$, where λ is the penetration length. Since $\kappa \gg 1$ in the high T_c superconductors, this limit is not unreasonable. It is unclear, however, how much inclusion of screening via a fluctuating gauge field would modify the behavior of Eq. (8).

Note that if we set all the A_{ij} to zero, the model is just the XY ferromagnet, a popular model of magnetism. It is in the correct universality class to describe the transition to the Meissner phase in a superconductor, if one neglects screening [3], because the Meissner phase, like the ferromagnet, has the same value for the order parameter everywhere. If one has no disorder, but puts in values for the A_{ij} corresponding to a uniform field in some direction, then the model describes a transition to the vortex lattice state. In the magnetic analogy, this corresponds to an antiferromagnet because the order parameter varies periodically in space.

If the A_{ij} are restricted to the values 0 and π, the model becomes the XY spin glass, for which the lower critical dimension is believed [10] to be 4. However, it has been argued [11, 12, 13], that the gauge glass is in a different universality class from the XY spin glass, because, unlike the XY spin glass, the gauge glass does not posses the "reflection" symmetry, $\phi_i \to -\phi_i \ \forall\, i$ [11]. Consequently, the lower critical dimensions of the two models could be different. This turns out to be the case as we shall see below.

4 Finite Size Scaling

Since one can only study a rather modest range of sizes in the simulations, finite size effects are significant. In order to extrapolate results to the thermodynamic limit one uses the techniques of finite-size-scaling. It is particularly useful [13, 12] to consider the change in free energy ΔF when one imposes a twist Θ along one of the space directions, x say. More precisely, the periodic boundary conditions, $\phi_i = \phi_{i+L\hat{x}}$ are replaced by the twisted boundary conditions, $\phi_i = \phi_{i+L\hat{x}} + \Theta$. By a simple redefinition of the phases ϕ_i one can replace this situation by a system with periodic boundary conditions and an extra contribution, Θ/L, to the vector potential on bonds in the x-direction.

By Monte Carlo methods one can calculate derivatives of the free energy w.r.t. Θ, so, for a single sample, we define a current, I, and a stiffness, Y, by

$$I \equiv \frac{\partial F}{\partial \Theta} = \frac{1}{L} \sum_i \langle \sin \Delta_i \rangle_T \quad , \tag{9}$$

$$Y \equiv \frac{\partial^2 F}{\partial \Theta^2} = \frac{1}{L^2}\Big\{ \sum_i \langle \cos \Delta_i \rangle_T - \frac{1}{T} \sum_{i,j} \Big[\langle \sin \Delta_i \sin \Delta_j \rangle_T - \langle \sin \Delta_i \rangle_T \langle \sin \Delta_j \rangle_T \Big] \Big\} \quad , \tag{10}$$

where $\Delta_i = \phi_i - \phi_{i+\hat{x}} - A_{i,i+\hat{x}}$, F is the total free energy and $i + \hat{x}$ refers to the nearest neighbor site in the x-direction from i. Note that both I and Y are gauge invariant so they are still useful even if one includes fluctuating gauge fields.

Above T_c, ΔF, and hence both I and Y, go to zero rapidly with increasing system size because the system is insensitive to boundary conditions when L is much greater than the vortex glass correlation length ξ. If T_c is finite, then, below T_c, I and Y vary with L as L^θ where θ (> 0), is an exponent describing the low temperature phase. In other words, I and Y *increase* with increasing L below T_c, the opposite of what happens above T_c. Precisely at T_c, the both I and Y are independent of size. Hence if T_c is finite, I and Y should come together at T_c and splay out again at lower temperatures. By contrast, if $T_c = 0$, then, at $T = 0$, I and Y vary as L^θ but with $\theta < 0$. Consequently, I and Y decrease with L even at $T = 0$.

For the gauge glass, the average values of I and Y, averaged over different configurations of the A_{ij}, are both zero, i.e.

$$[Y]_{\text{av}} = [I]_{\text{av}} = 0 \quad , \tag{11}$$

because the configuration in which the vector potentials in the x direction have been increased by Θ/L has the same weight in the configurational average as the original choice of vector potentials. One is therefore interested in the root mean square fluctuation between samples. This means that many samples must be averaged over, typically several thousand. If T_c is finite, the finite size scaling form for the r.m.s. current, ΔI is therefore

$$\Delta I \equiv [I^2]_{\text{av}}^{1/2} = \tilde{I}(L^{1/\nu}(T - T_c)) \qquad (T_c > 0) \quad , \tag{12}$$

where ν is the correlation length exponent. We shall concentrate on the r.m.s. current in what follows, rather than the stiffness, because sample to sample fluctuations in the stiffness have an asymmetric distribution with a long tail, which makes it difficult to get good statistics [13]. If $T_c = 0$ then ΔI decreases with size even at $T = 0$, *i.e.* $\Delta I \sim L^\theta$ where θ is negative and related to the exponent ν giving the divergence of the correlation length as $T \to 0$ by $-\theta = 1/\nu$ [10]. The finite size scaling form is then

$$L^{1/\nu} \Delta I = \tilde{I}(L^{1/\nu} T) \qquad (T_c = 0) \quad . \tag{13}$$

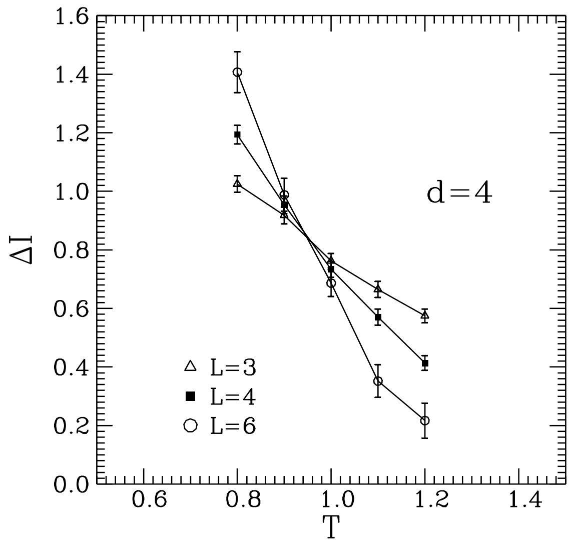

Figure 1: The r.m.s. current, $\Delta I = [I^2]_{av}^{1/2}$, for $d = 4$ determined by Monte Carlo simulations for different sizes and temperatures. The curves for different sizes are expected to come together at T_c and, if there is order in the low temperature state, to splay out again at lower temperatures. The data does indeed follow this behavior.

Tests to ensure equilibration were carried out as described elsewhere [15].

5 Results

Since the physically most interesting case of $d = 3$ is also the hardest to get unambiguous results we start with our results in $d = 4$ [14]. Fig. 1 shows clearly that the data for the r.m.s. current for different sizes come together at $T = T_c \simeq 0.95$ and then splay out again on the low temperature size, just as expected. This provides unambiguous evidence that there is a vortex glass transition in four dimensions (and presumably also in higher dimensions). A scaling plot corresponding to Eq. (12) is shown in Fig. 2. From the fit we estimate [14]

$$T_c = 0.96 \pm 0.01, \quad \nu = 0.7 \pm 0.15 \quad (d = 4) \quad . \tag{14}$$

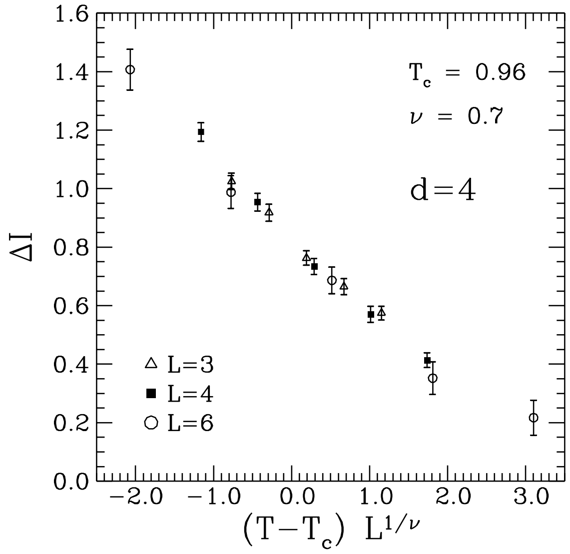

Figure 2: The same data as in Fig. 1 but in a finite size scaling plot, with $T_c = 0.96$ and $\nu = 0.7$.

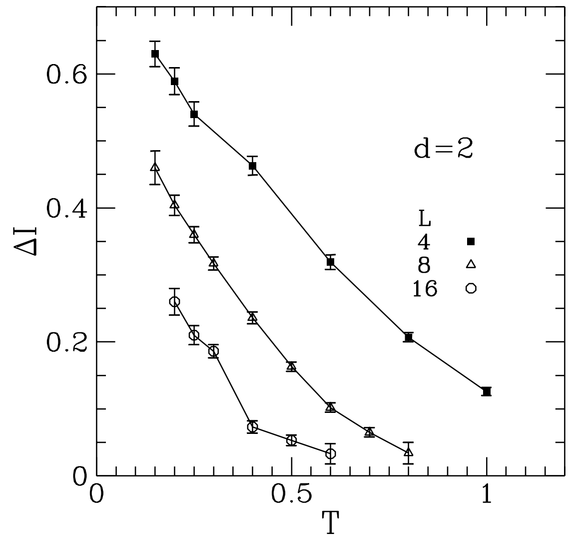

Figure 3: The r.m.s. current, $\Delta I = [I^2]_{av}^{1/2}$, for $d = 2$ determined by Monte Carlo simulations for different sizes and temperatures. The curves for different sizes do not come together, even at the lowest temperature. This behavior indicates a transition at $T = 0$.

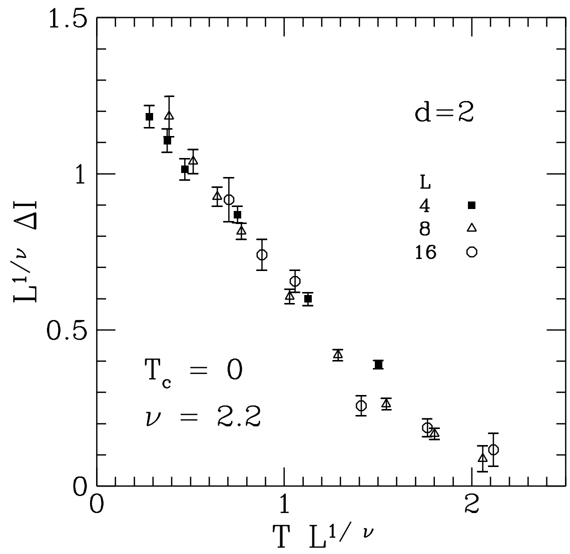

Figure 4: The same data as in Fig. 3 but in a finite size scaling plot, with $T_c = 0$ and $\nu = 2.2$.

Next we discuss the case of $d = 2$. The results for ΔI [14] are shown in Fig. 3. Notice that they are quite different from Fig. 1, since, even at the lowest temperature, ΔI decreases with increasing size. This is precisely what is expected at a zero temperature transition, and the scaling plot in Fig. 4 corresponding to Eq. (13) works very well. From the fit we estimate

$$T_c = 0, \quad \nu = 2.2 \pm 0.2 \quad (d = 2) \quad . \tag{15}$$

The value for ν agree with earlier work [12], in which a different finite-size-scaling technique was used.

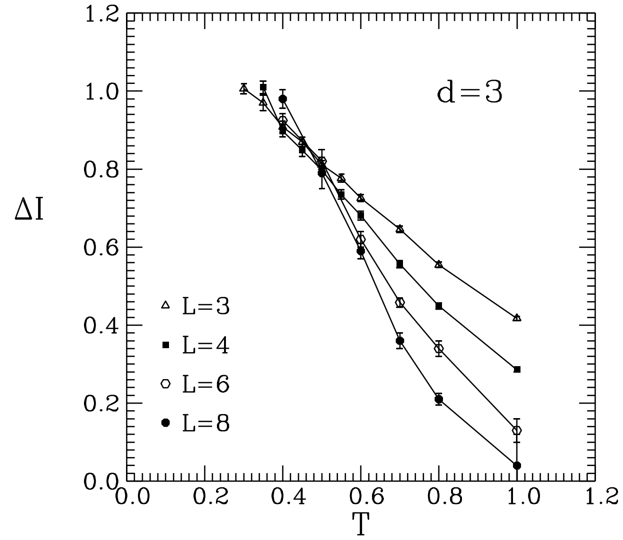

Figure 5: The r.m.s. current, $\Delta I = [I^2]_{av}^{1/2}$, for $d = 3$ determined by Monte Carlo simulations for different sizes and temperatures. The curves for different sizes are expected to come together at T_c and, if there is order in the low temperature state, to splay out again at lower temperatures. The data does indeed become independent of size for $T \simeq 0.50$. At lower temperatures, most of the data is independent of size but for $T = 0.4$ the data for $L = 8$ is significantly greater than that of the lower sizes. More precisely the values for $T = 0.4$ are: 0.980 ± 0.024 ($L = 8$, 1200 samples), 0.925 ± 0.017 ($L = 6$, 2000 samples), 0.898 ± 0.015 ($L = 4$, 2000 samples), 0.908 ± 0.020 ($L = 3$, 2000 samples). In general the data for $L = 8$ used 1000 samples and that for smaller sizes used 2000 or more samples. The error bars are obtained from the variance of the estimates from different samples and represent one standard deviation.

Recent experiments [16] on very thin (16Å) films of YBCO have provided striking confirmation that $T_c = 0$ for the vortex glass in two dimensions. Furthermore, non-linear effects in the current-voltage characteristics set in when the current density exceeds a value, J_{nl} which is varies with temperature as $T^{1+\nu}$ [12]. According to the conventional flux creep theory, there is no divergent length scale as $T \to 0$, which corresponds to setting $\nu = 0$. The experiments [16] find $1 + \nu = 3.0 \pm 0.3$ in excellent agreement with the results presented here and in Ref. [12], but in clear disagreement with the flux creep theory. We emphasize, then, that the vortex glass picture leads to measurable consequences even when $T_c = 0$.

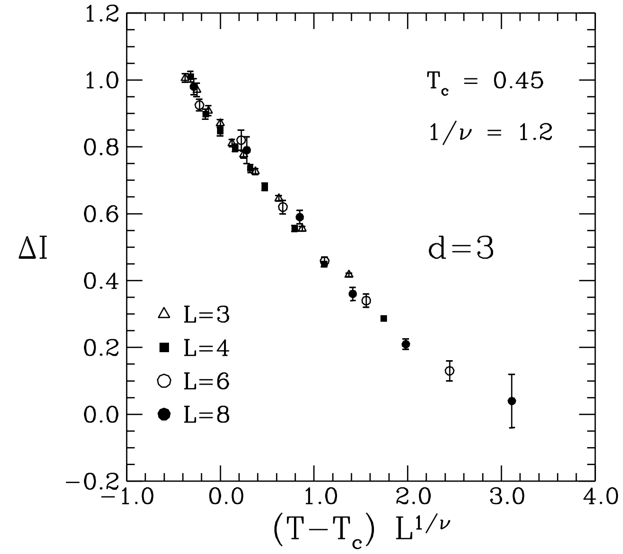

Figure 6: The same data as in Fig. 5 but in a finite size scaling plot, with $T_c = 0.45$ and $\nu = 1.2$.

Our final set of data, for $d = 3$ [13], is shown in Fig. 5. The curves do come together at about $T = 0.5$ and do tend to splay out somewhat below this temperature, though the evidence for this is not as compelling as for $d = 4$. Based on this, it appears that there is a finite transition temperature, $T_c \simeq 0.5$, though the possibility that $T_c = 0$ and $d = 3$ is the lower critical dimension cannot be completely excluded. Collapsing the data for ΔI onto a scaling plot, see Fig. 6, we find $T_c = 0.45 \pm 0.05$, $\nu = 1.3 \pm 0.4$. It is gratifying that this value of ν is in reasonably good agreement with experimental estimates[17], though we should caution that the effects of systematic errors (due to corrections to finite size scaling) have not been incorporated in the estimate of the error bar and that both the experimental and theoretical values may be only effective exponents, valid in a restricted range of temperature and size, since it is unclear if the asymptotic critical region has been reached.

6 Transport Properties

As mentioned above, experiments determine the vortex glass transition temperature critical exponents from the I-V characteristics. It would obviously be interesting to compute the same quantity by simulations on a simplified model. This can be done [18] by working in the vortex representation and including the Magnus force which acts on a vortex in the presence of an applied current. This causes a net flow of vortices which gives rise to a voltage. Applying this idea to the gauge glass in two dimensions, [19] one finds again that $T_c = 0$ and obtains a value of ν in fair agreement with experiments and the other theoretical estimates [12, 14]. Work is in progress [19] to compare the experimental and theoretical scaling functions.

Note that in applying the Monte Carlo simulation to determine transport properties, one is interpreting the number of Monte Carlo sweeps as time. Since Monte Carlo "dynamics" is purely relaxational, this seems intuitively reasonable when the real dynamics is overdamped. Presumably this is the case here, where the vortices are both pinned to sites, and, when they do move, are subjected to frictional forces [20]. What is less well known is that all the standard results of linear response theory for conventional Hamiltonian dynamics, such as the fluctuation-dissipation theorem and the Kubo formula for transport properties, are also valid for discrete-time Monte Carlo dynamics. In the appendix, we give a derivation of this.

7 Conclusions

To conclude, we have shown that a Monte Carlo calculation of the change in free energy due to a twist in the boundary conditions combined with finite size scaling is a very powerful tool for systems with XY-like symmetry. We have shown that it clearly distinguishes between the finite temperature transition in the $d = 4$ gauge glass and the zero temperature transition of the two-dimensional model. The three-dimensional gauge glass seems to be close to the lower critical dimension, but does appear to have a finite transition temperature, in agreement with experiment. It has recently been possible to compute directly the I-V characteristics of the two-dimensional model using the vortex representation. One remaining unsolved problem is to understand the role of screening.

8 Questions

A. Hebard: What microscopic parameters affect the crossover length which determines whether the system is three-dimensional with a finite transition temperature, or two-dimensional with a transition at zero temperature?

A. P. Young: One has to compare the thickness of the film with the correlation length in the direction perpendicular to the film. If the thickness is less than the correlation length even well away from T_c the behavior will always look two-dimensional. This seems to be the case for the 16Å films in the experiments of Ref. [16]. In the opposite extreme, the film is so thick that it is much greater than the correlation length at all temperatures except for an immeasurably small range of temperature around T_c, and the behavior will be three-dimensional. The 3000Å films in Ref. [16] seem to be in this limit. For films of intermediate thickness, a crossover will be observed between two and three dimensional behavior at the temperature where the out-of-plane correlation length becomes equal to the film thickness. This has been observed [16] in films of intermediate thickness.

M. L. Lapidus: Could you please elaborate on the possible effects of "screening"

A. P. Young: Inclusion of screening is expected to lead to a different critical behavior very close to the transition [3]. It is also possible that screening might eliminate the vortex glass transition in three-dimensions, though, to my knowledge, there are no calculations which substantiate this possibility.

Acknowledgments: This work was supported in part by the NSF grant No. DMR 91-11576. It is a pleasure to acknowledge M. P. A. Fisher for informative discussions and a stimulating collaboration. Some of the results presented here were obtained in collaboration with Joseph Reger.

Appendix

In this appendix we demonstrate that the fluctuation-dissipation theorem and the Kubo formula for transport coefficients, which are well known for continuous time Hamiltonian dynamics, are also valid for discrete-time stochastic Monte Carlo dynamics. The applicability of the fluctuation-dissipation theorem has been discussed before, *e.g.* the review by Kawasaki [21]. However, there is a crucial aspect of the derivation which is not very clear in Ref. [21], which we would like to emphasize here. We are not aware of any previous discussion of the Kubo formula in the context of Monte Carlo dynamics.

We denote a state of the system by α. The probability that the system is in state α at time t is denoted by $P(\alpha, t)$. Here t is an *integer* which indicates how many Monte Carlo updates have been performed. t is increased by unity for every (attempted) Monte Carlo update so that one "sweep" through the lattice, as conventionally defined, increases t by N, where N is the number of lattice sites. The time development of P is determined by a master equation [21]

$$P(t+1) - P(t) = -\Gamma P \quad , \tag{16}$$

where the matrix Γ has elements given by

$$\Gamma_{\alpha\beta} = \delta_{\alpha\beta} \sum_{\gamma} w_{\gamma\alpha} - w_{\alpha\beta} \quad , \tag{17}$$

in which $w_{\alpha\beta}$ is the probability that the system, assumed in state β at time t, makes a transition to state α at time $t+1$, *i.e.* it is a conditional probability. The second term in Eq. (17) arises from transitions into state α from some other state β, while the first term describes transitions out of state α into another state γ. Since the sum of the probabilities is unity for all times it follows that

$$\sum_{\alpha} \Gamma_{\alpha\beta} = 0 \quad . \tag{18}$$

We assume that the $w_{\alpha\beta}$ do not depend on t so all updates are equivalent to each other. (This corresponds to choosing the site where the move will be made at random, rather than according to sequential updating). The $w_{\alpha\beta}$ can be chosen arbitrarily as long as they have the attributes of probabilities, *i.e.* they are non-negative and are properly normalized,

$$\sum_{\alpha} w_{\alpha\beta} = 1 \quad , \tag{19}$$

and, in addition, satisfy the detailed balance condition

$$w_{\alpha\beta} P_{eq}(\beta) = w_{\beta\alpha} P_{eq}(\alpha) \quad , \tag{20}$$

where $P_{eq}(\alpha)$ is the equilibrium distribution,

$$P_{eq}(\alpha) = \frac{e^{-E_\alpha/T}}{Z} \quad , \tag{21}$$

in which $E(\alpha)$ is the energy of state α and we have set Boltzmann's constant to unity. The detailed balance condition ensures that P_{eq} is a stationary distribution as required, or, equivalently,

$$\sum_{\beta} \Gamma_{\alpha\beta} P_{eq}(\beta) = 0 \quad . \tag{22}$$

If we set

$$w_{\alpha\beta} = P_{eq}^{1/2}(\alpha)\ \hat{w_{\alpha\beta}}\ P_{eq}^{-1/2}(\beta) = e^{-(E_\alpha - E_\beta)/2T} \hat{w}_{\alpha\beta} \tag{23}$$

then, from the detailed balance condition, the $\hat{w}_{\alpha\beta}$ are symmetric. Consequently, if the $\hat{w}_{\alpha\beta}$ are changed (still keeping them symmetric and ensuring that the normalization condition, Eq. (19) is maintained) then the equilibrium distribution is unchanged, so $(\Gamma + \delta\Gamma)P_{eq} = 0$, where $\delta\Gamma$ is the resulting change in the matrix Γ. It then follows from Eq. (22) that

$$\delta\Gamma P_{eq} = 0 \quad , \tag{24}$$

which will be important later.

Note that Γ is not symmetric but, if we wish, we can make the Master equation symmetric by defining

$$\hat{P}(\alpha) = \frac{P(\alpha)}{P_{eq}^{1/2}(\alpha)} \tag{25}$$

so $\hat{P}$ satisfies the equation of motion

$$\hat{P}(t+1) - \hat{P}(t) = -\mathcal{L}\hat{P} \quad , \tag{26}$$

where

$$\mathcal{L}_{\alpha\beta} = P_{eq}^{-1/2}(\alpha)\ \Gamma_{\alpha\beta}\ P_{eq}^{1/2}(\beta) \tag{27}$$

is symmetric. Note that Γ and $\mathcal{L}$ have the same eigenvalues (which are real because $\mathcal{L}$ is symmetric). However, we shall not need this symmetric representation of the problem in what follows.

Let us now assume that the system has come to equilibrium and we then add a small time dependent perturbation,

$$\delta\mathcal{H} = -Bf(t) \quad , \tag{28}$$

where B is some variable of the problem (*e.g.* it could be the magnetization in a spin problem) and $f(t)$ is small so we need only compute the response to first order in $f(t)$. In order to determine the response of the system, we must determine the changes in $w_{\alpha\beta}$ and Γ induced by $\delta\mathcal{H}$. The change in $w_{\alpha\beta}$ comes from two sources: (i) the change in the energies E_α and E_β in Eq. (23) and (ii) the change in $\hat{w}_{\alpha\beta}$, *i.e.*

$$\delta w_{\alpha\beta}(t) = \delta w^{(1)}_{\alpha\beta}(t) + \delta w^{(2)}_{\alpha\beta}(t) \tag{29}$$

where (for $\alpha \neq \beta$)

$$\delta w^{(1)}_{\alpha\beta}(t) = w_{\alpha\beta}\frac{f(t)}{2T}(B_\alpha - B_\beta) \tag{30}$$

and

$$\delta w^{(2)}_{\alpha\beta}(t) = \delta\hat{w}_{\alpha\beta}(t)e^{-(E_\alpha - E_\beta)/2T} \ . \tag{31}$$

The changes in $w_{\alpha\alpha}$ are determined by the normalization condition, Eq. (19). There will be two corresponding changes in $\delta\Gamma$,

$$\delta\Gamma(t) = \delta\Gamma^{(1)}(t) + \delta\Gamma^{(2)}(t) \quad . \tag{32}$$

Note that $\delta\Gamma^{(2)}(t)$, which comes from the change in $\delta w^{(2)}$, will —em not affect the linear response because it gives zero when acting on P_{eq}, see Eq. (24). This point does not seem to made clearly in Ref. [21]. Hence, we consider only $\delta\Gamma^{(1)}(t)$, which is given by

$$\delta\Gamma^{(1)}_{\alpha\beta}(t) = \frac{f(t)}{2T}(B_\alpha - B_\beta)\Gamma_{\alpha\beta} \qquad (\alpha \neq \beta) \tag{33}$$

$$\delta\Gamma^{(1)}_{\beta\beta}(t) = -\frac{f(t)}{2T}\sum_{\alpha\neq\beta}(B_\alpha - B_\beta)\Gamma_{\alpha\beta} \quad . \tag{34}$$

The change in the probability distribution at time t is given by

$$\delta P(\alpha, t) = -\sum_{t'=-\infty}^{t-1}\sum_\beta \left[(1-\Gamma)^{t-t'-1}\,\delta\Gamma^{(1)}(t')\right]_{\alpha\beta} P_{eq}(\beta) \quad , \tag{35}$$

where we have used the formal solution of Eq. (16),

$$P(t) = (1-\Gamma)^{t-t'}P(t') \quad , \tag{36}$$

(remember that t takes integer values). The change in the expectation value of a variable, A, at time t is then given by

$$\overline{\delta A(t)} = \sum_\alpha A_\alpha \delta P(\alpha, t) \quad . \tag{37}$$

One finds that the $B_\alpha \Gamma_{\alpha\beta}$ term in Eq. (33) does not contribute because of Eq. (22), the terms in Eqs. (33) and (34) contribute equally, and so from Eqs. (22), (33) and (35), Eq. (37) can be expressed as

$$\overline{\delta A(t)} = \frac{1}{T} \sum_{t'=-\infty}^{t-1} f(t') \sum_{\alpha,\beta} A_\alpha \left[(1-\Gamma)^{t-t'-1} \Gamma \right]_{\alpha\beta} B_\beta P_{eq}(\beta) \quad . \tag{38}$$

Writing the single factor of Γ in Eq. (38) as $1-(1-\Gamma)$, and defining

$$\hat{A}(t) = (1-\Gamma)^t \hat{A} (1-\Gamma)^{-t} \quad , \tag{39}$$

where the variables A and B are now represented by diagonal matrices with elements

$$\hat{A}_{\alpha\beta} = \delta_{\alpha\beta} A_\alpha \quad , \tag{40}$$

Eq. (38) becomes

$$\overline{\delta A(t)} = \frac{1}{T} \sum_{t'=-\infty}^{t-1} f(t') \sum_{\alpha,\beta} \left[\left(\hat{A}(t-t'-1) - \hat{A}(t-t') \right) \hat{B} \right]_{\alpha\beta} P_{eq}(\beta) \quad , \tag{41}$$

where we have used Eq. (18). It is easy to show [21] that

$$\sum_{\alpha,\beta} \left[\hat{A}(t_1) \hat{B}(t_2) \right]_{\alpha\beta} P_{eq}(\beta) = \langle A(t_1) B(t_2) \rangle \equiv C_{AB}(t_1 - t_2) \quad , \tag{42}$$

where $\langle A(t_1) B(t_2) \rangle$ denotes an equilibrium Monte Carlo average, which only depends on the time difference $t_1 - t_2$, and which is an even function of its argument, *i.e.*

$$C_{AB}(-t) = C_{AB}(t) \quad , \tag{43}$$

since the fluctuations are classical. Hence Eq. (41) becomes

$$\overline{\delta A(t)} = \frac{1}{T} \sum_{t'=-\infty}^{t-1} f(t') \left[C_{AB}(t-t'-1) - C_{AB}(t-t') \right] \quad . \tag{44}$$

Defining the linear response function, $\chi_{AB}(t)$ in the usual way,

$$\overline{\delta A(t)} = \sum_{t'=-\infty}^{\infty} \chi_{AB}(t-t') f(t') \quad , \tag{45}$$

we obtain

$$\begin{aligned} T\chi_{AB}(t) &= C_{AB}(t-1) - C_{AB}(t) \qquad (t \geq 1) \\ &= 0 \qquad\qquad\qquad\qquad\quad\;\; (t \leq 0) \quad . \end{aligned} \tag{46}$$

Remember that t takes on integer values. Eq. (46) is of the same form as the standard fluctuation theorem (FDT) for classical Hamiltonian systems

$$\begin{aligned} T\chi_{AB}(t) &= -\partial_t C_{AB}(t) \qquad (t>0) \\ &= 0 \qquad\qquad\qquad (t<0) \quad . \end{aligned} \tag{47}$$

It is interesting that the FDT holds *exactly* for Monte Carlo simulations, despite the replacement of deterministic Hamiltonian dynamics by a stochastic dynamics and of continuous time by discrete time.

Next we discuss the Kubo formula for transport properties. We suppose, for example, that an electric field is applied across the sample in one direction. The electric field couples to the total electric dipole moment of the lattice, p, (we assume that the response at $\mathbf{k}=0$ is required), so $\delta\mathcal{H}$ is given by

$$\delta\mathcal{H} = -f(t)\; p \quad . \tag{48}$$

In order to define transport properties, we need to assign the amount of real time, Δt, associated with a single update. It presumably makes sense to choose $\Delta t \simeq \tau_{mic}/N$ since each particle can move in the microscopic time τ_{mic}. The current density (integrated over the system), which we denote by j, is then given by

$$j(t) = \frac{[p(t+1)-p(t)]}{\Delta t} \quad . \tag{49}$$

The perturbation induces a time-dependent response in the polarization, which is given by Eq. (44) as

$$\overline{\delta p(t)} = \frac{1}{T}\sum_{t'=-\infty}^{t-1} f(t')\;\langle\; p(t)\,[\; p(t'+1)-p(t')\;]\;\rangle \quad . \tag{50}$$

The resulting current density (integrated over the system) is given by

$$\overline{\delta j(t)} = \frac{\left[\overline{\delta p(t+1)} - \overline{\delta p(t)}\right]}{\Delta t} \quad . \tag{51}$$

From Eqs. (50) and (43) this can be expressed as

$$\overline{\delta j(t)} = N\sum_{t'=-\infty}^{\infty} \sigma(t-t') f(t') \quad , \tag{52}$$

where $\sigma(t)$, the time-dependent conductivity, is given by

$$\begin{aligned} \sigma(t) &= \frac{\Delta t}{NT}\langle j(t)j(0)\rangle \qquad (t\ge 1) \\ &= \frac{\Delta t}{2NT}\langle j(0)j(0)\rangle \qquad (t=0) \\ &= 0 \qquad\qquad\qquad\qquad (t<0) \quad . \end{aligned} \tag{53}$$

The d.c. conductivity is therefore given by

$$\begin{aligned}\sigma(\omega=0) &= \frac{\Delta t}{2NT}\langle j(0)j(0)\rangle + \frac{1}{NT}\sum_{t=1}^{\infty}\Delta t\langle j(t)j(0)\rangle \\ &= \frac{1}{2NT}\sum_{t=-\infty}^{\infty}\Delta t\langle j(t)j(0)\rangle \quad ,\end{aligned} \tag{54}$$

where we have used Eq. (43) to obtain the last expression. Eq. (54) corresponds to the Kubo formula for classical Hamiltonian systems written in the form

$$\sigma(\omega=0) = \frac{1}{2NT}\int_{-\infty}^{\infty} dt\ \langle j(t)j(0)\rangle \quad . \tag{55}$$

Note that for both the FDT and Kubo formula, one can deduce the continuous-time expression from the discrete-time version, but the converse is not true because many finite differences have the same continuum limit. Note also that both the continuous-time and discrete-time results can also be rephrased to relate the conductance, Σ ($\equiv L^{d-2}\sigma$ for a system of size $N = L^d$), to fluctuations in the total current, I ($\equiv L^{-1}j$), *e.g.*

$$\Sigma(\omega=0) = \frac{1}{2T}\int_{-\infty}^{\infty} dt\ \langle I(t)I(0)\rangle \quad , \tag{56}$$

with no factors involving the system size.

The Kubo formula, Eq. (54), has recently [19] been used to determine the linear resistance of the two-dimensional gauge glass in the vortex representation.

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