Vortex glass transition in a frustrated 3D XY model with disorder

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The anisotropic frustrated three dimensional (3D) XY model with disorder in the coupling constants is simulated as a model of a point disordered superconductor in an applied magnetic field. From a finite size scaling analysis of the helicity modulus it is concluded that the data is consistent with a finite temperature transition with isotropic scaling and the correlation length exponent is found to be $\nu = 1.50 \pm 0.12$, consistent with 3D gauge glass universality.

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The hypothesis of a vortex glass in disordered high temperature superconductors has spurred much research and many discussions during more than one decade and continues to be a very controversial issue. The essence of this suggestion is that random point disorder in superconductors may conspire with the vortex line interaction to pin the vortices and that this takes place through a sharp transition into a phase with vanishing linear resistance.

Computer simulations have for quite some time played an important role in the examination of critical phenomena and have also recently been used in the study of some vortex glass models. One important such model is the three dimensional (3D) gauge glass, which is an isotropic 3D XY model with randomness included through a random vector potential added to the phase difference of the superconducting order parameter. The evidence has for quite some time pointed at a finite temperature transition in this model, but strong evidence for a real phase transition has been obtained only recently through the use of the exchange Monte Carlo (MC) technique. The value of the correlation length exponent was then found to be $\nu = 1.39 \pm 0.20$. It is however generally recognized that the 3D gauge glass models is too much of a simplification to allow for any safe conclusions regarding the behavior of disordered superconductors in applied magnetic fields. Most seriously, the gauge glass is an isotropic model with no net field which means that the possibility of anisotropic scaling is excluded at the outset.

Two studies with the necessary ingredients of disorder and applied field have so far been reported in the literature. The first is an examination of a frustrated 3D XY model with randomness in the couplings, and the data was there interpreted as evidence for a phase transition with $\nu \approx 2.2$. The crossing of the data for different sizes expected from finite size scaling, was however not entirely convincing, possibly because of the open boundary conditions employed in the simulation. The second study gives results for a 3D random pinning model with strong disorder. The value of the correlation length exponent was there found to be $\nu \approx 0.7$, undistinguishable from $\nu \approx 0.67$ in the pure zero field 3D XY model. This is at odds with the common expectation that a vortex glass transition should be in a different universality class than the pure model.

In this paper we present results from large scale simulations on a frustrated 3D XY model with disorder in the coupling constants. The quantity in focus is the helicity modulus and we find that the data is consistent with a finite temperature glass transition with isotropic scaling and obtain the correlation length exponent $\nu = 1.50 \pm 0.12$. The agreement with $\nu = 1.39 \pm 0.20$ for the 3D gauge glass model suggests a common universality class.

The model we simulate is given by the Hamiltonian

$$\mathcal{H} = - \sum_{\text{bonds } i\mu} J_{i\mu} \cos(\theta_i - \theta_{i+\mu} - A_{i\mu} + \delta_{i\mu}), \quad (1)$$

where $\theta_i$ is the phase of the superconducting wave function at site $i$ of a periodic $L_x \times L_y \times L_z$ lattice and the sum is over all bonds in directions $\mu = x, y, z$. An applied magnetic field in the $z$ direction corresponding to $1/5$ flux quantum per plaquette is obtained through the quenched vector potential with the choice $A_{i\mu} = y_i 2\pi / 5$, and $A_{iy} = A_{iz} = 0$. The randomness is included through disorder in the coupling constants,

$$J_{i\mu} = J_{i\parallel} (1 + p \epsilon_{i\mu}), \quad \mu = x, y,$$

$$J_{i\mu} = J_{i\perp}, \quad \mu = z,$$

where $\epsilon_{i\mu}$ are independent variables from a Gaussian distribution with $\langle \epsilon_{i\mu} \rangle = 0$ and $\langle \epsilon_{i\mu} \rangle^2 = 1$. The disorder strength $p = 0.4$ together with the anisotropy $J_{i\parallel} = J_{i\perp}/40$ were chosen since they were found sufficient to prohibit the formation of Abrikosov lattices. The simulations are performed with fluctuating twist boundary conditions: the $\delta_{i\mu}$ in Eq. are the twist variables and the total twist in the respective directions are $\Delta_{i\mu} = L_{i\mu} \delta_{i\mu}$. The simulations are performed with $L = L_x = L_y$ and a fixed aspect ratio, $L_z = 5/3$. The temperature is given in units of $J_{i\perp}$.

The quantity in focus in our analysis is the helicity modulus which is defined from the change in free energy density, $f$, due to an applied twist, $\delta_{i\mu}$: $Y_{i\mu} = \partial^2 f / \partial \delta_{i\mu}^2$. To use the helicity modulus as a signal of the stiffness of the system the derivative should be evaluated...
at the twist that minimizes the free energy. In ordered systems this minimum is always at zero twist and the helicity modulus may then be evaluated by means of a correlation function determined with periodic boundary conditions, $\Delta_\mu = 0$. For disordered systems, however, the minimizing twist will in general be different from zero and one then needs to make simulations with the twist variables $\Delta_\mu$ as additional dynamical variables and collect histograms $P_\mu(\Delta_\mu)$. The helicity moduli are then determined from the free energies $F_\mu = -T \ln P_\mu$, as discussed below. To analyze the critical behavior we use the standard scaling relation for the helicity modulus in 3D,

$$LY \sim g \left(t L^{1/\nu}\right),$$  \hspace{1cm} (2)

where $t = (T - T_c)/T_c$ and $g$ is a scaling function. This expression presumes isotropic scaling; the more general scaling relations are given in Ref. 10. A naive analysis of $\Upsilon(L)$ rather than the correct scaling quantity $LY$, led to an erroneous conclusion regarding the existence of a vortex glass phase in Ref. 10.

Our simulations are performed with exchange MC which is a method for simultaneously simulating multiple copies of a particular configuration of disorder with each copy at a different temperature. According to certain rules these copies may now and then interchange temperature and therefore effectively perform random walks in temperature space. These random changes in temperature greatly help the different copies avoid getting trapped in restricted parts of the phase space and therefore makes it possible to sample the whole phase space and obtain the true thermodynamic averages. In our simulations the temperatures were chosen according to the equation

$$T_m = T_{\text{min}} \left(\frac{T_{\text{max}}}{T_{\text{min}}}\right)^{m/N_T}, \quad m = 0, \ldots, N_T - 1,$$  \hspace{1cm} (3)

with $T_{\text{max}} = 0.24$ and $T_{\text{min}}$ as given in Table I. Before doing the actual exchange MC the initial spin configurations for the $N_T$ temperatures were obtained by slowly cooling the system with standard MC simulations. The number of temperatures, the acceptance ratio for the exchange step, and the number of disorders simulated for the different system sizes are shown in Table II. The exchange steps are attempted once every 16 sweeps.

The exchange MC method ensures that all the different copies remain at thermal equilibrium as soon as equilibrium has been reached. The approach to equilibrium may however be very slow since information and configurations have to propagate all the way from high to low temperatures. We have carefully examined the approach to equilibrium and especially for our largest sizes the times for equilibration are indeed very long. For the next largest size, $L = 20$, equilibration is only reached after about $2.9 \times 10^6$ sweeps, and to make thermalization at all possible for our largest size, $L = 25$, we chose not to go to quite that low temperatures for the largest size, cf. Table II. This was decided since the time required for thermalization may increase very rapidly with decreasing temperature. Still, about $4.5 \times 10^6$ sweeps were necessary to reach equilibrium for $L = 25$.

![FIG. 1: $P_\mu(\Delta_\mu)$ for a certain disorder realisation. Note that the peaks of the histograms become higher and sharper as the temperature is lowered. This kind of data is used for the determination of $\Upsilon$ through Eq. 9. The inset gives the corresponding quantity for the $x$ direction.](image)

For each system size, disorder configuration and temperature the main output from the simulations is histograms $P_\mu(\Delta_\mu; \tau)$, where $\tau$ enumerates bins corresponding to $2^{18} = 262144$ sweeps over the lattice. The further analysis is then based on the average

$$P_\mu(\Delta_\mu) = \frac{1}{\tau_{\text{max}}} \sum_{\tau=1}^{\tau_{\text{max}}} P_\mu(\Delta_\mu; \tau),$$  \hspace{1cm} (4)

and the helicity modulus is determined from the curvature at the minimum of the associated free energy by fitting a second order polynomial to the free energy in a narrow interval around the minimum, $\Delta_0$, which is also

| $L_x$ | $L_z$ | $N_d$ | $N_T$ | $T_{\text{min}}$ | $X_{\text{acc}}$ (%) | $\tau_{\text{eq}}$ | $\tau_{\text{max}}$ | sweeps/10^6 |
|---|---|---|---|---|---|---|---|---|
| 10 | 6 | 600 | 12 | 0.09 | 30 | 1 | 15 | 0.3 + 3.9 |
| 15 | 9 | 600 | 24 | 0.09 | 30 | 4 | 12 | 1.0 + 3.1 |
| 20 | 12 | 600 | 36 | 0.09 | 32 | 11 | 21 | 2.9 + 5.5 |
| 25 | 15 | 200 | 36 | 0.15 | 27 | 17 | 31 | 4.5 + 8.1 |

TABLE I: Parameters describing the simulations. For systems of size $L \times L_x \times L_z$ we simulated $N_d$ disorder configurations with $N_T$ temperatures in the range $T_{\text{min}} \le T < T_{\text{max}}$, cf. Eq. 3. The acceptance ratio for the exchange step is given by $X_{\text{acc}}$. Of the bins corresponding to $2^{18} = 262144$ sweeps $\tau_{\text{eq}}$ are first discarded and the remaining $\tau_{\text{max}}$ are used for calculating averages. The same information is also given in terms of the number of sweeps for equilibration and for collecting data.
determined in the fit,
\[ \bar{F}_\mu(\Delta_\mu) \sim Y_\mu \frac{V}{2L_\mu^2}(\Delta_\mu - \bar{\Delta}_\mu^0)^2. \] (5)

However, it turns out that the values of \( Y_\mu \) obtained in this way are biased towards too large values. The origin of this bias as well as the method employed to eliminate it from the data is discussed below after the discussion of the results.

We now focus on disorder averaged quantities for which the bias mentioned above has already been eliminated. With \([\ldots]_{\text{av}}\) denoting the average over disorder configurations we define
\[
Y_{\perp} = \frac{1}{2}[Y_x + Y_\mu]_{\text{av}}, \tag{6a}
\]
\[
Y_\parallel = [Y_z]_{\text{av}}. \tag{6b}
\]

Our results for \( L Y_{\perp} \) are shown in Fig. 2. To a very good accuracy the data for the different sizes cross at a single temperature. To further verify the scaling according to Eq. (2) we fit our data for \( L Y_{\perp} \) near \( T_c \) to a fourth order polynomial expansion of \( g(tL^{1/\nu}) \) and obtain the values \( \nu = 1.50 \pm 0.12 \) and \( T_c = 0.123 \pm 0.003 \). The collapse which is shown in Fig. 2 is excellent and holds in a surprisingly large temperature interval. The error estimates are obtained with a resampling technique and correspond to one standard deviation.

A vortex glass transition should also be seen in the parallel component of the helicity modulus and since the anisotropy exponent enters the scaling relation in different ways for \( Y_\parallel \) and \( Y_{\perp} \), a scaling analysis of \( L Y_\parallel \) constitutes an additional test that the scaling actually is isotropic. The crossing of \( L Y_\parallel \) at \( T_c \) for different sizes and the scaling collapse are shown in the insets of Figs. 2 and 3 respectively. From the not so smooth curves it is clear that the precision in \( Y_\parallel \) is much worse than for \( Y_{\perp} \).

This may be traced back to the less good quality of the histograms \( P(\Delta_x) \), as shown in the inset of Fig. 1. Nevertheless, the data for \( L Y_\parallel \) (see inset in Fig. 3) collapses nicely when using the same values of \( \nu \) and \( T_c \) as in the main figure. This therefore constitutes additional evidence for a vortex glass transition in the model. We now turn to the bias mentioned above and also discuss similarities and differences with the more common method to determine the root mean square current \( I_{\text{rms}} \), in analyses of models with disorder.

As mentioned above the determination of \( Y \) from a twist histogram suffers from a bias towards too large values. To investigate the reason for this bias we performed additional simulations with fluctuating twist boundary conditions of the pure zero-field 3D XY model and collected histograms \( P(\Delta; \tau) \) where \( \tau \) enumerates the bins. This data was then used to calculate averages over \( \tau_{\text{aver}} \) consecutive bins \( \bar{P}(\Delta; \tau_{\text{aver}}) \), which in turn were used to determine the helicity modulus. By repeating this procedure for several values of \( \tau_{\text{aver}} \) the dependence of \( Y \) on \( \tau_{\text{aver}} \) was determined. From this kind of analysis it was found that the bias decays as \( 1/\tau_{\text{aver}} \) to a very good precision. Another finding is that the bias may be made to vanish altogether by making use of \( \Delta^0 = 0 \) in Eq. (5) instead of using \( \Delta^0 \) as a free parameter. (\( \Delta^0 = 0 \) is the known value of the minimizing twist in the pure system.) The latter observation suggests that the bias is related to the usual complication in determining the width (variance) of a distribution when the true average is not known. Since \( Y \) is inversely related to the variance of the distribution \( P(\Delta) \) around the maximum it follows that the estimates based on runs of length \( \tau_{\text{aver}} \) would be expected to decay towards the true value as
\[ Y(\tau_{\text{aver}}) = \frac{1}{1 - b/\tau_{\text{aver}}} Y(\infty), \tag{7} \]
where $b$ is a free parameter related to the decorrelation time in the simulations. For small values of $b/\tau_{\text{av}}$, the expected behavior is therefore entirely in accordance with the $1/\tau_{\text{av}}$ decay discussed above.

Returning to our data for the vortex glass model, the procedure used to determine the data points in Fig. 2 consists of three steps: (i) Determine $\Upsilon_\mu(\tau_{\text{av}})$ for each disorder configuration and several values of $\tau_{\text{av}}$ by fitting histogram $P_\mu(\Delta, \tau)$ to Eq. $\alpha$. (ii) Calculate the disorder averaged quantities $\Upsilon_\perp(\tau_{\text{av}})$ and $\Upsilon_\parallel(\tau_{\text{av}})$, cf. Eqs. $\alpha$. (iii) Fit this data to Eq. $\alpha$ to obtain the unbiased estimates $\Upsilon_\perp(\tau_{\text{av}}) \equiv \Upsilon_\perp(\infty)$ and $\Upsilon_\parallel(\tau_{\text{av}}) \equiv \Upsilon_\parallel(\infty)$. The last step is illustrated in Fig. 4 for $T = 0.125$ close to $T_c$. The error bars on the last point for each size are the errors associated with the disorder average.

Note also that there is a bias in the determination of the root mean square current $I_{\text{rms}}$ that is very similar to the bias in $\Upsilon$ discussed above. For $I_{\text{rms}} = \sqrt{\langle I^2 \rangle}$, the origin of this bias is that the statistical error $\delta I$ gives a term $(\delta I)^2 \geq 0$. Since $\delta I$ would be expected to vanish with simulation time as $\sim 1/\sqrt{1/\tau_{\text{av}}}$, the bias in $I_{\text{rms}}$ would vanish as $1/\tau_{\text{av}}$, which is essentially the same as the behavior of $\Upsilon(\tau_{\text{av}})$. There is however a difference in that the bias in $I_{\text{rms}}$ is easily eliminated by performing two independent simulations, $\alpha$ and $\beta$, for each disorder and measuring the quantity $[I_\alpha I_\beta]_{\text{avg}}$. Since the bias in $\Upsilon$ is of a very different origin it cannot be eliminated with such methods.

To summarize, we have performed a finite size scaling analysis of the helicity modulus in a frustrated 3D XY model with disorder in the coupling constants. The data is consistent with isotropic scaling and the correlation length exponent is found to be $\nu = 1.50 \pm 0.12$. The good agreement with $\nu = 1.39 \pm 0.20$ of the 3D gauge glass suggests that the two models actually do belong to the same universality class.

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![FIG. 4: The figure shows the elimination of the bias in $\Upsilon_\perp$ by fitting $\Upsilon_\perp(\tau_{\text{av}})$ to Eq. $\alpha$ with $b$ and $\Upsilon_\perp(\infty)$ as free parameters. The time is in units of the bin size which is $2^{18} = 262144$ sweeps.](image)

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[14] To get an unbiased estimate of the variance of a distribution based on $N$ independent values $x_i$, one should make use of $\sigma^2 = 1/(N-1) \sum (x_i - \bar{x})^2$. The prefactor here differs from the naively expected $1/N$ since the value of the average $\bar{x}$ in general is different from the true average of the distribution. The connection with Eq. $\alpha$ follows since this may be written $\sigma_{\text{naive}}^2(N) = (1 - 1/N)\sigma^2$. 
