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Accelerated simulations of XY spin glasses

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We present numerical simulation results for the XY spin-glass model in two and three dimensions, using stochastic differential-equation methods with Fourier acceleration. We show that the dynamics of these methods are much faster than Metropolis and suffer much less from critical slowing down, without changing static quantities. We also show that renormalized physical quantities are not affected by systematic errors. We use this method to show that, in two dimensions, the Ising-type chiral variables of this model follow thermal activation dynamics.

The Ising spin glass has been studied extensively in two and three dimensions by means of numerical simulations.[1] As is well known, the relaxation time for these simulations increases very rapidly as the temperature is decreased, thus limiting the system size and the temperature range that can be studied. However, one can use the discreteness of the Ising variables to write very efficient codes, and thus keep the required computer time within reach. Furthermore, new algorithms have been proposed by Swendsen[1] to accelerate the relaxation of these systems. This is not so for models where the variables take continuous values. For this reason, the XY and Heisenberg spin glasses are still not very well studied even in two dimensions.

In this Rapid Communication we show how to reduce drastically the severity of critical slowing down in spin-glass models with continuous vairables, by simulating the system using dynamics that are much faster than Metropolis or heat bath. Thus, we were able to conduct (for $d=2$) the first study of the dynamics of the chiral degrees of freedom[2,3] (to be defined below), and demonstrate that they follow a thermal activation law. This lends strong support to the idea that these degrees of freedom behave like an Ising spin glass,[2] as a recent simulation by Kawamura and Tanemura[3] indicated.

To speed up the dynamics of the system, we used Fourier acceleration which was first studied in lattice field theories.[4-7] For such translationally invariant theories, perturbative calculations show clearly why Fourier acceleration works.[4,5] These calculations fail for frustrated models, and so until now it was not known whether our method is effective in the simulations of such models. We found that it works very well. We tested the following stochastic differential equation methods: Langevin,[4,5] hybrid,[6] accelerated Langevin,[4,5] accelerated hybrid,[7] and found the last method to be the fastest. Therefore, we will sketch here only the last method leaving the details to the references and to a future publication.[8] The Hamiltonian of the model is

$$H=-\beta\sum_{\langle ij\rangle}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{1}$$

where $\mathbf{S}_i=(\cos\theta_i,\sin\theta_i)$, and $0\le\theta_i\le 2\pi$. The sum is over nearest neighbors, i and j, on a square ($d=2$) or simple-cubic ($d=3$) lattice. β is the inverse temperature, and J_{ij} are the random bonds and have values ± 1 with equal probability. The molecular dynamics Lagrangian, corresponding to Eq. (1), is given by[6,7]

$$L=\tfrac{1}{2}\sum_{i,j}p(i)M(i,j)p(j)-H(\{\theta_i\})\ , \tag{2}$$

where the $p(i)$ are variables conjugate to the angles θ_i. M is an arbitrary but positive-definite matrix, which for simplicity is taken to be diagonal in momentum space, e.g.,

$$M(k)=1-\frac{x}{2}-\frac{x}{2d}\sum_{\mu=1}^{d}\cos k_\mu\ . \tag{3}$$

d is the dimensionality of the system, and $0\le x\le 1$ is an acceleration parameter. For $x=0$, L is local and standard molecular dynamics is recovered. As $x\to 1$, the low-momentum components of $M(k)$ become increasingly important making $M(i,j)$, and therefore L, increasingly nonlocal. The new nonlocal couplings generated by M accelerate the relaxation of the system but can still be shown to lead the *same* static limit as for the local case.[4-7] It has been shown that this choice of M eliminates critical slowing down in free theories[4,5] with uniform couplings, and reduces it near critical points.[7] In this paper we show that this choice also works very well for spin glasses.

The discretized equations of motion (accurate to order dt^2), corresponding to the above Langrangian, are

$$p\left(i,t+\frac{dt}{2}\right)=p\left(i,t-\frac{dt}{2}\right)+(dt)F^{-1}[M^{-1}(k)F(-\partial_{\theta_i}H)]\ , \tag{4a}$$

$$\theta(i,t+dt)=\theta(i,t)+(dt)p\left(i,t+\frac{dt}{2}\right)\ , \tag{4b}$$

where dt is the time step, and F is a fast-Fourier-transform (FFT) operator.[9] To ensure the ergodicity of molecular dynamics,[6] we "refresh" the momenta periodi-

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cally, i.e., we replace $p(i,t+dt/2)$ by

$$F^{-1}\left\{\sqrt{M^{-1}(k)}F\left[\eta\left[i,t+\frac{dt}{2}\right]\right]\right\}, \tag{5}$$

where η is a Gaussian random variable. This is equivalent to doing a Langevin step. Note that the dependence on J_{ij} is through the term $\partial_{\theta_i}H$ in Eq. (4a). This mixture of molecular dynamics and Langevin is what we refer to as the hybrid method. Clearly, Langevin dynamics is obtained in the limit of refreshing every step, while molecular dynamics is obtained by not refreshing at all. It can be shown[5,6] that for large t and arbitrary $M(i,j)$, the ensemble of configurations $\{\theta_i\}$ has the correct distribution e^{-H} (up to order dt^2). We ran the simulation with the time step $dt=0.1$ and the acceleration parameter $x=0.99$, and refreshing the momenta every 25 iterations. We found that these parameters are optimal in the sense that they give the shortest autocorrelation in the data, and systematic errors that are very small compared to the statistical ones.

Using this algorithm, we always start from a disordered configuration, and typically ignore the first 5×10^4 to 10^5 sweeps, depending on the temperature, and measure over the next 10^5, for both $d=2$ and $d=3$. This proved to be enough to get very good statistics because the relaxation time for our methods is very short. We have checked that starting from an ordered configuration, $\theta_i=0$, leads to the same results.

We now describe the various quantities that we measured. Information about the dynamics are contained in the autocorrelation function

$$q(t)=\frac{1}{N}\left\langle\left\langle\sum_i \mathbf{S}_i(t_0)\cdot\mathbf{S}_i(t+t_0)\right\rangle_T\right\rangle_J , \tag{6}$$

where N is the total number of sites on the lattice ($N=16^2$ for $d=2$, and $N=8^3$ for $d=3$), and t_0 is the initial time at which measurements are started. Thermal averages are denoted by $\langle\cdots\rangle_T$ and sample averages by $\langle\cdots\rangle_J$. We typically averaged over 10 to 25 samples which was enough to get good statistics because for each sample we ran at least of the order of hundreds times the autocorrelation time. The average autocorrelation time[1,10,11] τ_{SG} is given by

$$\tau_{SG}=\int_0^\infty q(t)dt . \tag{7}$$

We also measured the spin-glass susceptibility given by

$$\chi_{SG}=\frac{1}{N}\sum_{i,j}\langle\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle_T^2\rangle_J . \tag{8}$$

Aside from these usual spin-glass quantities, we measured the average relaxation time τ_{ch} for the chiral variables defined by[2,3]

$$\kappa_\alpha=\sum_{\langle ij\rangle}\mathrm{sgn}(J_{ij})\sin(\theta_i-\theta_j) , \tag{9}$$

where the summation is directed along the contour of plaquette α in the counterclockwise direction. Note that κ_α is invariant under global rotations but changes sign under any global reflection, $\theta_i\rightarrow 2\theta_0-\theta_i$, where θ_0 defines the axis of reflection. The average relaxation time for these chiral variables is obtained from

$$\tau_{ch}=\int_0^\infty q_{ch}(t)dt , \tag{10}$$

where

$$q_{ch}(t)=\frac{\left\langle\left\langle\left[\sum_\alpha\kappa_\alpha(0)\kappa_\alpha(t)\right]^2\right\rangle_T\right\rangle_J}{\left\langle\left\langle\left[\sum_\alpha\kappa_\alpha(0)\kappa_\alpha(0)\right]^2\right\rangle_T\right\rangle_J} . \tag{11}$$

This is analogous to Eq. (6) and is normalized so that $q_{ch}(0)=1$.

We now discuss our results. In Fig. 1(a) [Fig. 1(b)] the

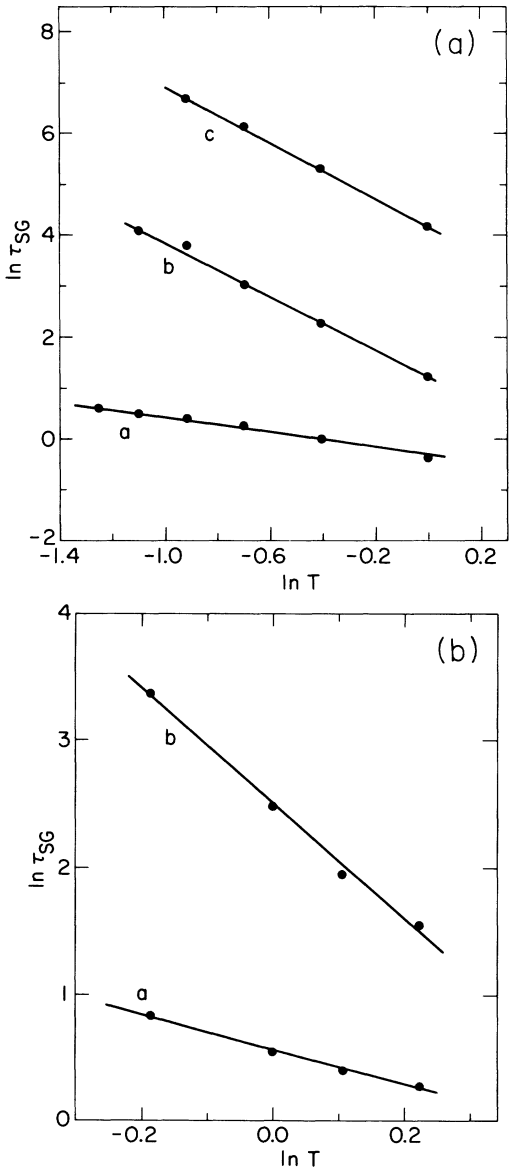

FIG. 1. Plots of $\ln\tau_{SG}$ vs T in (a) two dimensions and (b) three dimensions. Here τ_{SG} is the number of sweeps multiplied by $dt=0.1$. The labels on the curves are for accelerated hybrid (a), hybrid (b), and Langevin (c). The slopes are given in the text.

plots of $\ln\tau_{SG}$ vs $\ln T$ for $d=2$ ($d=3$) show that the dynamics suffer from ordinary critical slowing down, i.e.,[1,11] $\tau_{SG} \propto T^{-z_{av}\nu}$, where ν is the correlation length critical exponent and z_{av} is the average dynamic critical exponent. The same behavior was found by Jain and Young,[11] who found that $z_{av}\nu$ is 5.16 ± 0.18 for $d=2$, and 8.54 ± 0.57 for $d=3$, using Metropolis dynamics. Using different dynamics, we found that for $d=2$, $z_{av}\nu = 2.79 \pm 0.06$ (Langevin), 2.66 ± 0.10 (hybrid), and 0.82 ± 0.05 (accelerated hybrid) while for $d=3$, $z_{av}\nu = 4.58 \pm 0.25$ (hybrid), and 1.41 ± 0.08 (accelerated hybrid). So we see that our slowest dynamics (Langevin) suffers less critical slowing down than Metropolis, while the Fourier accelerated hybrid method is the fastest and suffers the least critical slowing down. This important result is the first numerical verification of the conjecture that Fourier acceleration *reduces* the dynamic critical exponent.[4,5,7] The values for $z_{av}\nu$, with acceleration, are 3 times smaller than without, and 6 times smaller than for Metropolis. For the Langevin method at $T=0.5$, we found $\tau_{SG} \approx 5000$ sweeps, while for the accelerated hybrid $\tau_{SG} \approx 13$, a relative acceleration factor of about 380 in sweeps and 230 in cpu time because of the overhead in performing FFT's.[9,12] This gain increases as T decreases.

It is important to note that hybrid dynamics relaxes faster than Langevin, but that both have the *same* dynamic critical exponent [Fig. 1(a)]. In other words, we have established that hybrid dynamics forms a large *universality* class which contains Langevin and microcanonical (when ergodic) as limiting cases of the rate at which we randomize the momenta. Fourier acceleration reduces the dynamic critical exponent and changes the universality class of the dynamics.

What about systematic errors? After all, our methods approximate a differential equation of motion with a difference equation which should introduce some systematic errors in the solutions. This problem has been addressed in detail both numerically and analytically.[5-7] Here we only mention that we expect the discreteness of the time step not to affect renormalized physical quantities, such as critical exponents. Our results give the first numerical confirmation of this. Figure 2(a) shows a plot of $\ln\chi_{SG}$ vs $\ln T$ for Langevin and for accelerated hybrid. The data from the accelerated hybrid method are in excellent agreement with the results of Ref. 11. The Langevin results are in slight disagreement because the systematic errors for this method are larger, and because χ_{SG} is not measured in renormalized physical units. However, the slopes of both lines are the same. This means that, to within our statistical accuracy, the susceptibility exponent has the same value in both methods independent of systematic errors.[13] We find $\gamma = 1.85 \pm 0.04$, which agrees with the results of Refs. 3 and 11. Figure 2(b) shows the same thing in three dimensions but only for the accelerated hybrid method.

Now we discuss our results for the dynamics of the chiral variables [Eq. (9)] on a two-dimensional lattice of size 16.[2] We measured the relaxation time and found that it follows a thermal activation law, $\tau_{ch} \propto e^{\Delta E\beta}$, $\beta = T^{-1}$, as was found for the Ising spin glass by Young[1] and McMillan.[1] Young[1] found that $\Delta E\beta \approx 9\beta^2$, while McMillan[1]

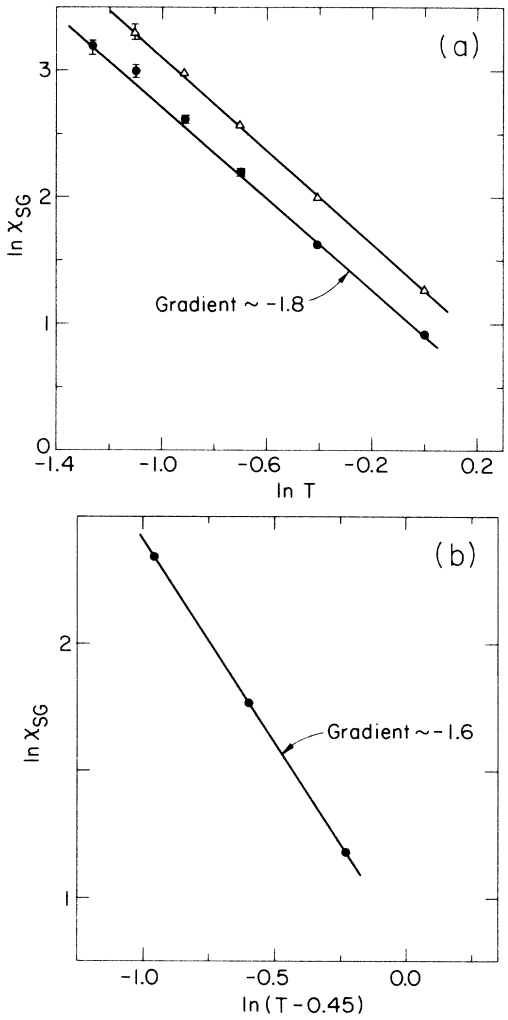

FIG. 2. (a) $\ln\chi_{SG}$ vs $\ln T$ in two dimensions. The slope for accelerated hybrid (●) is $\gamma = -1.85 \pm 0.04$ and Langevin (△) is $\gamma = -1.87 \pm 0.02$. (b) $\ln\chi_{SG}$ vs $\ln(T-0.45)$ for accelerated hybrid in three dimensions. The slope is $\gamma = -1.58 \pm 0.01$. These results agree with Refs. 3 and 11.

found $\Delta E\beta = 14.16\beta - 6.59 + 0.785\beta^{-1}$. However, the results of one do not rule out the other. The same holds in our case, where we can fit the data for τ_{ch} using $\Delta E\beta = 0.5\beta^2$, or $\Delta E\beta = 3.8\beta - 8.84 + 7.96\beta^{-1}$, the former giving a slightly better fit, which we show in Fig. 3. Recall that Ref. 3 measured the chiral susceptibility and found that, for low enough temperature, it can be mapped onto that of the Ising spin glass by rescaling the temperature, $\beta = 4\beta_I$, where β_I is the Ising inverse temperature. With this rescaling our fits become $\Delta E\beta = 8\beta_I^2$ and $\Delta E\beta = 15.2\beta_I - 8.84 + 1.99\beta_I^{-1}$. We see that at low enough temperatures, i.e., ignoring the β_I^{-1} term, our coefficients of β_I and β_I^2 agree very well with the Ising coefficients of Young and McMillan. We have therefore shown that both qualitatively and quantitatively, the dynamics of the chiral variables is that of Ising rather than XY spin-glass variables. These results for the dynamics, combined with previous results for the statics,[3] strongly

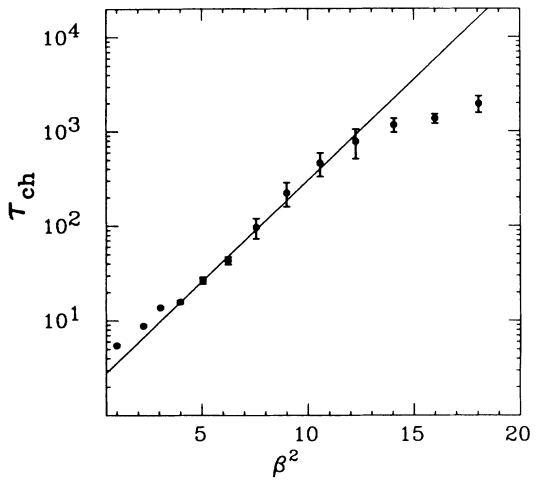

FIG. 3. A plot of $\ln\tau_{ch}$ (for $d=2$) vs β^2, the squared inverse temperature. The line is from a χ^2 fit and has a slope of 0.5. Here τ_{ch} is the number of sweeps, and the plateau after $\beta=3.5$ is due to finite-size effects.

confirm the idea that for $d=2$ the chiral variables behave just like an Ising glass.[3] If the Ising-like behavior of these chiral variables persists in three dimensions, it would raise the interesting question of how the finite-temperature phase transition of the Ising spin glass would manifest itself in this XY spin glass where the phase transition is believed to be at zero temperature. The possibility of chiral ordering in three dimensions was recently conjectured by Kawamura and Tanemura.[3]

Note that the very long relaxation time of chiral variables is not due to critical slowing down but to thermal activation. In this case, Fourier acceleration did speed up this relaxation but by decreasing the coefficient multipling $e^{\Delta E\beta}$, and *not* by changing the heights of the potential barriers. For this reason we are allowed to compare our results for $\Delta E\beta$ with those of Young and McMillan.

We examined finite-size effects by measuring χ_{SG} ($d=2,3$) and χ_{ch} ($d=2$) for $L=4$, 8, 16. Our results for χ_{SG} agree with those of Ref. 11. For example for $d=2$ and $L=16$, we found that the finite-size effects become important for $\beta>3.5$. Measurements of χ_{ch} indicate the onset of these effects at $\beta\geq 3.5$, which agrees with the data of Ref. 3. Finally, by studying τ_{ch} vs T (Fig. 3), we see a plateau due to finite-size effects for $\beta>3.5$. So we have three independent estimates for β where finite-size effects become important. All estimates give $\beta\geq 3.5$ for $d=2$ and $L=16$. This agrees with previous results.[3,11]

To summarize, we have found that Fourier acceleration greatly reduces the dynamic critical exponent, thus greatly reducing the relaxation times for both the XY spin-glass variables and the chiral variables. We were, therefore, able to conduct the first study (in $d=2$) of the dynamics of these chiral variables and to show that they follow thermal activation over potential barriers. We also showed that to within our error bars, the systematic errors due to the discretization of the field equations of motion do not change renormalized physical quantities such as critical exponents. Further work is in progress to perform a detailed study in three dimensions.

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