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Dynamical phase transitions in the classical Heisenberg model

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Abstract. Damage spreading in the 2D and 3D Heisenberg model is considered. For the 3D model, there is a critical temperature $T_1 = 1.15$ between a frozen phase and a chaotic phase at low temperature. There is another critical temperature $T_2 \sim 0.3$ below which the final damage depends on its initial value. For the 2D case, there is a transition at $T_0 \sim 0.5$ between a frozen phase and a low-temperature chaotic phase which might be characterized by the existence of infinite critical points.

Damage spreading is one of the most puzzling aspects of the dynamics of statistical models: one considers the time evolution of two configurations submitted to the same thermal noise and, typically, one finds a chaotic phase where the damage spreads all over the system and a frozen phase where it disappears. The 2D Ising model was the first model studied with this technique [1]; since this seminal work, many other models have been analysed. For instance, the 3D spin glass was studied using heat-bath [2] and Glauber dynamics [3]. It is not surprising that the results depend strongly on the dynamics used. This point has been carefully analysed in [4]. Also, more complex models have been considered: the ANNNI model [5], several 2D problems [6], the Ising model with increasing range of interactions [7], the XY model [8, 9], etc.

In this paper, the spreading of damage in the 3D and 2D Heisenberg model is analysed. For the 3D case, there is a sharp transition at $T_1 = 1.15$. Above T_1 the damage does not spread, i.e. the system is in a frozen phase. Below T_1 the system is in a chaotic one: the damage spreads but its final value does not depend on the initial one if $T_2 < T < T_1$ where $T_2 = 0.3$; for temperatures lower than T_2, the final damage depends on the initial one. In the 2D case results are more interesting. Again, there is a transition at $T_0 \simeq 0.5$ between a frozen phase and a low-temperature chaotic phase which might be characterized by the existence of infinite critical points.

The classical Heisenberg model on a cubic $L \times L \times L$ lattice is considered. The boundary conditions are periodic in all directions. There is a spin $\boldsymbol{s}_i$ on each lattice site with components $(\cos(\phi)\sin(\theta), \sin(\phi)\sin(\theta), \cos(\theta))$, where ϕ and θ are the usual spherical coordinate angles. The energy of a given configuration C is

$$H(C) = -\sum_{\langle i,j\rangle} \boldsymbol{s}_i^{(C)} \cdot \boldsymbol{s}_j^{(C)}$$

where the sum is over all pairs of nearest neighbours on the lattice. The dynamics is the following one. For each site i, a random direction in space is chosen, i.e. $\cos\theta'$

and $\cos\phi'$ are random variables between -1 and 1. The spin $\boldsymbol{s}_i$ is put in the new direction and the energy of the new configuration C' is evaluated. Then the usual Metropolis schedule is followed: if $H(C') \leq H(C)$, then the change is accepted; if $H(C') > H(C)$, it is accepted with a probability given by $\exp[(H(C) - H(C'))/T]$. In practice, a random number z is generated and the new configuration is accepted if $z \leq \exp[(H(C) - H(C'))/T]$.

The distance between two configurations is defined in the following way. Let $\{\boldsymbol{s}_i^{(A)}\}$ and $\{\boldsymbol{s}_i^{(B)}\}$ be the two considered configurations, and let $s_{ij}^{(A)}$ be the jth component of spin i of configuration A; then, we have

$$
\begin{aligned}
d_{AB}(t) &= \frac{1}{N}\sum_{i=0}^{N}(1 - \boldsymbol{s}_i^{(A)} \cdot \boldsymbol{s}_i^{(B)}) \\
&= \frac{1}{N}\sum_{i=0}^{N}(1 - \sum_{j=1}^{3} s_{ij}^{(A)} s_{ij}^{(B)}).
\end{aligned}
$$

The spins $\boldsymbol{s}$ are normalized to one, so $\boldsymbol{s}_i^{(A)} \cdot \boldsymbol{s}_i^{(B)}$ is just the cosine of the angle between both spins. It is clear that $0 \leq d \leq 1$. In order to study the dynamics of the model, the time evolution of the distance between two configurations which evolve with the same thermal noise, i.e. the same sequence of random numbers, is measured. $d(t)$ depends on the lattice size L, the temperature T, the initial conditions and the noise; so the meaningful quantity to be considered is the average of $\langle d(t) \rangle$ over many samples. In the thermodynamics limit, one expects that $\langle d(t) \rangle$ goes to zero at large times in a frozen phase and it goes to a finite value in a chaotic phase.

Numerical simulations of the 3D model have been performed for different systems sizes: $N = 8^3, 12^3$ and 20^3. The observation time was 500 MC steps, starting with a randomly chosen configuration. Typically 50–500 samples were considered depending on the size of the system. In each case, once the initial configuration is chosen, a copy of it is made and the damage is introduced. Three different cases were considered: (a) a random chosen spin was flipped, (b) $N/2$ spins were flipped and (c) all the spins were flipped. So, the initial distances were: $1/N, 0.5$ and 1.0.

In figure 1 the average final distance is shown in terms of temperature for the 3D classical Heisenberg model. From figure 1 it is clear that there is a change in the behaviour of the system at $T_1 \simeq 1.2$. Above this temperature the final distance between the two configurations is zero. Between T_1 and $T_2 \simeq 0.3$ the final distance in non-zero but does not depend on the initial value; below T_2, it depends on the initial distance.

The value of T_1 could be determined more precisely using a finite-size scaling method [8, 10, 11]. The first two moments of the distance probability distribution were measured:

$$
\begin{aligned}
\tau_1(L, T, s) &= \sum_t t d(t) \left(\sum_t d(t)\right)^{-1} \\
\tau_2(L, T, s) &= \sum_t t^2 d(t) \left(\sum_t d(t)\right)^{-1}
\end{aligned}
$$

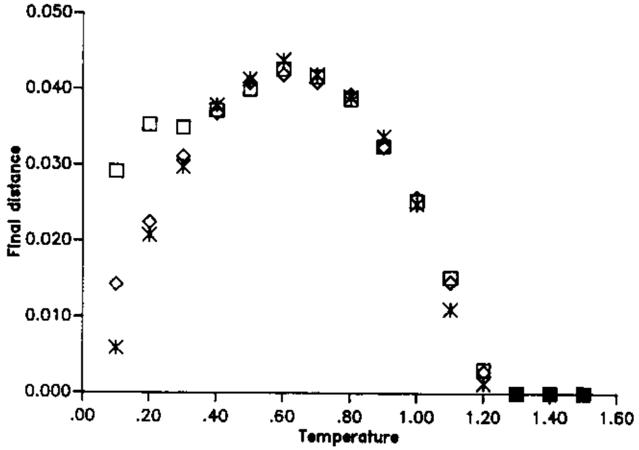

Figure 1. Final distance as a function of temperature for the 3D model on a cubic 20^3 lattice. Different symbols correspond to different initial distances: squares (□) for $d(0) = 1$; diamonds (◇) for $d(0) = 0.5$ and stars ($\star$) for $d(0) = 1/N$. The error bars are smaller than the symbol sizes. There is a sharp transition at $T_1 \simeq 1.2$ between a frozen phase and a chaotic one. Below $T_2 \sim 0.3$ the final distance depends on the inital one.

where τ_1 is a measure of a characteristic time and τ_2 is a measure of a square characteristic time. They both depend on the size, the temperature and the sample s. At the critical temperature T_1, one expects the following scaling for τ_1:

$$\tau_1(L, T, s) \sim u(L) f_1(v(L)(T - T_1), s)$$

where $u(L)$ gives the size dependence at $T = T_1$. For τ_2, the expected scaling is

$$\tau_2(L, T, s) \sim u^2(L) f_2(v(L)(T - T_1), s).$$

Since τ_2 is a measure of the squared characteristic time one expects that the ratio $R = \tau_1^2/\tau_2$ does not depend on L at $T = T_1$:

$$R(L, T, s) \sim f_3(v(L)(T - T_1), s).$$

Performing the average over samples:

$$\langle R(L, T, s)\rangle \sim g(v(L)(T - T_1)).$$

So, all the curves $\langle R\rangle$ plotted as a function of T should cross at the same temperature T_1.

In figure 2 curves $\langle R\rangle$ for different sizes are shown as a function of T. All of them cross at the same point, which gives the critical temperature $T_1 = 1.15 \pm 0.05$.

The second critical temperature is less well defined but from figure 1, one can conclude it is approximately $T_2 \simeq 0.3$.

For the Heisenberg model in 2D the technical details are the same as above but now the spins are on a square $L \times L$ lattice. In figure 3, the average final distance for a 100^2 lattice can be seen as a function of T. There is a change in the behaviour of the system at $T_0 \sim 0.5$. Above T_0 the system is clearly in a frozen phase. Below

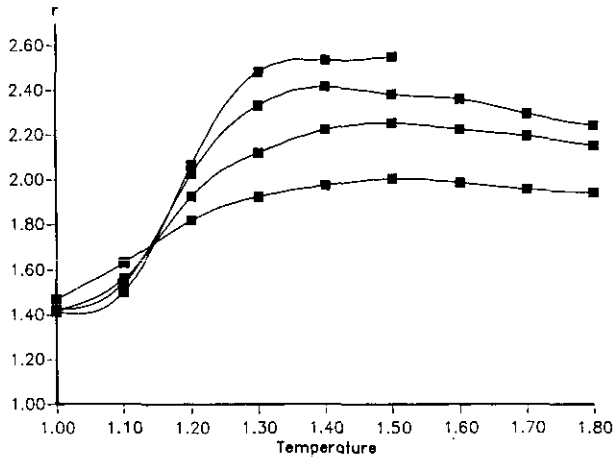

Figure 2. $\langle R\rangle$ curves for differents system sizes in the 3D case. From top to bottom: $N = 20^3, 16^3, 12^3$ and 8^3. All the curves cross at the same point, which gives accurately the critical temperature $T_1 = 1.15$.

T_0 the system seems to be in a chaotic phase where the final distance depends on the initial one. However, it should be noted that for very low temperatures there could be another frozen phase. At least for $d(0) = 1/N$, this is very clear. If finite-size scaling is used to determine precisely T_0, again there are unexpected results. In figure 4 the curves $\langle R\rangle$ are shown as a function of temperature for different sizes. The curves, instead of crossing at T_0, fall on top of each other below $T_0 = 0.5$. As far as we know this is the first time such a result has been found in a dynamical phase transition, but it is well known in the study of equilibrium ones. In fact, this kind of behaviour takes place for the XY model [12] and in the six-state clock model [13]. It is a sign of a Kosterlitz–Thouless (KT) phase, which is characterized by the existence of infinite critical points. So, our results suggest that there may be infinite critical points in the low-temperature regime of the 2D Heisenberg model.

It should be pointed out that our results are about dynamical properties of the model. In fact, the critical temperature found in the 3D model does not correspond to the usual equilibrium one, since the last numerical estimation of the equilibrium critical temperature gives $T_c = 1.45 \pm 0.05$ [14] which agrees with analytical calculations [15,16]. The dynamical phase transition we found takes place well below that value. The same considerations are valid for the 2D model. It is well known it has no equilibrium transition at finite temperature [17,18] but there is a clear change in the dynamical behaviour of the model at $T_0 \sim 0.5$ with an interesting low-temperature phase. Perhaps the same could be applied to the XY model where the dynamical phase transition and the equilibrium one seem to take place roughly at the same temperature [8,9]; however they might not necessarily be related to each other. It should be noted that there is no peculiarity in the behaviour of $\langle R\rangle$ below the transition temperature [8]. It should also be noted that there are rigorous resuls which bind equilibrium properties like the correlation function with dynamical one if heat-bath dynamics is used [19] but these results do not hold with Metropolis dynamics.

In conclusion, the study of damage spreading in statistical systems seems to be a powerful tool to study a new whole kind of phenomena. Indeed, it is one way to analyse properties of the models which are different from equilibrium ones. It

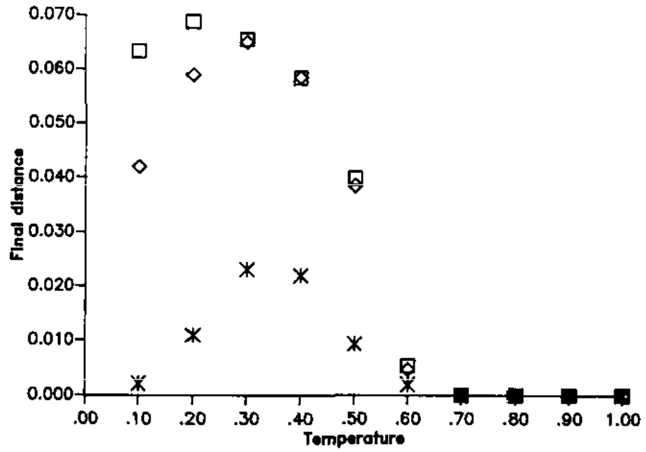

Figure 3. Final distance as a function of temperature for the 2D case. The system size is 100^2. The different symbols mean different initial distances: squares (□) for $d(0) = 1$, diamonds (◇) for $d(0) = 0.5$ and stars ($\star$) for $d(0) = 1/N$. There is a phase transtion at $T_0 \sim 0.6$ between a frozen phase and a chaotic one. The error bars are smaller than the symbol sizes.

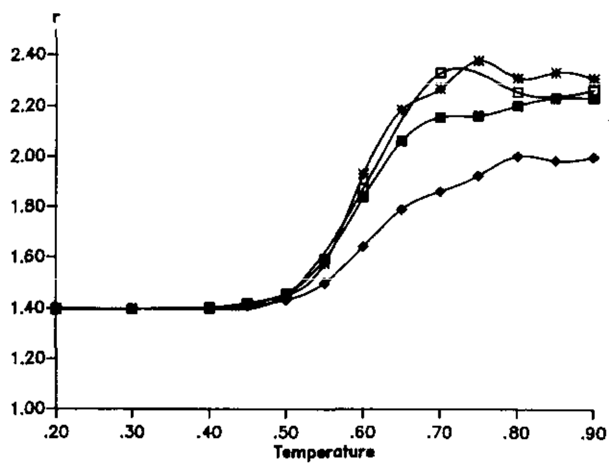

Figure 4. (R) curves for the 2D case and different system sizes: stars ($\star$) for $N = 100^2$, empty squares (□) for 60^2, full squares (■) for $N = 40^2$ and diamonds (◆) for $N = 20^2$. All the curves fall on top of each other below $T_0 \simeq 0.5$. This kind of behaviour is expected for a phase with infinite critical points.

would be interesting to repeat our numerical experiments using heat-bath dynamics. In principle, the results may be completely different. One can guess they would be related to the equilibrium properties of the Heisenberg model; of course, it would be nice to generalize the exact results of [19] to continuous variables and heat-bath dynamics. Finally, many problems remain open: the XY model in 3D, the Heisenberg spin glass, etc. They could be the subject of future work.

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