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LETTER TO THE EDITOR

Simulation of domain wall dynamics in the 2D anisotropic Ising model

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Abstract. In this letter we first show that the movement of a domain wall in a highly anisotropic Ising model of spins in two dimensions can be mapped to a random walk movement of labelled walkers in one dimension. This movement is correlated in the sense that the transition probability of a given walker, labelled i, depends upon the current positions of its labelled neighbours ($i-1$ and $i+1$). A Monte Carlo simulation of the walk for various numbers of walkers (up to a maximum of 50) and for quite long times (up to a maximum of 25×10^4 Monte Carlo steps) yields useful and interesting information about the dynamics. We verify that (i) the centre of mass of the walkers executes an unbiased random walk for all times starting from the lowest times; and (ii) the moment of inertia of the walkers asymptotically reaches a constant value which scales with the number of walkers.

The results on the relaxation of a straight vertical wall indicate the existence of a characteristic time t^* such that the behaviour of an individual walker for times $t<t^*$ is a random walk whose variance in position follows a t^{α_-} ($\alpha_-\simeq0.5$) law, whereas the value of the exponent for $t>t^*$ is approximately such as to indicate an independent unbiased random walk. It was found that the time t^* scales with system size with an exponent $\phi\simeq2$. We also discuss the relation of this work to the dynamics in the 2D Ising model, identifying ϕ with the dynamical exponent z. The random walk equivalence also provides a geometrical interpretation of the known results for the solid-on-solid (SOS) model.

Consider Ising spins located on a square lattice as shown in figure 1. In the figure a spin configuration in the presence of a wall separating regions of opposite spins is

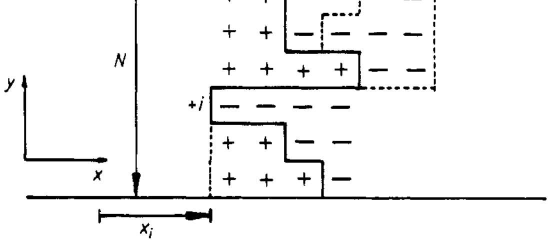


Figure 1. A configuration of the interface. The broken line is an example of an overhanging configuration. These configurations are excluded since $J_x \gg k_BT$.

shown. We want to simulate the dynamics of the system starting from a straight vertical wall with a spin-flip dynamics satisfying detailed balance. The anisotropy, $J_x \gg k_B T \gg J_y$ has two major implications: (i) excitations of spins inside the domains can be neglected and only spins at the interface have significant transition rates; (ii) we can ignore 'overhanging' configurations.

The flip of interface spins of the ith row leads to a movement of the coordinate X_i of the interface by one unit to the left or one unit to the right. The coordinate X_i thus makes a correlated random walk whose transition probabilities can be obtained from the spin-flip transition rate

$$W = \frac{1}{\tau} \frac{\exp(-\Delta E/k_B T)}{1+\exp(-\Delta E/k_B T)}$$

where ΔE is the change in system energy when the spin flips and τ is the characteristic time of a spin flip (table 1). For configurations 2, 4, 7 and 9 we must consider a pausing probability proportional to $\tanh(2\beta J_y)$.

We studied the time dependence of the variance of the centre of mass $V_{CM}(t)$ and the moment of inertia of the interface $I_N(t)$, as well as the variance V_1 of the position X_i of a generic walker i. These quantities are defined in table 2. All walkers are equivalent because we use periodic boundary conditions in the y direction.

The centre of mass is related to the magnetisation of the system through $M = 2NX_{CM}$. The moment of inertia is a measure of the width of the interface and is related to the variances V_1 and V_{CM} in the following way:

$$I_N(t) = V_1(t) - V_{CM}(t). \tag{1}$$

The mean magnetisation is of course zero, as can be seen by looking at the transition probabilities given in table 1; the sum total of probabilities for all the configurations to move to the left is the same as that for movement to the right.

It is expected that the equilibrium thermodynamic susceptibility for a finite system of size N and periodic boundary conditions in the y direction is infinite because of the degeneracy of a translation of the interface in the x direction. The susceptibility is proportional to the variance of the centre of mass of the domain wall.

The equilibrium value of the moment of inertia is finite and can be expressed in terms of $\overline{\Delta^2} = \langle (X_i - X_{i-1})^2 \rangle$. For a subsystem of size L, $2 < L \ll N$, the moment of inertia, I_L (table 2), is given by [1]

$$I_L(\infty) = \overline{\Delta^2}\left(\frac{L}{6} - \frac{1}{6L}\right). \tag{2}$$

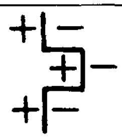
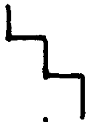
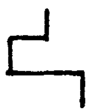
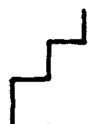
where [2]

$$\overline{\Delta^2} = \frac{1}{2\sinh^2(\beta J_y)} \qquad \Delta = X_i - X_{i-1}.$$

It is expected that the above relation is also valid for the entire system, $L = N$, with $\overline{\Delta^2}$ corrected for the effect of the periodic boundary conditions used in the y direction.

We have studied systems of size $N = 10$, 20, 30, 40 and 50 at a temperature $x = J_y/K_B T = 0.1$, for up to 25 000 MCS/N (Monte Carlo steps per walker). The number of samples for the averages at each MCS/N was taken as 500. The results were not significantly affected if we chose random or sequential updating of the X_i coordinate. The latter option was adopted because of CPU time-saving considerations.

Table 1. One-step transition probabilities for nine different configurations of neighbours of walker i. $p_{\rightarrow}^{k}$ is the probability of increase of X_i by one unit; $p_{\leftarrow}^{k}$ is the probability of decrease of X_i by one unit; p_0^k is the pausing probability. Their sum must be one. $\beta = 1/k_B T$.

k	Configuration	$p_{\rightarrow}^{k}$	$p_{\leftarrow}^{k}$	p_0^k
1		$\frac{\exp(-2\beta J_y)}{2\cosh(2\beta J_y)}$	$\frac{\exp(2\beta J_y)}{2\cosh(2\beta J_y)}$	0
2		$\frac{\exp(-2\beta J_y)}{2\cosh(2\beta J_y)}$	$\frac{\exp(-2\beta J_y)}{2\cosh(2\beta J_y)}$	$\tanh(2\beta J_y)$
3		$\frac{1}{2}$	$\frac{1}{2}$	0
4		$\frac{1}{2}$	$\frac{\exp(-2\beta J_y)}{2\cosh(2\beta J_y)}$	$\frac{1}{2}\tanh(2\beta J_y)$
5		$p_{\leftarrow}^{1}$	$p_{\rightarrow}^{1}$	0
6		$\frac{1}{2}$	$\frac{1}{2}$	0
7		$p_{\leftarrow}^{4}$	$p_{\rightarrow}^{4}$	p_0^4
8		$p_{\rightarrow}^{4}$	$p_{\leftarrow}^{4}$	p_0^4
9		$p_{\leftarrow}^{4}$	$p_{\rightarrow}^{4}$	p_0^4

The variances of the centre of mass for all sample sizes studied are shown on a logarithmic scale in figure 2 showing that they are parallel straight lines, whose slope is the exponent α in the power-law time dependence, and whose intercept at the origin is the logarithm of the diffusion coefficient D_∞.

These parameters are shown in table 3 for various sample sizes. The exponent obtained is independent of the sample size and is approximately 1. The size dependence of D_∞ was found to be of the form $\ln D_\infty = (0.04 \pm 0.1) - (0.99 \pm 0.02) \ln N$.

Table 2. Definitions of centre of mass, moment of inertia of a subsystem of size L $(2 < L \leq N)$, variance of single walker position and variance of the centre of mass.

Quantity	Definition
$\langle X_{CM}(t)\rangle$	$\left\langle \frac{1}{N}\sum_{i=1}^{N} X_i \right\rangle$
$I_L(t)$	$\left\langle \frac{1}{L}\sum_{i=1}^{L}\left(X_i - \frac{1}{L}\sum_{i=1}^{L} X_i\right)^2\right\rangle$
$V_1(t)$	$\langle X_i^2\rangle - \langle X_i\rangle^2$
$V_{CM}(t)$	$\langle X_{CM}^2\rangle - \langle X_{CM}\rangle^2$

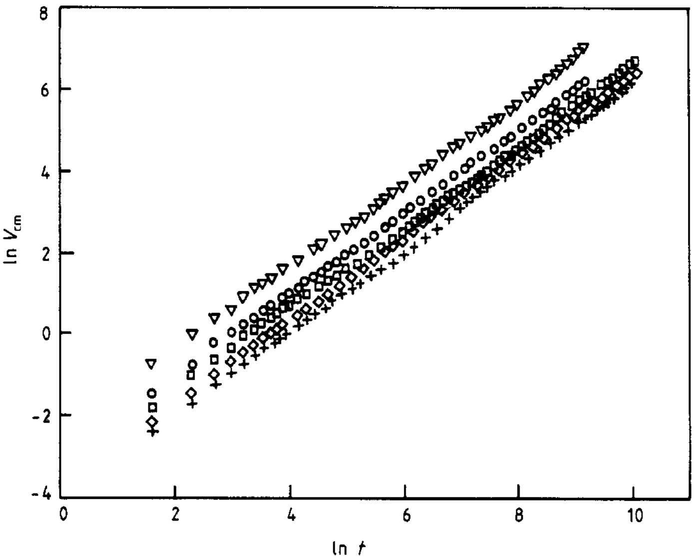


Figure 2. Plot in logarithmic scale of $V_{CM}(t)$ for all sample sizes studied. The estimated error of each point is ~0.07; t is in units of MCS/N in this and subsequent figures. Plots are for $N = 10$ (∇), 20 ($\bigcirc$), 30 ($\square$), 40 ($\diamond$) and 50 (+).

Table 3. Values of diffusion coefficient D_∞ and time exponent α for V_{CM} and the moment of inertia $I_N(\infty)$ for various sample sizes. Errors estimated from least-squares linear regression in α and in ln D_∞ are 0.05 and 0.03 respectively. $\Delta I_N(\infty)$ is the error in $I_N(\infty)$.

N	α	$\ln D_\infty$	$I_N(\infty)$	$\Delta I_N(\infty)$
10	1.003	−2.36	36.0	1.6
20	0.993	−2.97	77.1	4.8
30	0.986	−3.31	118.6	14.4
40	1.007	−3.67	158.0	19.4
50	1.011	−3.99	198.6	25.5

The quantities $V_{CM}(t)$ and $V_1(t)$ were plotted on a log-log scale and a typical behaviour ($N = 10$) is shown in figure 3. The variance of a single walker position, V_1, shows two distinct behaviours. For times greater than a characteristic time t^*, i.e. $t > t^*$, the curve $\ln V_1$ is coincident with that of $\ln V_{CM}$ and for $t < t^*$ we have the behaviour $V_1 \sim t^{\alpha_-}$, α_- being an exponent slightly larger than 0.5. The values of $\ln t^*$, the exponent α_- and the intercept at the origin were registered for various sample sizes (table 4). The behaviour of $I_N(t)$ for $N = 10$ is shown in figure 4 and we can see the asymptotic approach to a constant value $I_N(\infty)$; values of $I_N(\infty)$ for other values of N are shown in table 3.

In order to obtain the temperature dependence of $\overline{\Delta^2}(T)$, we also recorded the moment of inertia $I_2(t)$ of a two-walker subsystem of a system of size $N = 40$; it has an expected limiting behaviour of the form $I_2(\infty) = \frac{1}{4}\overline{\Delta^2}(T)$. In table 5 we show the values of $\overline{\Delta^2}(x)$, with $x = J_y/k_B T$, obtained from (2) together with those from simulation.

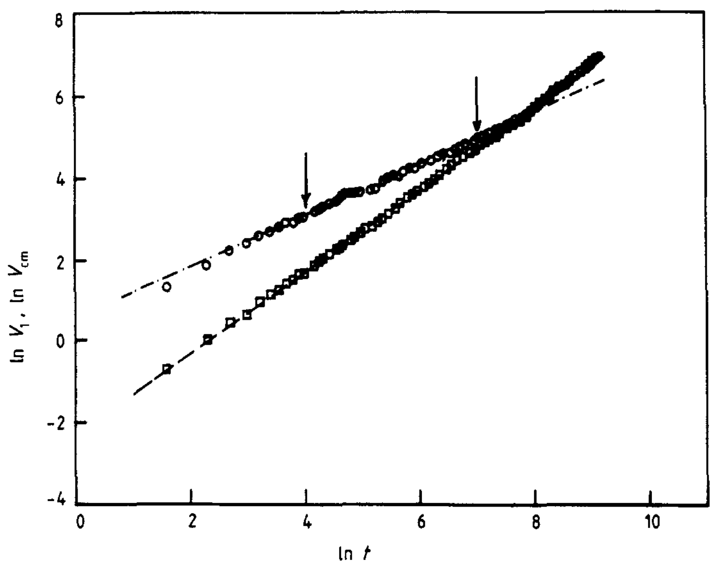


Figure 3. $\ln V_1(t)$ (○) and $\ln V_{CM}(t)$ (□) plotted against $\ln t$ for $N = 10$. The estimated error of each point is ~0.07.

Table 4. Values of exponent α_- and crossover time t^* obtained from the graphs $\ln V_1$ against $\ln t$ for $t < t^*$. For the least-squares fit that gives α_- and $\ln f(\simeq 1)$ we use points such that $4 < \ln t < 7$. The estimated error in α_- is 0.02 and the error in $\ln f(\simeq 1)$ is 0.1. The error in $\ln t^*$ is indicated in the table as $\Delta_{\ln t^*}$.

N	α_-	$\ln f(\simeq 1)$	$\ln t^*$	$\Delta_{\ln t^*}$
10	0.63	0.5	7.7	0.4
20	0.58	0.8	9.1	0.3
30	0.50	1.3	9.4	0.3
40	0.57	0.9	10.4	0.3
50	0.56	0.9	10.9	0.3

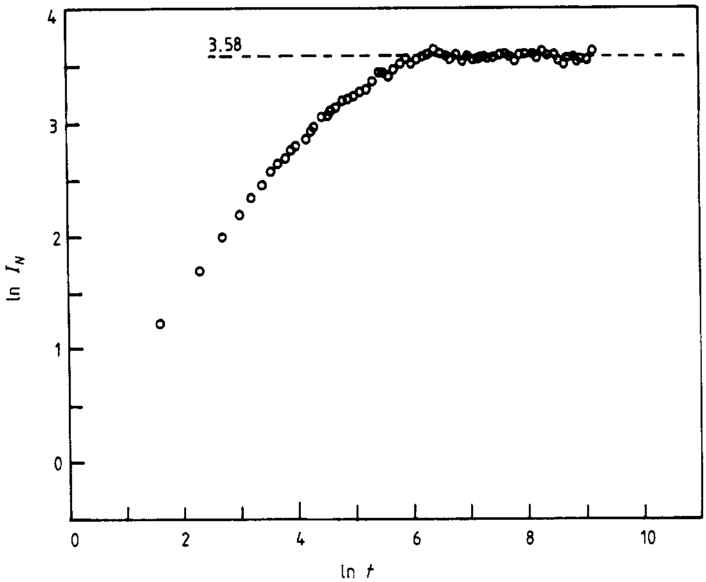


Figure 4. Moment of inertia, $I_N(t)$, as a function of time on a log-log scale ($N=10$). The broken curve represents the least-squares fit.

Table 5. Comparison of theoretical values $\overline{\Delta^2_{\rm th}}(x)$ given by equation (2) with simulation results $\overline{\Delta^2_{\rm sim}}(x)$; $\overline{\Delta^2}(x)=4\times I_2(\infty)$.

x	$\overline{\Delta^2_{\rm th}}(x)$	$\overline{\Delta^2_{\rm sim}}(x)$	error
0.1	49.83	47.06	5.73
0.2	12.34	11.66	0.34
0.3	5.39	5.07	0.63
0.4	2.96	2.78	0.02
0.5	1.84	1.72	0.02

Let us now discuss these results. First we shall look at the variance of the centre of mass. $V_{\rm CM}$ has an approximate behaviour $V_{\rm CM}=t/N$ (t measured in MCS/N) which indicates a simple random walk motion for the CM. This can be justified schematically in the following way. In one MCS the CM moves the step $a=1/N$. Thus if it were moving as a simple RW, diffusion coefficient D would be

$$\frac{(\text{step size})^2}{(\text{step time})}=\frac{1}{N^2\tau_{\rm MCS}}.$$

Since $V_{\rm CM}=Dt$, we obtain

$$V_{\rm CM}=\frac{1}{N}\frac{t}{N\tau_{\rm MCS}}.$$

Thus when time is measured in the units of Monte Carlo steps per walker we obtain the observed behaviour of $V_{\rm CM}=t/N$ and $D_\infty=1/N$. The fact that $V_{\rm CM}$ does not attain a limiting value indicates that we have infinite susceptibility.

Now let us examine V_1 and a scaling relation. One can describe the behaviour $V_1(t) \sim t^{\alpha_-}$ for $t < t^*$ and $V_1(t) \sim t/N$ for $t > t^*$, by a single scaling function

$$V_1(t) = t^{\alpha_-} f\left(\frac{t^{1/\phi}}{N}\right). \tag{3}$$

if it is assumed that $f(x)$ goes as $x^{\phi(1-\alpha_-)}$ for $x \gg 1$ and is essentially constant for $x \ll 1$. This gives for t^* the behaviour $t^* \sim N^\phi$ and indicates that in the large-N limit ϕ and α_- must obey

$$\phi\alpha_- = \phi - 1. \tag{4}$$

Relation (4) is needed in order to obtain the $(1/N)$ dependence of the diffusion coefficient for large times.

The scaling relation has been tested, giving the value of ϕ in the following way. We calculate α_- from a least-squares linear fit of the plot of $\ln V_1$ against $\ln t$ using points in the interval $4 < \ln t < 7$. Then we determine the intersection of this straight line with the straight line fitted to the plot of $\ln V_{CM}$ against $\ln t$ and then find $\ln t^*$. By plotting $\ln t^*$, thus obtained, against $\ln N$ we obtain the value $\phi = 1.9 \pm 0.3$. The large estimated error is due to large uncertainty in the estimation of t^*. We see that relation (4) is approximately satisfied. It is to be remarked that the anomalous diffusive behaviour of a single walker, for short times, is expected because of correlation between different walkers. However, since the walk is of finite memory we expect [3] a Gaussian behaviour in the asymptotic region of the variable X_i.

Now let us discuss the results relating to the moment of inertia and $\overline{\Delta^2}$. From (1), t^* can be interpreted as the equilibration time; after this time an individual walker and the centre of mass execute a random walk whose variance is linear in t (the variances are two parallel straight lines). This explains why the moment of inertia approaches a constant value. These observations lead to the following N dependence of the asymptotic value of the moment of inertia (interpreted as wall thickness):

$$\begin{aligned} I_N(\infty) &= V_1(t^*) - V_{CM}(t^*) \\ &= N^{\phi\alpha_-} f(\simeq 1) - N^{\phi-1} \\ &\sim N^{\phi-1}. \end{aligned}$$

From the plot of $\ln I_N(\infty)$ against $\ln N$ we once more obtain the value of the exponent $\phi = 2.08 \pm 0.07$, in good agreement with the value determined before and with (2), thereby supporting the self-consistency of our interpretation.

The temperature dependence of $\overline{\Delta^2}(J_y/k_B T)$ as given by relation (2) is confirmed, as we show by data in table 5. Thus we are confident that our algorithm correctly reproduces the equilibrium thermodynamic behaviour.

Some related models are worthy of consideration here. The model of correlated random walkers (in 1D) may be useful for a geometrical understanding of critical dynamics in the 2D Ising model with non-conserved order parameter [4]. According to the restricted dynamical scaling hypothesis [5] the characteristic relaxation time of the magnetisation scales (in the appropriate critical regime) with the thermal correlation length as

$$\tau \sim \xi^z.$$

This relation defines the critical dynamical exponent z. It is known [6] that $z = 2$ in the 1D spin model and recently [7] this value was interpreted as due to pure random motion of a domain wall. However, for the 2D spin model, an exact solution is not available and the values thus far obtained (see e.g. [8]) were derived either through approximate analytical methods or Monte Carlo simulation. A single geometrical interpretation is therefore useful in order to gauge the relevance of such results. In the following we show how our work does determine z.

According to universality, the dynamical exponent should be independent of the ratio between the nearest-neighbour exchange couplings. We are thus free to consider the extremely anisotropic limit, $J_x \gg k_B T \gg J_y$; therefore, the transition temperature is very high and the domain wall extending along the y direction moves essentially along the x axis. Furthermore we may choose to consider relaxation at the critical temperature ($\xi = \infty$) and in this case the above relation can be replaced by

$$\tau \sim L^z$$

where L is some characteristic length of the system. This follows from single finite-size scaling and obviously L is the sample size in Monte Carlo simulation. In our case, L is the system size along the y direction, or the number N of the walkers.

We observe that the motion of the walkers is highly correlated due to the weak but non-zero J_y coupling; the jump rates of a walker are strongly influenced by the position of its two neighbours. Actually it is quite easy to see that the motion of a walker is purely random if it is situated between its neighbours, otherwise a biased random walk occurs which forces it to be between its neighbours. Therefore there is an internal force which effectively stretches the wall to its maximum width N. There is then a purely diffusive motion of each random walker (a segment of the wall) as well as that of their centre of mass. The center of mass executes this diffusive motion with the mass equal to N. This is confirmed by the N dependence of the diffusion coefficient D_∞. Furthermore, the CM random walk drags, for sufficiently long times, the individual walker. This gives rise to a scaling law (3) and justifies the correct asymptotic result found for the moment of inertia. We may thus identify the characteristic time of magnetisation fluctuation with that found for the crossover between the two regimes observed for each walker. We therefore conclude that $z = \phi$ and our results suggest $z = 2.08 \pm 0.07$, consistent with very recent Monte Carlo simulations [9].

Obviously, it is of interest to extend this type of analogy and such simulations to higher-dimensional Ising systems as well as to other models (e.g. the Potts model). These will be subjects of future research.

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