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Simulation of domain wall dynamics in the SOS approximation of the 2D anisotropic Ising model: field-driven case

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Abstract. We consider an Ising system in two dimensions with anisotropic ferromagnetic interactions in the strong anisotropic limit and study, via numerical simulation, the dynamics of the interface separating two domains. Since the system is highly anisotropic ($J_x \gg J_y$ with $J_x \gg k_B T$) and we neglect the overhang configurations, the model in some aspects is an SOS (solid on solid) model. In this case the domain wall moves in one direction (x) and we are in the so-called 'strip geometry' ($L \times \infty$), L being the size of the system in the y direction. The dynamics of this interface can be reduced, as has been already shown, to the correlated motion of random walkers. Our previous study at high temperature ($J_y < k_B T$) has shown that for the equilibrium case where the mean position of the centre of mass (CM) does not change, the exponents z and α of the scaling relation describing the dynamics of the width of the wall have values 2 and 0.5, respectively. An equality $z - 2\alpha = 1$ was also obtained from cross-over arguments. In this paper we extend our study, by including a uniform external magnetic field, to the non-equilibrium case where CM mean position of the interface moves with time. We consider both the high- and low-temperature cases ($J_y/k_B T = 0.1$ and 1), and obtain the equality $z - 2\alpha = -\alpha_{CM}$; α_{CM} being the exponent characterizing the size dependence of the diffusion coefficient of the CM, i.e. $D \sim L^{\alpha_{CM}}$ in the long-time regime. For equilibrium we get $\alpha_{CM} \sim -1$. For the low-temperature, field-driven case we find the exponent approaching the value -0.5 as the magnetic field increases from 0 to $H/J_y = 2$. Since the static exponent α obtained is always near 0.5, our results in the low-temperature case correspond to $z = 2$ for equilibrium and approach the value $z = \frac{3}{2}$ predicted by Kardar, Parisi and Zhang in the non-equilibrium situation. The values of the exponent z obtained in different cases (equilibrium and non-equilibrium) by calculating the CM exponent α_{CM} are the same as those obtained from known equalities: $z + \alpha = 2$ (non-equilibrium) and $z - 2\alpha = d - 1$ (equilibrium). Therefore we propose that the single equality $z - 2\alpha = -\alpha_{CM}$ may apply far more generally and the study of CM dynamics may therefore provide an alternative (or complementary) way of analysing the results of domain growth simulations. We also note that our results are in agreement with two-dimensional results on the restricted solid on solid model (RSOS).

1. Introduction

Many studies have been reported of the simulation of dynamics of an interface that moves just in one direction. Various models have been considered: the single-step model [1, 2], ballistic deposition models [3–6], random deposition with surface diffusion [2, 7], Eden models [8–13], and the restricted SOS model [14], both in two and higher

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dimensions. For 'strip geometry' ($L \times \infty$), considered here, the interface is defined by the variables h_i ($i = 1, \ldots, L$). The interface width, ξ, is given by

$$\xi^2 = \left\langle 1/L \sum_{i=1}^{L} (h_i - h_{\mathrm{CM}})^2 \right\rangle \tag{1}$$

with $h_{\mathrm{CM}} = 1/L \sum_{i=1}^{L} h_i$, the position of the centre of mass. This quantity, ξ, obeys a finite-size scaling relation [3]:

$$\xi(L, t) = L^{\alpha} f_{\xi}(t/L^{z}). \tag{2}$$

The interface width saturates for large times ($t \gg L^z$) at a size-dependent value,

$$\xi(L, \infty) \sim L^{\alpha} \tag{3}$$

and is L independent for small times ($t \ll L^z$):

$$\xi(L, t \ll L^z) \sim t^{\alpha/z}. \tag{4}$$

To this behaviour corresponds a scaling function that reaches a constant value for large x and behaves like $x^{\alpha/z}$ for small x. Edwards and Wilkinson [15] derived a Langevin equation for the variables h_i, and following that Kardar *et al* [16] analysed the general non-equilibrium case and predicted that the inclusion of the drift velocity for the interface mean position introduces a nonlinear term in that equation. In the absence of the nonlinear term, $z = 2$ and $\alpha = 0.5$ was obtained for two dimensions. When the nonlinear term is added a value of z equal to $\frac{3}{2}$ is obtained, but the value of α is the same. Furthermore, the exponent equality, $z + \alpha = 2$, emerged from the renormalization group treatment. This behaviour was found to be consistent with simulation results, except for random deposition with surface diffusion where, despite the non-equilibrium character of the model, $z = 2$ was observed [2, 7].

In our previous simulation study [17] of the 2D anisotopic Ising model for temperature corresponding to $J_y/k_{\mathrm{B}}T = 0.1$, we had found that in equilibrium the exponents z and α take the values 2 and 0.5, respectively. We include here the magnetic field in our model thereby creating a non-equilibrium situation which makes the interface mean position increase with time in the x direction. We consider various values of the magnetic field and temperatures. Henceforth, we express both J_y and H in energy units; thus $Jy/k_{\mathrm{B}}T$ and $H/k_{\mathrm{B}}T$ are dimensionless. In the next section we define the model and the various quantities used and discuss in some detail the CM movement and its relation with other quantities. The details of the simulation experiment are given in the section of results and discussion. Our conclusions, which include discussion on the limitations of our study and possible future work, are in the last section.

2. The model

The model considered is a two-dimensional anisotropic Ising model where the anisotropy is strong, $J_x \gg J_y$, and the coupling constant J_x obeys $J_x \gg k_{\mathrm{B}}T$. The initial configuration of the interface separating two domains is a straight line extending along the y direction and positioned at $x = 0$. This interface moves just in the x

direction and one can describe it at any time-step by the variables h_i. We use periodic boundary conditions such that $h_i = h_{i+L}$. Starting from the spin-flip transition rates for spins on the two sides of the interface we construct the probability that in a single time-step the variable h_i increases or decreases by one unit, or retains its value [17]. These probabilities depend on the local configuration of the interface, namely on the values of h_{i-1} and h_{i+1}. Only three parameters a_1, a_2, a_3 are needed to write these transition probabilities for all the nine possible local configurations:

$$a_1 = \{1 + \exp[4J_y/k_B T(1 - H/2J_y)]\}^{-1}$$

$$a_2 = \{1 + \exp[4J_y/k_B T(1 + H/2J_y)]\}^{-1}$$

$$a_3 = [1 + \exp(-2H/k_B T)]^{-1}.$$

In figure 1 we indicate, in a concise form, the transition probabilities p_+ $(h_i \to h_i + 1)$, p_0 $(h_i \to h_i)$ and p_- $(h_i \to h_i - 1)$ for all possible configurations around h_i. In the figure, the full black circle represents the position of the walker h_i along the x direction while circles with $-$ and $+$ signs represent walkers h_{i-1} and h_{i+1}, respectively. The probabilities underneath a configuration are given in the following order: p_+, p_0, p_-. At every time-step a variable h_i is randomly chosen to move and is changed according to these probability rules.

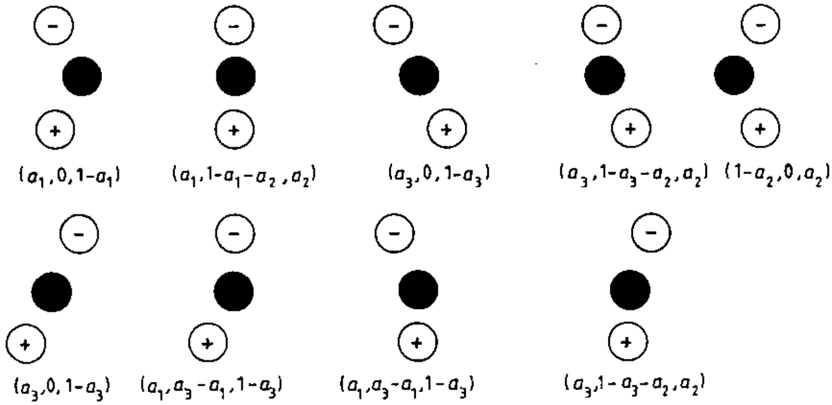

Figure 1. Various possible local configurations of the walker h_i and the associated stepping probabilities. The relative positions of walkers h_{i-1} and h_{i+1} are indicated by $\ominus$ and $\oplus$, respectively, and the probabilities are given as (p_+, p_0, p_-). See the text for details.

Besides the interface width already defined, we introduce two other quantities, the variance of the position h_i of a single segment of interface, V_1, and the variance of the centre of mass V_{CM}. These two quantities are related to the interface width by [17]

$$\xi^2(L,t) = V_1(t) - V_{CM}(t). \tag{5}$$

The variable h_i is seen to perform a random walk where non-trivial correlations with neigbouring walkers h_{i-1} and h_{i+1} arise because of the non-zero exchange constant J_y along the direction parallel to the interface. Since this walk has no memory, i.e. the transition probabilities at any time-step do not depend on the configuration at previous times, it is expected that the Gaussian limit of the random walk must be achieved for large times [18]. The variances V_1 and V_{CM} have, therefore, a diffusive behaviour for large times and grow linearly with time, with a diffusion coefficient that is L dependent. Moreover, the magnetic field H causes the CM position to move in the increasing x direction.

Since the interface width aproach a constant value for large times the large-time diffusion constants of V_1 and V_{CM} must be equal. We designate this common diffusion constant as D and write its size dependence as $D \sim L^{\alpha_{CM}}$. At the other end, for small times and sufficiently large systems, V_1 is L independent. Moreover, for this small-time regime ξ^2 and V_1 are approximately equal, since V_{CM} is small in this regime. So we can write a finite-size scaling expression for $V_1(L,t)$:

$$V_1(L,t) = t^{2\alpha/z} f(t/L^z). \tag{6}$$

For small times $f(x)$ is constant and for large times it should behave as $x^{1-2\alpha/z}$ in order to obtain the time-linear behaviour in the asymptotic regime. The diffusion coefficient D, for large times, behaves, therefore, like $1/L^{z-2\alpha}$ and we obtain

$$z - 2\alpha = -\alpha_{CM}. \tag{7}$$

In d dimensions, in the cases where the CM behaves as a simple random walker, the exponent α_{CM} is equal to $-(d-1)$ and equation (7) reduces to

$$z - 2\alpha = d - 1 \tag{8}$$

predicting for two dimensions ($d = 2$) $\alpha = 0.5$ and $z = 2$, characteristic of equilibrium situations. The last exponent relation was also found to be relevant for a random deposition model in which particles diffuse to nearby sites where the binding is strongest [19]. In the next section we describe the results of our simulation for the exponents α_{CM} and α.

3. Results and discussion

Our Monte Carlo simulations were done for system sizes $L = 8, 16, 32, 64$, and 128 and times up to 25 000 MCS/L (MCS/L Monte Carlo steps per walker). For each system size 500 runs were made. Simulations were done for two temperatures corresponding to (a) $J_y/k_BT = 1$, and (b) $J_y/k_BT = 0.1$. In the low-temperature case, case (a), the external magnetic field values chosen were $H/J_y = 0$, 0.4 and 2 and in case (b) the values were 0.4, 2 and 4. The exponent α was obtained using equation (3) by fitting $\ln\xi(L,\infty)$ against $\ln L$ to a straight line. We obtain the diffusion coefficient, D, by fitting a straight line to the curves V_{CM} against t in the long-time regime. A subsquent straight-line fit of $\ln D$ against $\ln L$ yields the exponent α_{CM}. The errors quoted (table 1) in the exponents correspond to fitting probabilities equal to or larger than 0.9. We discuss low- and high-temperature results separately.

Table 1. Results of the straight-line fits of $\ln \xi(L,\infty)$ against $\ln L$ and $\ln D$ against $\ln L$, giving α and α_{CM}, respectively.

H/J_y	$J_y/k_{\mathrm{B}}T$	α	α_{CM}
0	1	0.54 ± 0.04	-1.0 ± 0.1
0.4	1	0.50 ± 0.03	-0.71 ± 0.07
2	1	0.50 ± 0.01	-0.49 ± 0.05
0.4	0.1	0.51 ± 0.03	-0.99 ± 0.07
2	0.1	0.55 ± 0.04	-0.98 ± 0.07
4	0.1	0.50 ± 0.05	—

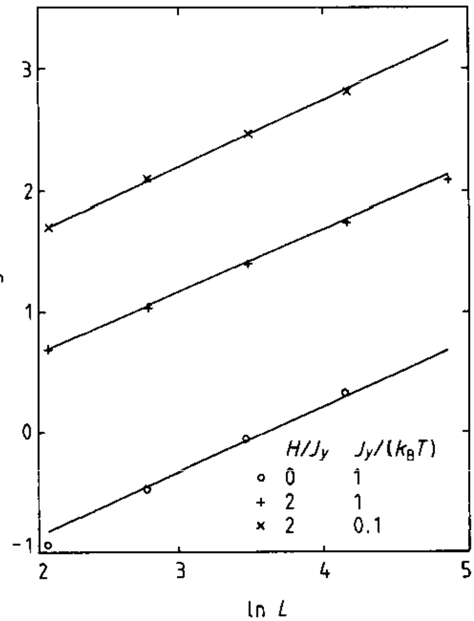

Figure 2. Plot of $\ln \xi(L,\infty)$ against $\ln L$ and the corresponding straight-line fits for $J_y/k_{\mathrm{B}}T = 1$ and $H/J_y = 0, 2$ and for $J_y/k_{\mathrm{B}}T = 0.1$ and $H/J_y = 2$.

3.1. Low-temperature results

For all magnetic fields the α values obtained are shown in table 1. For the case $H = 0$ data for $L = 8$ were not included in the fit. The exponent values obtained are close to 0.5 as expected. For $H/J_y = 0$ and 2 we show ξ against L in a log–log plot in figure 2.

The fits of V_{CM} against t for $H/J_y = 0, 0.4$ include data only for times greater than 1000 MCS/L. For this time interval all the systems reached the asymptotic regime, as seen from the $\xi(L,t)$ behaviour. For $H/J_y = 2$, times greater than 5000 MCS/L are needed. The results of the straight-line fit of $\ln D$ against $\ln L$ are in table 1, and the corresponding data are plotted in figure 3. In the zero-field case we get an exponent α_{CM} near -1 and therefore $z = 2$, a behaviour expected for equilibrium. For higher magnetic fields this exponent approaches $\alpha_{\mathrm{CM}} = -0.5$, corresponding to $z = 1.5$. A further insight into this data analysis can be obtained by plotting $V_{\mathrm{CM}} \times L^{-\alpha_{\mathrm{CM}}}$ against t for all system sizes. In figures 4 and 5 we plot these curves for the extreme cases $H/J_y = 0$ and 2. In the first case a good collapse of data can be seen at all

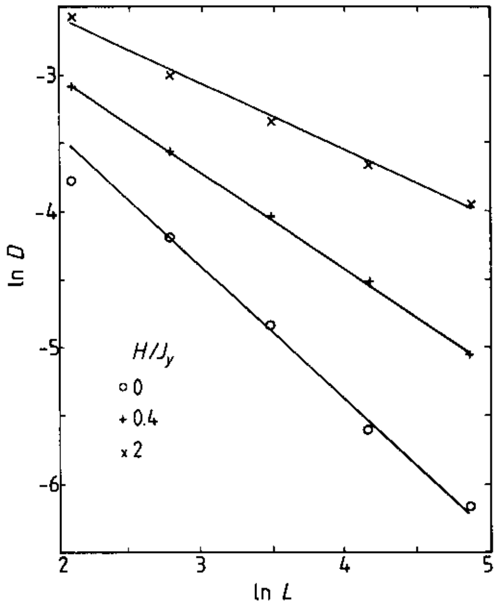

Figure 3. Plot of $\ln D$ against $\ln L$ for the cases $J_y/k_BT = 1$ and $H/J_y = 0, 0.4$ and 2.

times; for $H/J_y = 2$ collapse is obtained in the asymptotic regime. For smaller times V_{CM} scales actually like $1/L$.

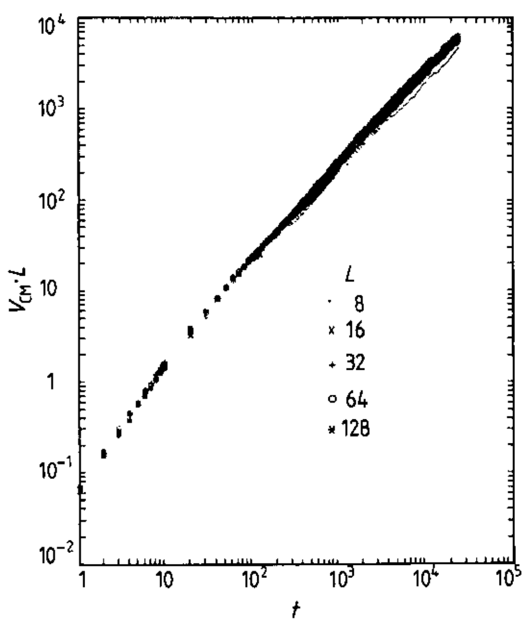

Figure 4. Plot of $V_{CM} \times L$ against t in log–log scale for the case $J_y/k_BT = 1$ and $H/J_y = 0$ showing the collapsing of the curves for the different system sizes L.

For temperatures lower than the one used by us the interface does not move for

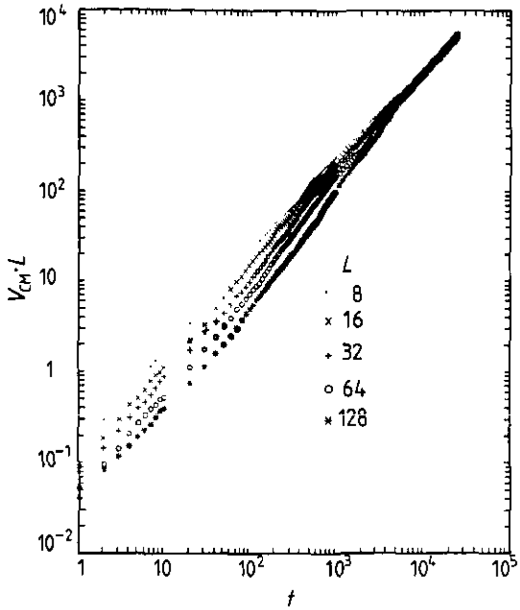

Figure 5. Plot, in log–log scale, of $V_{CM} \times L^{1/2}$ against t for the case $J_y/k_BT = 1$ and $H/J_y = 2$. Collapse of the curves is seen for large times.

$H/J_y < 2$ because the parameter a_1 is effectively zero. For $H/J_y = 2$, however, a_1 is always $\frac{1}{2}$ and the interface moves with an exponent $z = 1.5$ as our results show. For $H/J_y > 2$ the magnetic field wins over the coupling constant J_y and we reach the random deposition limit (h_i increases every micro-step if it is chosen to move). Note that in the random deposition limit V_{CM} is zero at all times and $\xi^2(L,t) = t$ (h_i is a Poisson process) [20]. The parameter a_2 for $H/J_y = 2$ is small but not zero and a_3 is near 1 but not exactly 1 as it would be for zero temperature.

Now we try to show that for field $H/J_y = 2$ and low temperatures the model under consideration is physically similar to the restricted SOS model (RSOS) [4], and therefore the fact that the results of the numerical simulation on the two models agree is not surprising. In the RSOS model the height h_i (when chosen to move) increases only when the interface steps $|h_i - h_{i+1}|$, as well as $|h_i - h_{i-1}|$, are both less than or equal to a given specified number N. Thus the RSOS model maintains interface steps between specified limits. In our model the situation is similar. When h_i is chosen to move at a given time-step the quantities $|h_i - h_{i+1}|$ and $|h_i - h_{i+1}|$ in principle also change; the sum of two quantities $|h_i - h_{i+1}|$ and $|h_i - h_{i-1}|$ can be taken as an indicator of local roughness. In our special case for all those local configurations in which the increment of h_i leads to the sum remaining the same (or decreasing), the probability of h_i increasing is one. For all other configurations the probability of the sum of height differences increasing (due to a change in h_i) is always half. Thus we see that probability rules under these special conditions, i.e. $H/J_y = 2$ and low temperatures damp the increase of local roughness. We simulated the RSOS model for the case $N = 1$ for the same system sizes and simulation time as used in the simulation of our Ising model; two thousand samples were used for averaging purposes. The plot of $V_{CM} \times L^{0.5}$ against t is shown in figure 6, demonstrating that a data collapse is again obtained in the asymptotic regime, confirming $\alpha_{CM} = -0.5$ in this model also.

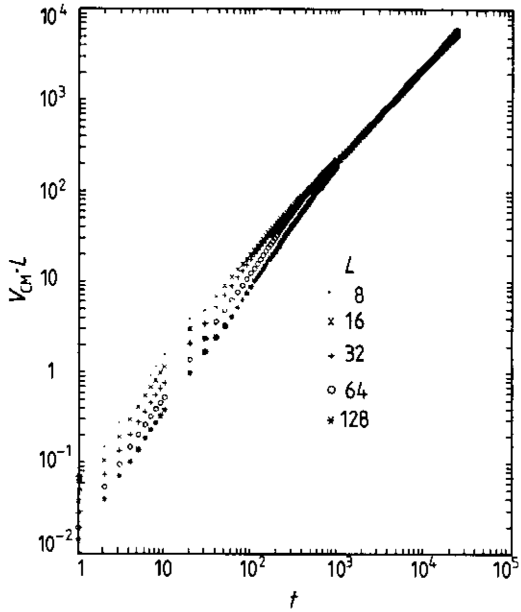

Figure 6. Plot, in log–log scale, of $V_{CM} \times L^{1/2}$ against t for the RSOS model. Here also collapse of the curves is obtained for large times.

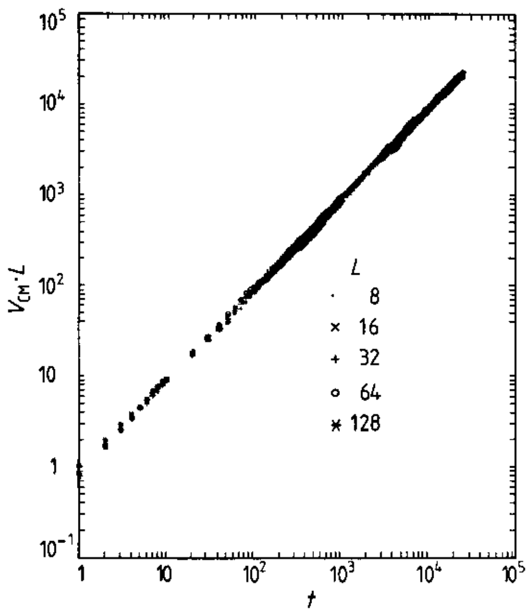

Figure 7. Plot, in log–log scale, of $V_{CM} \times L$ against t for the case $J_y/k_B T = 0.1$ and $H/J_y = 2$.

3.2. High-temperature results

The simulation time in this case was not enough to get the asymptotic value of $\xi(L,t)$ for the largest system ($L = 128$) and for all the magnetic fields studied. We enter the α values obtained for each case in table 1. As can be seen, they are all consistent with $\alpha = 0.5$ as expected. In figure 2 the curve $\ln \xi(L, \infty)$ against $\ln L$ is plotted for $H/J_y = 2$.

In order to obtain D, times greater than 10 000 MCS/L were used. The results of the fit of ln D against ln L to a straight line are also in the table. For $H/J_y = 0.4$ and $H/J_y = 2$ results are consistent with $\alpha_{\rm CM} = -1$. For the highest magnetic field simulated, however, we need higher simulation times and better statistics in order to get reliable measures of D in the asymptotic regime. The plot $V_{\rm CM} \times L$ against t for $H/J_y = 2$ is shown in figure 7. The collapse of the different curves shows again that $\alpha_{\rm CM} = -1$ describes the results well. For the case $H/J_y = 4.0$ a similar plot also gives the best superposition of curves for $\alpha_{\rm CM} = -1$.

In order that the effects of magnetic field be easily observable we should have $H > k_{\rm B}T$. However, in our case this forces H to be much greater than J_y and we find ourselves in the random deposition limit with the corresponding values of exponents. On the other hand, since the parameter λ (proportional to the interface growth velocity and, consequently, to the magnetic field) is a relevant coupling constant for $d = 2$ in the equation of Kardar *et al* [16], the magnetic field, however small, will *ultimately* change the exponents. The time needed to see this is, unfortunately, very large and we have not performed simulations to reach this limit.

4. Conclusion

The results for our model suggest that in the low-temperature regime there exists a cross-over, as the magnetic field increases, between $z = 2$ and 1.5. For magnetic fields higher than $H/J_y = 2$ a further set of simulations is needed in order to see if the z exponent continues to decrease as we approach the random deposition limit. It remains an unanswered question whether in the high-temperature case a decrease of z from 2 could be observed. Further simulations are needed with better statistics and larger times in order to probe the system under these conditions.

As we have shown, the size dependence of the large-time diffusion coefficient of the centre of mass can give information about the dynamic exponent z. This is confirmed by our simulation of the RSOS model. An analysis of this model [14] different from ours (based on equation (4)) gives $z = 1.5$ for two dimensions which agrees with ours: $\alpha_{\rm CM} = -0.5$ and $z - 2\alpha = -\alpha_{\rm CM}$. We believe that our method of analysis could be applied to other growth models in two dimensions as well as to higher dimension models, where some controversy about the values of the exponents remains [14]. Our study also indicates that it may be fruitful to develop theoretical work incorporating the behaviour of the variance of the centre of mass.

Acknowledgments

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