FINITE-SIZE SCALING STUDY OF THE BALLISTIC DEPOSITION

MODEL IN (1 + 1)-DIMENSIONS

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Abstract

We performed extensive Monte Carlo simulations of the ballistic deposition model in (1 + 1)-dimensions for several system sizes up to 1280 lattice constants, on the square lattice. Though the ballistic deposition model is generally accepted to belong to the Kardar-Parisi-Zhang (KPZ) universality class, strong corrections to scaling prevent numerical estimates of the exponents close to the asymptotic values. We obtained $\alpha \geq 0.40$, $\beta \geq 0.30$, and $z \geq 1.16$, which are consistent with the expected KPZ values of $\alpha = 1/2$, $\beta = 1/3$, and $z = 3/2$. We found a slow, and even non-monotonic, convergence of the exponents towards the asymptotic values, which corroborates previous claims in the literature of strong corrections to scaling.

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1. Introduction

The irreversible deposition of particles onto substrates is a complex, out-of-equilibrium process of fundamental interest with a concomitant technological interest. Consequently, there has been a surge of interest in models of deposition in the last two decades. [1-15] Depending on the incoming flux of particles and their mobility at the surface, one can have different regimes of kinetic growth. For example, at high surface mobility of adatoms one can expect significant restructuring on the time scale of film deposition, while for low surface mobility, adatoms irreversibly stick upon thermal deposition. Recent studies also focused on the post-deposition evolution of the exotic nanostructures developed during the deposition stage. [15-17]

Even in the simplest case of no surface diffusion, a series of simple, phenomenologically motivated models, have been proposed in the literature, namely solid-on-solid (SOS), Eden, restricted SOS (RSOS), random deposition (RD), and ballistic deposition (BD), which still capture relevant features observed in a diverse class of aggregation phenomena. An interesting feature of the BD model is that it allows for the growth of lateral correlations, contrary, for example, to the naive RD model. A variant of the standard BD model, the step model [4], produces compact, void free films, but other interesting variations of the basic theme have also been proposed on the literature. [9-10]

Even though the BD, step and Eden models show substantially different morphologies, the width or thickness of the growing interface scales similarly both spatially and in time. In fact, several studies on the BD, step model, and the Eden models show that they belong to the Kardar-Parisi-Zhang universality class. [11] However, simulation results present in the literature quote values close to, but different from, what is predicted by the KPZ universality class even in the most favorable case of $(1 + 1)$-dimensions. The justification has been the existence of strong corrections to scaling, leading to a rather slow convergence to the asymptotic values of the exponents. However, a detailed study of such finite-size effects can help understand the functional size dependence towards the asymptotic values, and, in principle, predict with better accuracy their actual asymptotic values. Moreover, since asymptotic values

are attained for quite large system sizes, the sub-asymptotic behavior is of interest to people working in the nanometer scale.

In this paper, we initiate the presentation of a series of extensive Monte Carlo simulations of the ballistic deposition model, with a detailed finite-size scaling study, [14] with the goal of offering a broader range of validity of these models. Specifically, within this work on the ballistic deposition model, we substantially expand previous numerical simulations.

This work is structured as follows: In Section 2 we briefly review case studies of kinetic growth models and introduce the necessary terminology to present our results in Section 3. Finally, we summarize our results in Section 4.

2. Some growth models

Though in the present work, we are primarily interested in the BD model, it is instructive to review related growth models and some of their properties. For example, the Eden model [12] was originally created to explain the growth of tumor cells. In this model, growth takes place by randomly choosing and occupying a vacant site on a lattice, which is usually called the seed or root site. Subsequent growth proceeds by randomly choosing and occupying a perimeter site of the cluster. As the number of particles added to the growing cluster increases, the roughening of the edges of the cluster is envisaged, i.e., roughening of the width of its interface. Eden clusters are, therefore, fairly compact, but some reminiscent voids are also present. [3, 4, 12]

In the single step model, particles of size two are vertically deposited on a substrate initially with alternating values of the heights of zero and one. Growth can only take place on those sites where the height difference between the landing site column and that of the neighboring columns is exactly one, thus increasing the value of the height of such column by two. Not surprisingly, one notices that such a restriction leads to compact void free films and rough interfaces. [4]

The ballistic deposition model was originally introduced by Vold and, independently, by Sutherland, [18] to study the process of sedimentation of suspensions of spherical colloidal particles about one micron in

size. In particular, interest was focused on the resulting density of deposits. However, in the past one and a half decades, research interest shifted towards the study of the growth of films, either off or in lattice, and, in particular, to the kinetics of growth associated with resulting film morphology. In the present work, we focus on the case of particles being vertically deposited by randomly choosing a column and letting the particle fall until it attaches to a neighboring particle upon touching it. The interesting case of slanted deposition at a given constant angle was also considered by P. Meakin, [4] but space restrictions prevent us from treating such a case. [14] In the case of vertical deposition, the landing site is the highest 'spot' of the randomly chosen column and of the corresponding nearest neighboring columns, i.e.,

$$h_i := \max (h_{i-1}, h_i + 1, h_{i+1}) \,, \tag{1}$$

where h_i represents the height of the column in positions i= 1, 2, …, L and the symbol ':=' denotes an update of the height, at column i, for a given deposition event. A typical configuration is shown in Figure 1 by the gray particles, while the white particles represent the next landing 'spot' of a particle falling on that randomly chosen column, in the next deposition event.

Though it is generally accepted that the ballistic deposition model belongs to the KPZ universality class, [11] the convergence to the theoretical predicted values of the exponents $\alpha = 1/2$, $\beta = 1/3$, and $z = 3/2$ is rather slow, requiring simulations of fairly large lattices. Our study makes use of finite-size scaling and large sampling to prevent having to simulate rather large lattices with few samples, or even worse, with a single sample. We are, therefore, interested in the functional size dependence of the various exponents. Finally, we note that from the three exponents referred above, only two of them are independent.

In the ballistic deposition model, the interface width is defined by

$$<w\,(t)> = \sqrt{<h^2\,(t)> - <h\,(t)>^2} \,, \tag{2}$$

where,

$$\langle h^n(t)\rangle = \frac{1}{L}\left\langle \sum_{i=1}^{L} h_i^n \right\rangle, \tag{3}$$

is the n-th moment of the heights, at time t, and L is the linear dimension of the system. The symbol '$\langle\ \rangle$' represents averages over many realizations.

As defined above, the width of the interface follows the scaling function proposed by Family and Vicsek, [6]

$$w(t) = L^\alpha f\left(\frac{t}{L^z}\right), \tag{4}$$

where the scaling function f (x), with $x = t/L^z$, is proportional to f (x)$\approx x^\beta$ for x $\ll$ 1 and f (x)$\approx$ const. for x $\gg$ 1. The exponent α is called the roughness exponent, for it is related to the interface width upon saturation. The exponent β is called the growth exponent and the exponent z is called the crossover or saturation exponent. Exponent z characterizes finite systems, since it represents the crossover time from the ballistic deposition regime to the saturation regime. This feature is rather typical of time-dependent, out-of-equilibrium systems, where correlations build up and are eventually curtailed by the finite size of the system. The analogous counterpart in systems in equilibrium happens at the critical point of a second order phase transition.

Since the interface grows at early times with little dependence on the size of the lattice and the scaling function in this region is proportional to $t^\beta/L^{z\beta}$, we get the following relation between exponents,

$$\alpha = \beta z. \tag{5}$$

3. Results

We extensively simulated the ballistic deposition model in the square lattice and now proceed to present our preliminary results for lattices of linear sizes, L, equal to 10, 20, 40, 80, 160, 320, 640, and 1280 lattice constants, which enabled us to perform a detailed finite size dependence study. The number of samples ranged from 10^4 samples for the 10 lattice constants case down to $2 \cdot 10^3$ for the 1280 lattice constants. We also simulated for about 30·L time steps, which enabled us to go deeply into the saturation regime, in particular for the smaller (L ≤ 160) lattice sizes. Notice that some authors adopt as a time step each deposition event, while we define each time step as the number of particles to fill up on the average a layer, which is equal to L in the present case. Periodic boundary conditions apply along the direction perpendicular to the incoming flux of particles.

For finite system sizes, which is always the case for any simulated system, the ballistic deposition model starts to saturate at some instant of time t_x, called the crossover time. From equation (4), we observe that the crossover time is consistent with the relation,

$$t_x \propto L^z ,$$
(6)

where the symbol '∝' means 'proportional to'. At early times, i.e., for $t \ll t_x$, ln w grows linearly with ln t, while for late times, i.e., for $t \gg t_x$, ln w takes a constant value. This behavior is clearly observed in Figure 2 for the ballistic deposition model simulated in the square lattice for lattices of sizes 10, 20, 40, 80, 160, 320, 640, and 1280 lattice constants.

From equation (6) we observe the characteristic dependence of the crossover time on the size of the system and also that the crossover time increases with the size of the system. (See also Figure 2.) We define the crossover time as the instant of time given by the intersection of the straight line describing the saturation regime and the straight line describing the growth regime. In the process of reckoning the slope of the latter straight line, we accounted for the presence of a transient regime in the initial stages of growth. [17] Figure 4 presents our results for exponent z for the same lattice sizes as in Figure 2. The

value of the exponent z increases monotonically with the size of the system from a value of 0.68 for a ten-lattice-constants lattice to 1.11 for a 1280-lattice-constants lattice. As $1/L \rightarrow 0$, one observes the increase in the absolute value of the local slope, an indication that the asymptotic limit has not yet been reached.

Exponent β characterizes the growth of the interface of the infinite system at all times. For a finite system size, β characterizes the growth of the interface at early times, i.e., before the system 'learns' that it is constrained to evolve inside a box. With these aspects in mind, we expect β to be fairly insensitive on the size of the system. Figure 5 shows the values of β for all simulated system sizes. We immediately notice strong corrections to scaling, particularly evident for lattices of sizes smaller than 160 lattice constants, leading to non-monotonic approach of the exponent β to the asymptotic value. Though by extrapolation one can quote a conservative value of $\beta \geq 0.30$, it is not clear it can converge to the 0.3 (3) value predicted by the KPZ universality class.

At late times the system had time to grow lateral correlations much longer than its own linear size, but since spatial correlations are limited by the size of the system, it sets a natural length scale, the saturation width of the interface. Due to equation (4) and Figure (2), we expect the value of the saturated width of the interface to scale as L^{α}. As with previous quantities the roughness exponent α did not saturate.

It is also instructive to observe the value of the α exponent given from the equation (5). Our results are shown in Figure 7. The values of α are taken from βz for a given size of the system. Once again results are far from converging to the asymptotic values, apart from being rather lower than direct measurements. Finally, the values of the z and α exponents have also to satisfy the following scaling relation

$$z + \alpha = 2 , \tag{7}$$

so we plot this quantity for the various system sizes. Once again we observe that the value of two is far from being reached though the trend is in the right direction. (See Figure 8.)

4. Conclusions

The ballistic deposition model shows strong corrections to scaling up to lattice sizes of 1280 lattice constants wide, leading to quite low convergence rates towards the asymptotic values of the exponents α, β, and z. We are in the process of simulating larger lattices to obtain better estimates.

Our study provides an example on how nanostructured materials may introduce more stringent demands on present day theories. In particular, the slow convergence of the exponents α, β, and z to their asymptotic limit may, in fact, prevent some real systems from being in the asymptotic regime.

References

[1] A.-L. Barabási and H.E. Stanley, *Fractal Concepts in Surface Growth*, Cambridge University Press, New York, 1995.

[2] F. Family and T. Vicsek, *Dynamics of Fractal Surfaces*, World Scientific, Singapore, 1991.

[3] H.E. Stanley and N. Ostrowsky, *On Growth and Form*, Martinus Nijhoff Publishers, Dordrecht, Netherlands, 1986.

[4] P. Meakin, *The Growth of Rough Surfaces and Interfaces*, Phys. Rep. **235**, 189 (1993).

[5] T. Halpin-Healy and Y.-C Zhang, Phys. Rep. **254**, 215 (1995).

[6] F. Family, and T. Vicsek, J. Phys. A**18**, L75 (1985).

[7] A.-L Barabási, R. Bourbonnais, M. Jensen, J. Kértesz, T. Vicsek, and Y.-C. Zhang, Phys. Rev. A**45**, 6951 (1992).

[8] P. Meakin, P. Ramanlal, L.M. Sander, and R.C. Ball, Phys. Rev. A**34**, 5091 (1986).

[9] H.F. El-Nashar, W. Wang, and H.A. Cerdeira, Surf. Science **391**, 1 (1997).

[10] W. Wang and H.A. Cerdeira, Phys. Rev. E**52**, 6308 (1995); Phys. Rev. E**47**, 3357 (1993).

[11] M. Kardar, G. Parisi, Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).

[12] M. Eden, Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Berkeley, California, edited by F. Neyman (University of California, Berkeley, 1961), Vol. 4, p. 223.

[13] P. Meakin, Phys. Rev. Lett. **51**, 1119 (1983).

[14] R. Miranda and A. Cadilhe, to be published elsewhere.

[15] K.J. Caspersen and J.W. Evans, Phys. Rev. B**64**, 075401 (2001).

[16] C.R. Stoldt, A.M. Cadilhe, C.J. Jenks, J.-M. Wen, J.W. Evans, and P.A. Thiel, Phys. Rev. Lett. **81**, 2950 (1998).

[17] A.M. Cadilhe, C.R. Stoldt, C.J. Jenks, P.A. Thiel, and J.W. Evans, Phys. Rev. B**61**, 4910 (2000).

[18] M.J. Vold, J. Colloid Interface Sci. **18**, 684 (1963); D.N. Sutherland, J. Colloid Interface Sci. **22**, 300 (1966).

List of figure captions

Figure 1.   Ballistic deposition model on a square lattice: gray particles represent a typical configuration while white particles represent a possible landing site.

Figure 2.   Plot of the width vs. time for systems of sizes 10, 20, 40, 80, 160, 320, 640, and 1280 lattice constants wide. Smaller sizes saturate at a smaller value of the width.

Figure 3.   Plot of the collapsed scaling function. Tails represent the initial transient behavior due to a clean substrate.

Figure 4.   Plot of the saturation exponent, z, vs. 1/L for the same system sizes referred to in Figure 2. Refer to the text for further details.

Figure 5.   Plot of the growth exponent, β, vs. 1/L for the same system sizes referred to in Figure 2. Refer to the text for further details.

Figure 6.   Plot of the roughness exponent, α, vs. 1/L for the same system sizes referred to in Figure 2. Refer to the text for further details.

Figure 7.   Plot of the roughness exponent, α, vs. 1/L for the same system sizes referred to in Figure 2. Filled triangles are calculated using equation (5), while filled rectangles are the values directly calculated as in Figure 6. Refer to the text for further details.

Figure 8.   The plot shows the quantity $\alpha + z$ vs. 1/L. Refer to the text for further details.
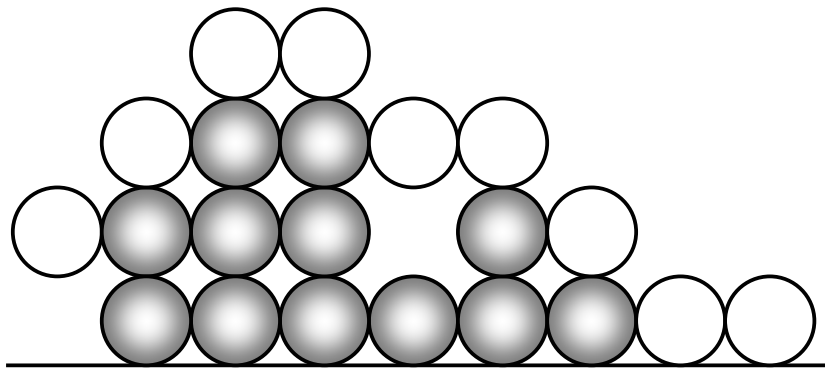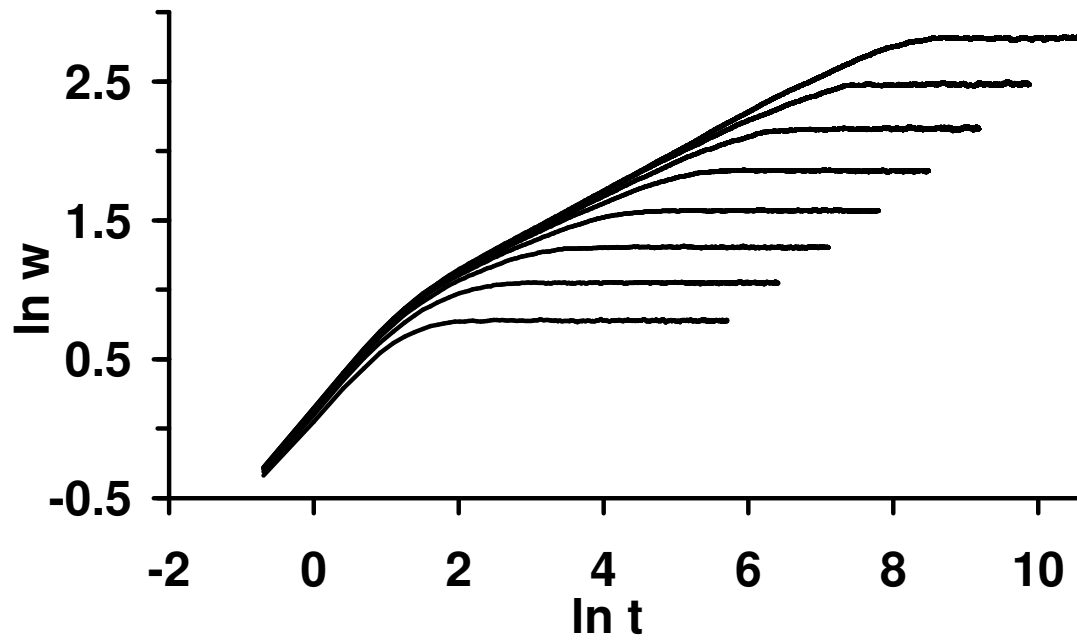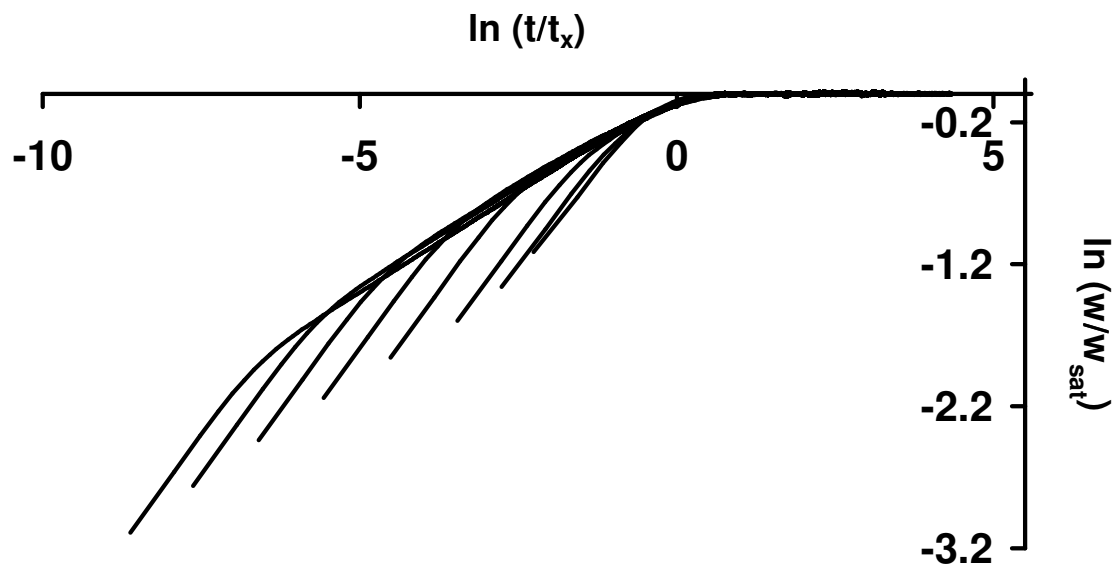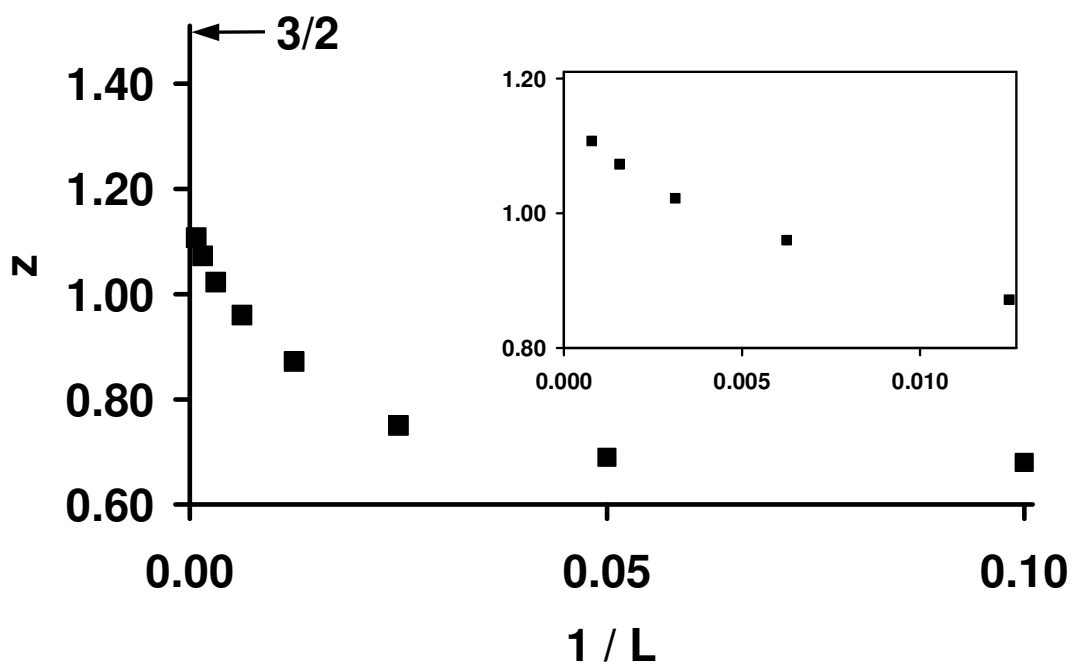
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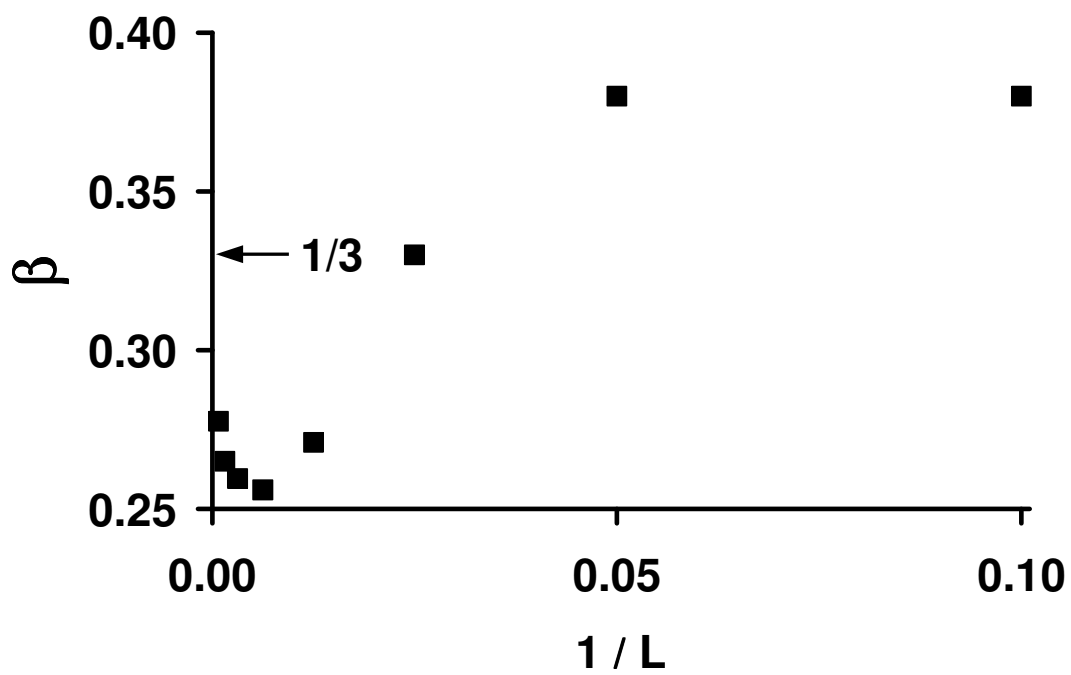
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Figure 8