Dynamic correlation function of lattice gas in c(2×2) phase

P. Argyrakis, M. Maragakis

Department of Physics, University of Thessaloniki, Greece

O. Chumak, A. Zhugayevych

Department of Theoretical Physics, Institute of Physics, Kyiv, Ukraine

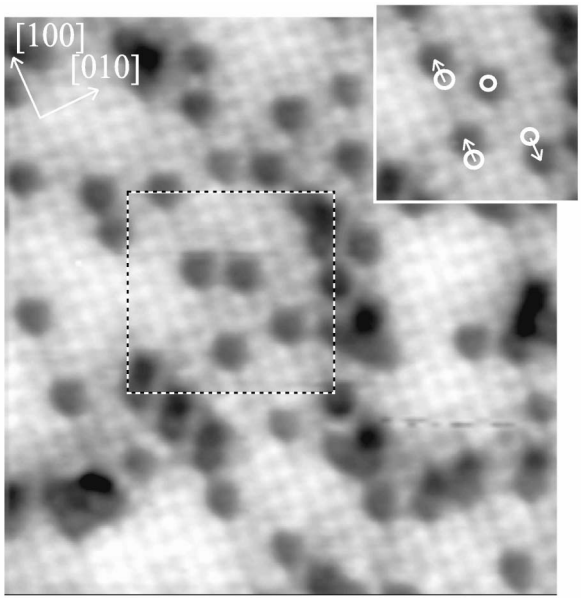

Fig. 1: STM movie: Diffusion of N adatoms on Fe(100) surface [M. Pedersen *et al.*, Phys. Rev. Let. 84, 4898 (2000)]

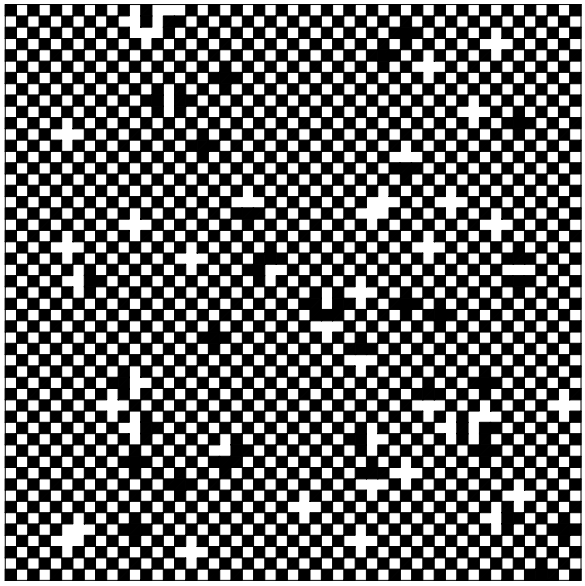

Fig. 2: MC simulations: Lattice gas with nearest neighbors repulsion in c(2×2) phase at half coverage and temperature $T = 0.8\ T_c$

Subject:

Kinetic phenomena in two-dimensional lattice gas with nearest neighbors repulsion in ordered c(2×2) (antiferromagnet) phase under the condition of low concentration of structural defects

Keywords:

lattice gas, kinetic phenomena, dynamic correlation function

PACS:

05.50.+q (Lattice theory and statistics)

68.43.De (Statistical mechanics of adsorbates)

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System specification

System:

- Square lattice of $L_0 \times L_0$ with periodic boundary conditions
- Lattice coordinates are denoted by a single letter: $x = (x_1, x_2)$
- Two particles cannot occupy the same point
- Particles interact via nearest neighbor repulsion so that

$$\beta H = \frac{1}{2} \sum_{x,e} \phi \; n_x n_{x+e},$$

  where $\beta = T^{-1}$, $\phi > 0$ – interaction parameter, n_x – number of particles at site x, e means a vector of unit length (the sum is over nearest neighbors)

We have two parameters: ϕ and c (average concentration of particles). The system is under the following conditions:

- subcritical temperatures, i.e. $\phi > \phi_c \approx 1.76$ so that $q = e^{-\phi}$ is a small parameter
- c is nearly $1/2$ so that c(2×2) phase is pronounced
- system is at thermodynamical equilibrium (and no domain walls)

Dynamics:

- Single-particle-jump approximation
- Master equation for an alone particle: $\dot{p}_x = -4p_x + \sum_e p_{x+e}$
- Transition rate from a given site is $e^{k\phi}$, where k is the number of nearest neighbors (i.e. overcoming of activation barrier)

Historical notes

- Lattice gas = Ising model with conserved spin dynamics
- Static properties are well studied
- Seminal papers: Glauber R J, JMP 4, 294 (1963); Kawasaki K, PR 145, 224 (1966); Heims S P, PR 138, A587 (1965)
- There is no efficient kinetic theory similar to BBGKI hierarchy in classic gas
- Diffusional approximation: O. Chumak

Objectives

- To develop an analytic method for studying kinetic phenomena in lattice systems in ordered phases, in particular, to obtain the dynamic correlation function: $\langle n_x(t) n_y(0) \rangle$
- To explain MC simulations (performed by P. Argyrakis and M. Maragakis) for the correlation function for fluctuations of number of atoms in a selected probe area at small times:

$$\langle \delta N(t) \delta N(0) \rangle = \sum_{x,y} \langle \delta n_x(t) \delta n_y(0) \rangle$$

- To substantiate the diffusional approximation (developed by O. Chumak) used in our previous papers

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Open problems

- To extend the method to $n^2 \sim q^4$ level that is necessary for accurate description of generation-recombination processes. The principal complication is that we must proceed from one-particle description to many-particle

BBGKI hierarchy for hard-core lattice gas

Master equation (time argument is omitted, symmetric distribution function is chosen):

$$\dot{p}(\{x\}) = \sum_{i=1}^{N} \sum_{|y-x_i|=1} \left[p(x_1, \ldots, \overset{i}{\widehat{y}}, \ldots, x_N) - p(t; \{x\}) \right] + 2N_{\mathrm{nn}}(\{x\}) p(\{x\}), \tag{1}$$

where $p(\{x\})$ is the probability of configuration $\{x\}$ and

$$N_{\mathrm{nn}}(\{x\}) = \sum_{1 \le i < j \le N} \mathrm{I}\{|x_i - x_j| = 1\} \tag{2}$$

is the number of nearest neighbor pairs in configuration $\{x\}$.

The lowest equations of the BBGKI hierarchy:

$$\dot{p}(x_1) = \sum_{|y-x_1|=1} [p(y) - p(x_1)] + 2(N-1) \sum_{|y-x_1|=1} p(x_1, y) + (N-1)(N-2) \sum_{|y-z|=1} p(x_1, y, z), \tag{3}$$

$$\dot{p}(x_1, x_2) = \sum_{|y-x_1|=1} [p(y, x_2) - p(x_1, x_2)] + \sum_{|y-x_2|=1} [p(x_1, y) - p(x_1, x_2)] + 2\mathrm{I}\{|x_1 - x_2| = 1\} p(x_1, x_2) + 2(N-2) \sum_{\substack{|y-x_1|=1 \\ \cup |y-x_2|=1}} p(x_1, x_2, y) + (N-2)(N-3) \sum_{|y-z|=1} p(x_1, x_2, y, z). \tag{4}$$

Snapshots

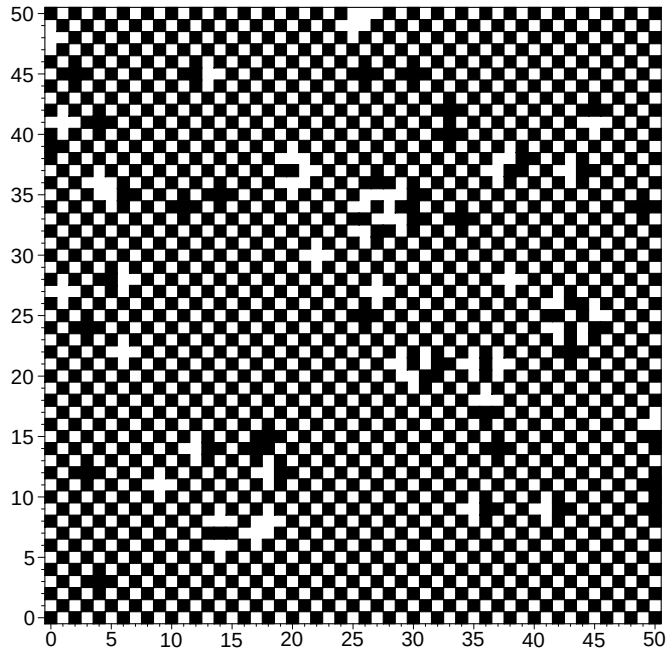


Fig. 3: Snapshot for $\phi = 2.0$ ($T = 0.8\ T_c$) and $c = 0.5$ (half coverage)

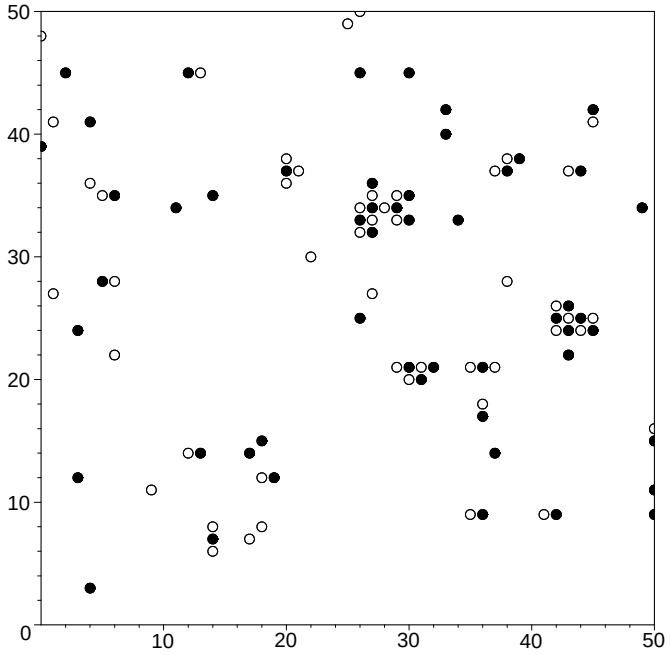


Fig. 4: "Defects only" view

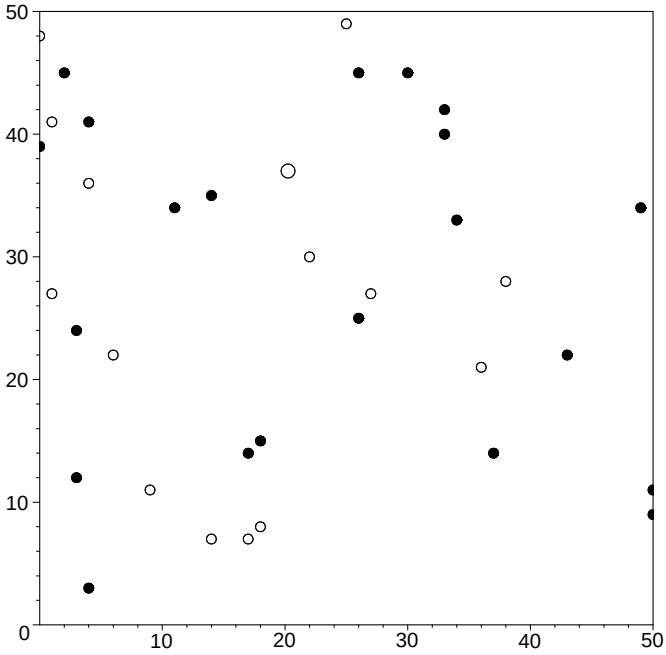
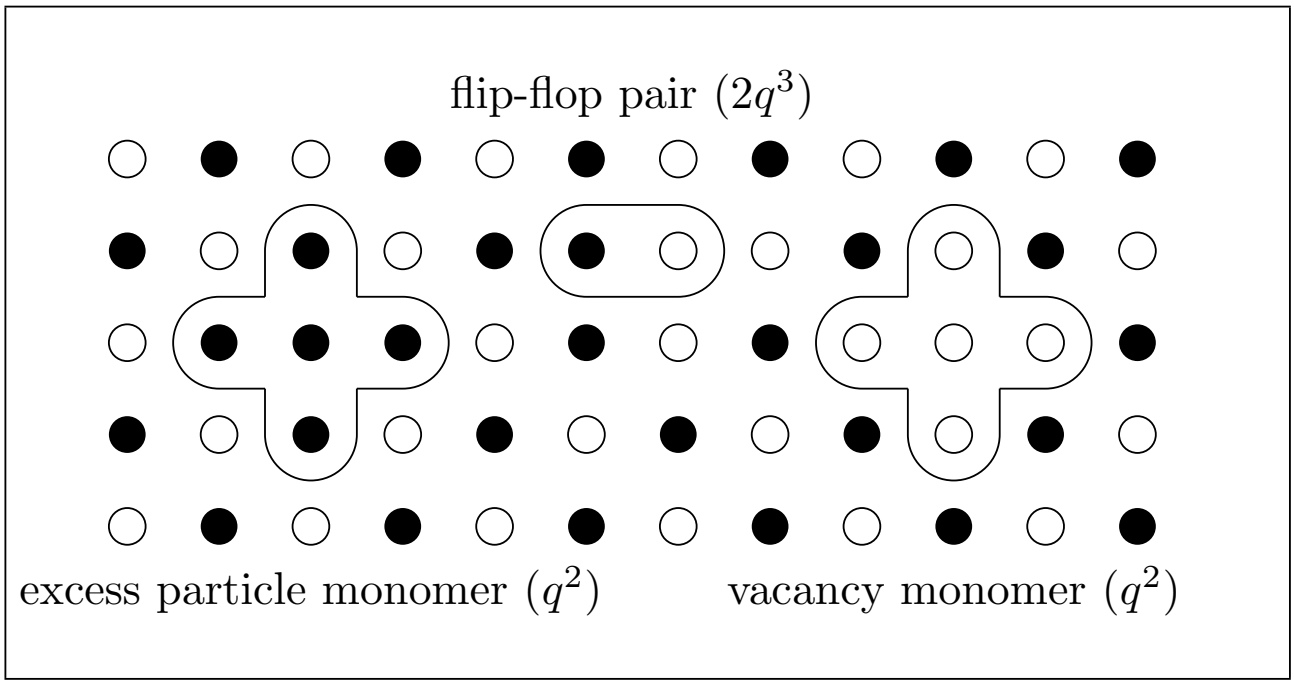


Fig. 5: Topological charges

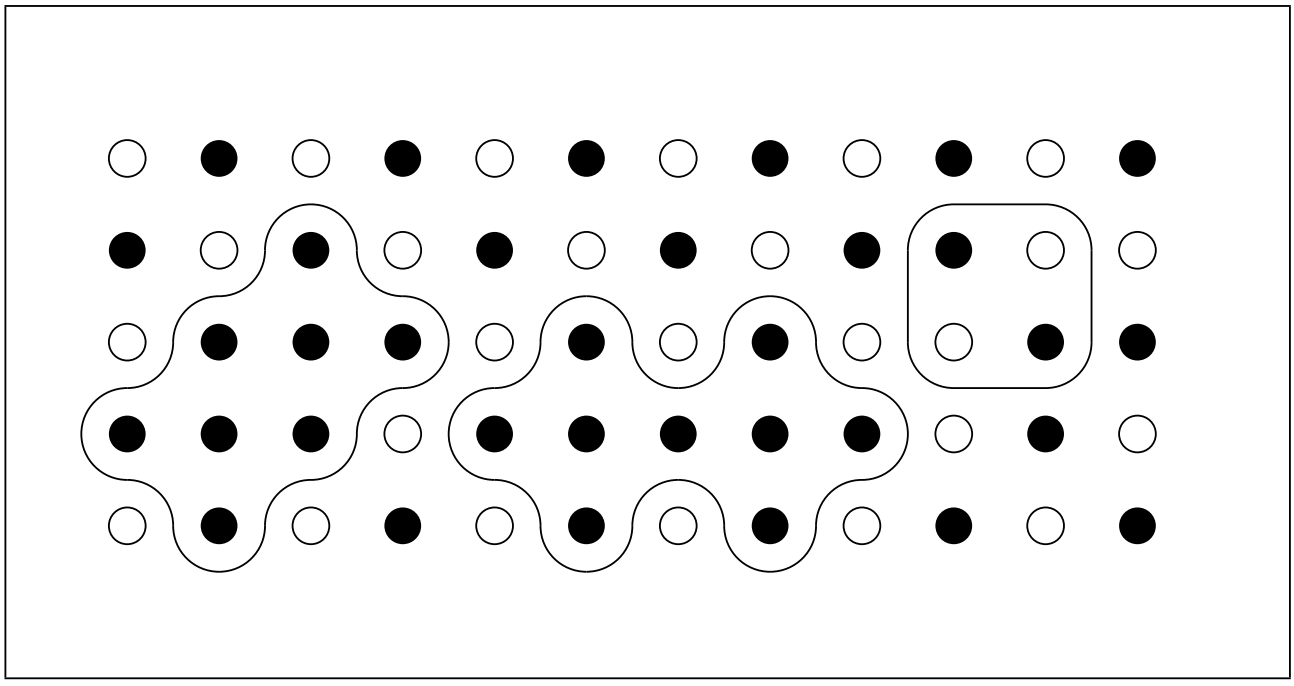
Structural defects

1) Level q^2: excess particles and vacancies with concentrations q^2 at exact half coverage

2) Level q^3:



2) Level q^4: isolated monomers, side and corner dimers, monomers at their jumps, isolated and double flip-flop pairs



Kinetic equation for monomers

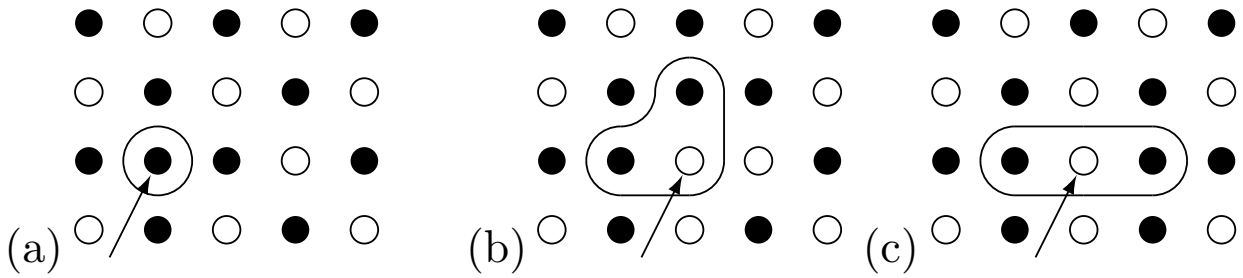


Fig. 6: Essential configurations for excess particle monomer: a) excess particle monomer (p_α); b,c) transient states ($p_\sigma^{ee'}$ and $p_\sigma^{e,-e}$). Centering is indicated by arrow. Defective sites are encircled

Kinetic equation for excess particle monomer (lattice dimension d is shown explicitly):

$$\begin{cases} \dot{p}_\alpha = -2d(2d-1)q^{-1}p_\alpha + q^{1-2d}\sum_{e\neq e'} p_{\alpha-e}^{ee'}, \\ \dot{p}_\sigma^{ee'} = -2q^{1-2d}p_\sigma^{ee'} + q^{-1}(p_{\sigma+e} + p_{\sigma+e'}), \quad e' \neq e. \end{cases} \tag{5}$$

Kinetic equation for flip-flop pairs

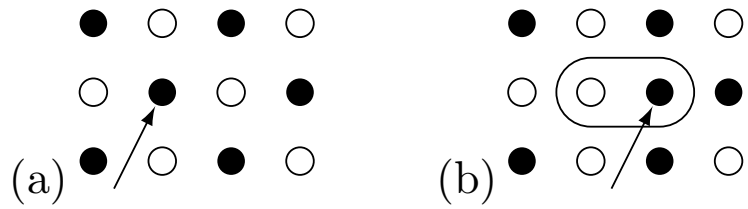


Fig. 7: Essential configurations for flip-flop pairs ((a) – p_0, (b) – p_e)

Kinetic equation:

$$\begin{cases} \dot{p}_0 = -2dp_0 + q^{1-2d}p_e, \\ \dot{p}_e = -q^{1-2d}p_e + p_0. \end{cases} \tag{6}$$

Fluctuations in probe area

Correlation function for fluctuations of number of atoms in a probe area:

$$\langle \delta N(t) \delta N(0) \rangle = n_e \sum_{x,y} G_{x-y} \left(4tq^{-1} \right) + n_v \sum_{x,y} G_{x-y}(4t) + O(q^3), \quad (7)$$

where G is given by its Fourier transform with $d = 2$:

$$G(t,k) = \exp \left\{ \frac{t}{d} \left[\left(\sum_{i=1}^{d} \cos k_i \right)^2 - d^2 \right] \right\} \quad (8)$$

and

$$n_{e,v} = \sqrt{\left(c - \frac{1}{2} \right)^2 + q^4} \pm \left(c - \frac{1}{2} \right) + O(q^4) \quad (9)$$

(upper sign is for excess particle monomers).

Validation by MC simulations. I

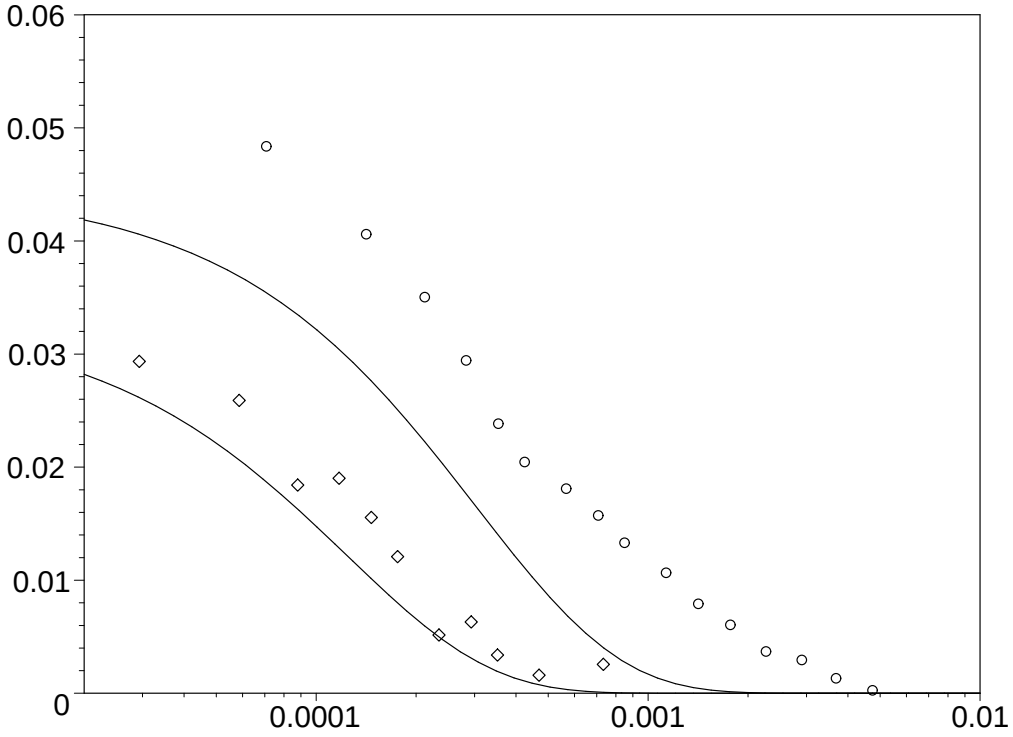


Fig. 8: Relative contribution of fluctuations due to flip-flop jumps for $L = 6$ and $\phi = \{2.41, 2.70, 3.00\}$ (from top to bottom), points denote MC data

Validation by MC simulations. II

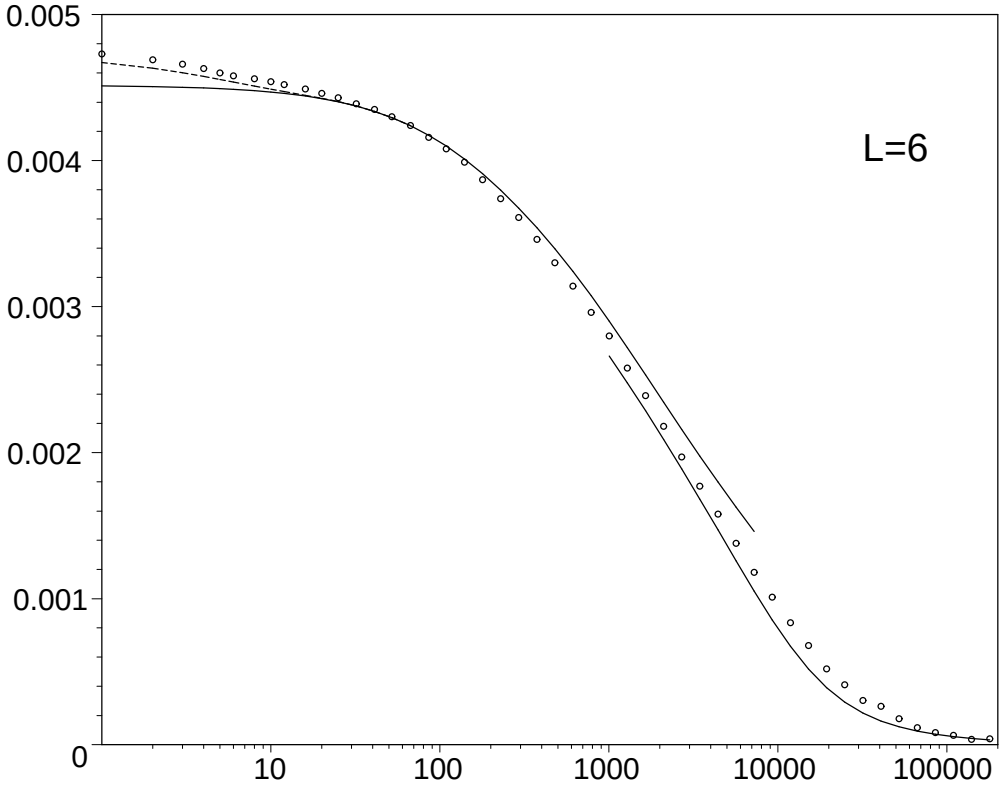


Fig. 9: Absolute value of fluctuations per site vs. MC steps for $L = 6$, $\phi = 2.70$, $c = 0.5$

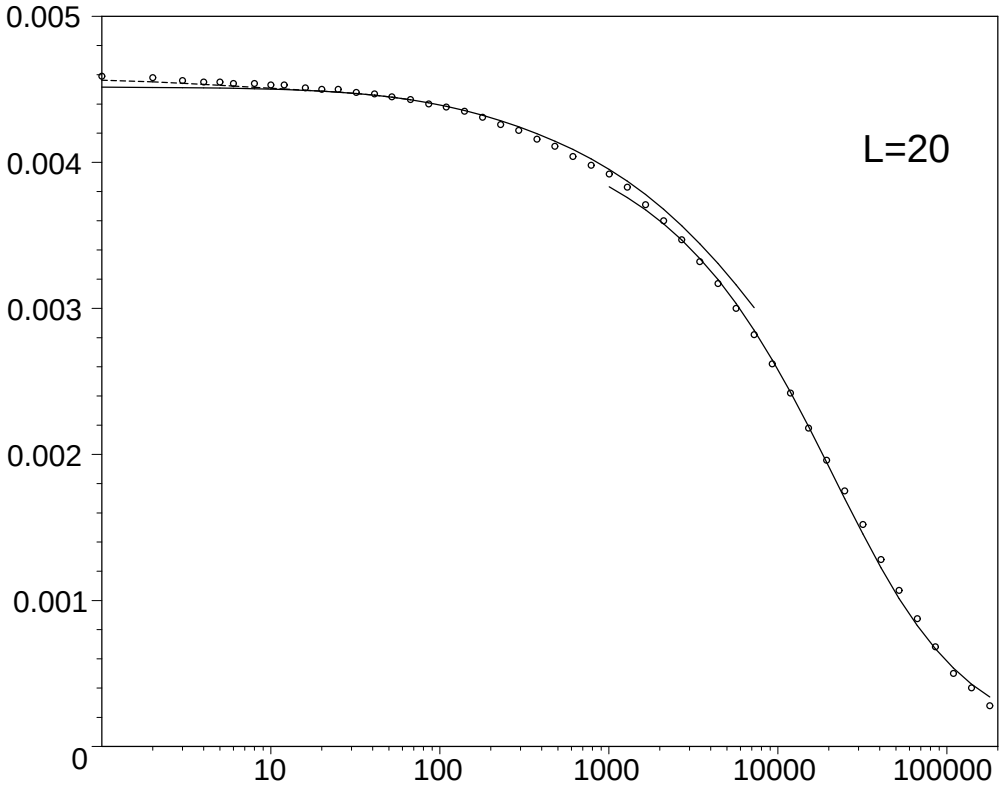


Fig. 10: Absolute value of fluctuations per site vs. MC steps for $L = 20$, $\phi = 2.70$, $c = 0.5$