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Correlation functions in a one-dimensional kinetic Ising model

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Abstract. In the limit of the strong magnetic field $H \to \infty$, the closed hierarchy of kinetic equations for correlation functions of an arbitrary order is derived for a one-dimensional kinetic Ising model. This hierarchy allows asymptotically exact solution in quadratures. For the first time the closed set of equation for generating functions of the domain distribution of the identically oriented spins have been obtained. The relations between kinetic parameters that make it possible to find exact solutions in quadratures are indicated.

1. Introduction

The Ising model being the simplest one among the models of cooperative phenomena has a significant place in theoretical physics and is described in many monographs and studies on statistical mechanics [1–5]. The equilibrium states, along with relaxational processes in different physical systems, can be presented in the terms of this model [6–9]. The original Ising model [10] was proposed for a description of the equilibrium magnetics whose microstate is characterized by the spin configuration on the one-dimensional lattice with each spin oriented along or opposite to the external magnetic field. In this model the interaction energy of the spins in an arbitrary configuration is equal to the sum of the interaction energy of the pairs' neighbour spins. After extension the field of applicability of the Ising model to non-equilibrium systems can be characterized by the probability of spin flip depending only on the orientation of its nearest neighbours. The theory of the equilibrium and non-equilibrium Ising model allows the calculation of the correlation function along with average magnetization [2, 3, 5, 8, 9]. The formalism of the Ising model has a wide application in adsorption, non-ideal gases, binary alloys etc [2, 3, 5–7]. Many problems in physics (calculation of unperturbed sizes and dipole moments of linear macromolecules along with their relaxational characteristics [11–14]), biophysics (description of helix-coli transition in biopolymers [15–18]) and chemical physics (calculation of equilibrium and kinetics of adsorption or chemical reaction on macromolecules of the small polymer molecules [19–22]) can be described in the framework of the kinetic Ising model. In this case the analogue of spin configuration is the infinite sequence of two symbols A and B, whose sense depends on the specifics of the problems under consideration [23]. In these terms the general one-dimensional kinetic Ising model is determined according to the scheme

$$\begin{array}{ccc} AAA & AAB & BAB \\ k_0 \downarrow\uparrow \tilde{k}_2 & k_1 \downarrow\uparrow \tilde{k}_1 & k_2 \downarrow\uparrow \tilde{k}_0 \\ ABA & ABB & BBB. \end{array} \tag{1}$$

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The six parameters $k_i, \tilde{k}_i$ $(i = 0, 1, 2)$, are the probabilities of corresponding transitions per unit time.

At the present time the exact solution of the kinetic Ising model at arbitrary values of the six parameters has not been found and the theoretical investigations in this field are connected with either development of approximation methods or using simplified modifications of a general model which have exact solutions [9]. The best known among these modifications was proposed by Glauber [24]. It corresponds to the following relations between kinetic parameters

$$2k_1 - k_0 - k_2 = 0 \qquad 2\tilde{k}_1 - \tilde{k}_0 - \tilde{k}_2 = 0 \qquad k_1\tilde{k}_0 = k_0\tilde{k}_1. \tag{2}$$

The relation (2) leads to thermodynamical equality for the rates of the elementary transformations (1)

$$k_a k_c = k_b^2 \tag{3}$$

$$k_a = \frac{\tilde{k}_0}{k_0} \qquad k_b = \frac{\tilde{k}_1}{k_1} \qquad k_c = \frac{\tilde{k}_2}{k_2}. \tag{4}$$

The conditions (2) upon the kinetic parameters of model (1) leave only three of them independent. Such parameters in Glauber's model [24] are the following

$$\alpha = \tilde{k}_1 + k_1 \qquad \beta = \frac{\tilde{k}_1 - k_1}{\tilde{k}_1 + k_1} \qquad \gamma = \frac{k_1 - k_0 + \tilde{k}_1 - \tilde{k}_0}{\tilde{k}_1 + k_1}. \tag{5}$$

α is equal to the average spin flip frequency, while the rest—β and γ—characterize equilibrium. Parameter $\beta = \tanh(H/T)$ depends on the relation of the energy of spin (μH), with the magnetic moment $\mu = 1$ in a magnetic field H, to temperature T, whereas $\gamma = \tanh(2J/T)$ is determined by the difference of interaction energy $2J$ between parallel and antiparallel spin configurations of the neighbour spins.

The exact analytical solution for two [24] and higher [25] points correlators in the Glauber model have been found only for the absence of magnetic field ($H = 0$), when

$$k_0 = \tilde{k}_0 \qquad k_1 = \tilde{k}_1 \qquad k_2 = \tilde{k}_2 \qquad \alpha = 2k_1 \qquad \beta = 0 \qquad \gamma = \frac{k_1 - k_0}{k_1}. \tag{6}$$

Keller [26] had proposed the second exact solvable case of the kinetic Ising model. It is determined by the following relationships

$$\tilde{k}_0 = \tilde{k}_1 = \tilde{k}_2 = 0 \tag{7}$$

which allow spin flips in only one direction [26]. In equilibrium due to condition (7) all spins have an orientation along the magnetic field. Therefore only the investigation of relaxational processes has theoretical interest. For the first time the problem of time evolution of probability $P(A)$ in a one-dimensional lattice of state A (equal to the problem of average magnetization dynamics) in the framework of the second model was solved by Keller [26] who used an arbitrary assumption, and after that, more rigorously, in [27]. The exact solution for the two-point correlation function was obtained in [28], and independently in [29]. In principle, algorithms, suggested in cited papers, make it possible to write down the equations for correlations of an arbitrary order, but require cumbersome probabilistic considerations. For this reason the authors of [28, 29] did not present equations for correlators whose order exceeds two.

The probabilistic approaches used in [28, 29], are based on considerations of all possible channels of transformations leading to the change of configurations of two-symbol sequences

and also on the fundamental property of statistical independence of arbitrary sequences U and V separated by AA dyad

$$P(UAAV) = \frac{P(UAA)P(AAV)}{P(AA)} \tag{8}$$

where $P(\ldots)$ represents the probability of the corresponding sequence. For the first time relation (8) was rigorously proved by Mityushin [30], and later was independently obtained in [31], where it was referred to as the 'shielding property' of AA dyad. Mityushin's proof of theorem (8) was based on considerations of Markovian processes with continuous time on space of the infinite two-symbols sequences, whose well developed mathematical theory [30, 32–34] is not efficient enough for obtaining a useful result in physics.

Our approach, proposed for the solution of the Keller model (7), is a traditional one, widely applied in theoretical physics for descriptions of magnetics with Pauli master equation. The first part of this paper contains general formulations of this approach to a one-dimensional kinetic Ising model (1). In the second part we demonstrate the truncation of an infinite equation hierarchy for correlation functions by the example of one- and two-point correlators. After that we present general equations for correlators of an arbitrary order and their generating functions which allow exact analytical solutions in quadratures. The third part contains the derivation of a closed system of partial derivative equations for generating the function of probability distribution by length of one-type symbol blocks and its exact solution for some particular cases.

2. General formulation of one-dimensional kinetic Ising model

Let us consider an infinite one-dimensional lattice contained in every ith site spin $\boldsymbol{\sigma}_i$, oriented along or opposite to an external magnetic field. Two values of a spin variable $\sigma_i = \pm 1$ correspond to the orientations of vector $\boldsymbol{\sigma}_i$. The system microstate is represented by the spin configuration $\{\sigma_i\}$, i.e. the concrete orientation of all spins in the sites of the lattice. The time evolution of probability $P(\{\sigma_i\}; t)$ of the system in microscopic state $\{\sigma_i\}$ at the time t is governed by the master equation [35]

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\{\sigma_i\}; t) = -\sum_i \Lambda_i^+ P(\{\ldots, \sigma_i, \ldots\}; t) + \sum_i \Lambda_i^- P(\{\ldots, -\sigma_i, \ldots\}; t). \tag{9}$$

The kinetic coefficients Λ_i^+ and Λ_i^- are correspondingly equal to the infinitesimal probability of spin flip from state σ_i to $-\sigma_i$ and *vice versa*, while other spins remain fixed. The concrete design of functions Λ_i^+, Λ_i^- is determined by the choice of model. In a general kinetic Ising model (1) the probability Λ_i^+ depends (apart from spin variable σ_i) on variables σ_{i-1} and σ_{i+1}

$$\begin{aligned}\Lambda_i^+ = {} & \tfrac{1}{8}(1+\sigma_i)\{(k_0 + k_2 - 2k_1)\sigma_{i-1}\sigma_{i+1} + (k_0 - k_2)(\sigma_{i-1} + \sigma_{i+1}) + (k_0 + k_2 + 2k_1)\} \\ & + \tfrac{1}{8}(1-\sigma_i)\{(\tilde{k}_0 + \tilde{k}_2 - 2\tilde{k}_1)\sigma_{i-1}\sigma_{i+1} + (\tilde{k}_2 - \tilde{k}_0)(\sigma_{i-1} + \sigma_{i+1}) \\ & + (\tilde{k}_0 + \tilde{k}_2 + 2\tilde{k}_1)\}\end{aligned} \tag{10}$$

and Λ_i^- can be obtained from Λ_i^+ by formal substitution σ_i for $-\sigma_i$.

The traditional approach which uses spin variables $\sigma_i = \pm 1$, is especially convenient for kinetic problems in the absence of a magnetic field, when the probability of both spin orientations are equal. When considering the problems with broken symmetry, it is convenient to apply other spin variables

$$s_i = \frac{1 + \sigma_i}{2} \tag{11}$$

which take values 0, 1. Thus, in this case each microscopic state of the system is represented by the given two-symbols sequence 1, 0 (or A, B). Instead of the traditional identity $\sigma_i^2 = 1$, the spin algebra in new variables (11) is determined by the following one

$$s_i^2 = s_i. \tag{12}$$

As may be proved by direct calculation, the stationary solution of the master equation (9) is the standard Gibbs distribution

$$P(\{\sigma_i\}) = \frac{1}{\mathcal{Z}} \exp\left\{\frac{J}{T}\sum_k \sigma_k\sigma_{k+1} + \frac{H}{T}\sum_k \sigma_k\right\} \tag{13}$$

where $\mathcal{Z}$ is the partition function of a system. One needs to express in relations (10) the kinetic parameters $\tilde{k}_i$ in terms of k_i using expressions (4) and equilibrium constants of elementary transformations (1)

$$k_a = \exp\left\{\frac{(4J+2H)}{T}\right\} \qquad k_b = \exp\left\{\frac{2H}{T}\right\} \qquad k_c = \exp\left\{\frac{(-4J+2H)}{T}\right\}. \tag{14}$$

It is evident that the exponential index in each of the expressions (14) corresponds to the change of free energy of the system, i.e.

$$\triangle F_k = 2J(\sigma_{k-1} + \sigma_{k+1}) + 2H \tag{15}$$

due to a flip of the kth spin, situated in the middle of triads (1). The right-hand side of equation (9) will be a linear form in parameters k_i $(i = 0, 1, 2)$. It is easy to check that the coefficients of this form are equal to zero at arbitrary values of the equilibrium parameters J and H. The statistical weight of any equilibrium configuration $\{\sigma_i\}$, characterized by the exponent in expression (13) resolves into a product of factors dependent upon the configuration of pairs of the neighbouring spins. Thus the expression for a normalized constant $\mathcal{Z}$ in (13) can be presented as the product of the transfer matrices $\mathbf{V}_k$ [5]

$$\begin{pmatrix} \exp((J+H)/T) & \exp((J-H)/T) \\ \exp((J-H)/T) & \exp((-J-H)/T) \end{pmatrix}. \tag{16}$$

Not only has the general solution of equation (9) not been found in the non-equilibrium case, but expressions for the time evolution of the average magnetization and correlation functions have only been obtained in a very few cases. Among all other correlators which have by definition the meaning to find the given symbols in the fixed sites of a one-dimensional lattice, it is sufficient without loss of generality to consider only the special type of correlation functions

$$\langle s_{i_1} s_{i_2} \ldots s_{i_n}\rangle = \sum_{\{s_i\}} s_{i_1} s_{i_2} \ldots s_{i_n} P(\{s_i\}; t) \tag{17}$$

when there are symbols A (or 1) in $i_1, i_2, \ldots, i_n$ sites. Because of stoichiometric conditions all other n-point correlation functions can be expressed in terms of correlators (17) and analogous ones of lower order.

In order to simplify the derivation of kinetic equations for correlation functions (17) we present the generating function as follows

$$\Psi(\{h_i\}; t) = \sum_{\{s_i\}} P(\{s_i\}; t) \exp\left\{\sum_j h_j^+ s_j + h_j^-(1 - s_j)\right\} \tag{18}$$

where h_j^+, h_j^- are the components of field h_j, conjugated to variable s_j. The correlators of an arbitrary order n can be obtained due to the relation

$$\langle s_{i_1} s_{i_2} \ldots s_{i_n}\rangle = \frac{\partial^n \Psi(\{h_i\}; t)}{\partial h_{i_1}^+ \ldots \partial h_{i_n}^+} \tag{19}$$

where after taking the nth derivative of function $\Psi(\{h_i\};t)$ with respect to corresponding fields one has to set all h_i to zero.

In order to obtain the equation for the generating function $\Psi(\{h_i\};t)$ one has to multiply both sides of the master equation (9) (written in variables $\{s_i\}$) by $\exp\{\sum_j h_j^+ s_j + h_j^-(1-s_j)\}$ and average them on all possible symbol sequences. As a result we obtain differential equations in partial derivatives of the third order

$$\frac{\partial}{\partial t}\Psi(\{h_i\};t) = -\sum_j \left\{[1-\exp(h_j^- - h_j^+)]\hat{D}_j^+ + [1-\exp(h_j^+ - h_j^-)]\hat{D}_j^-\right\}\Psi(\{h_j\};t) \quad (20)$$

where the differential operator is

$$\hat{D}_j^+ = \frac{\partial}{\partial h_j^+}\left[(k_0+k_2-2k_1)\frac{\partial^2}{\partial h_{j-1}^+ \partial h_{j+1}^+} + (k_1-k_2)\left(\frac{\partial}{\partial h_{j-1}^+} + \frac{\partial}{\partial h_{j+1}^+}\right) + k_2\right] \quad (21)$$

and $\hat{D}_j^-$ is formed from $\hat{D}_j^+$ by formal substitution h_j^+ on h_j^- and all of k_α on $\tilde{k}_\alpha$ ($\alpha = 0, 1, 2$).

Taking term by term the derivatives of both parts (20) with respect to the corresponding fields, setting all h_i to zero and using the simple operator equality

$$\frac{\partial}{\partial h_j^-} = 1 - \frac{\partial}{\partial h_j^+} \quad (22)$$

that enables us to eliminate the derivative on h_j^-, we obtain the hierarchy of kinetic equations for correlation functions (17). In the general case this infinite hierarchy is not closed, because the right-hand side of these equations will contain correlators of subsequently higher orders than those on the left-hand side. But, in at least two special cases of a kinetic Ising model it is possible to break the mentioned infinite hierarchy of equations. These cases are the Glauber model (2) and the Keller model (7), which have the following transition probabilities (10), respectively

$$\Lambda_i^G = \tfrac{1}{2}\alpha[(1+\beta)[1-\gamma+\gamma(s_{i-1}+s_{i+1})] + 2(\gamma-\beta)s_i - 2\gamma s_i(s_{i-1}+s_{i+1})] \quad (23)$$

$$\Lambda_i^K = s_i[(k_0+k_2-2k_1)s_{i-1}s_{i+1} + (k_1-k_2)(s_{i-1}+s_{i+1}) + k_2]. \quad (24)$$

The transition probabilities (23) and (24) for both of the models depend on three parameters, but the degree of polynomial Λ_i^k in variables s_i is one unit higher than degree of polynomial Λ_i^G.

3. Equations for correlations functions

The method of truncation of equation hierarchy for correlation functions can be easily demonstrated by example one and two-point correlators. To begin we write down these equations for the Glauber model

$$\frac{\mathrm{d}\langle s_i\rangle}{\mathrm{d}(\alpha t)} = -(1-\gamma\beta)\langle s_i\rangle - \gamma\beta(\langle s_{i-1}s_i\rangle + \langle s_i s_{i+1}\rangle) + \frac{1}{2}(1+\beta)[1-\gamma+\gamma(\langle s_{i-1}\rangle + \langle s_{i+1}\rangle)] \quad (25)$$

$$\frac{\mathrm{d}\langle s_i s_k\rangle}{\mathrm{d}(\alpha t)} = -2(1-\gamma\beta)\langle s_i s_k\rangle - \gamma\beta(\langle s_{i-1}s_i s_k\rangle + \langle s_i s_{i+1}s_k\rangle + \langle s_i s_{k-1}s_k\rangle + \langle s_i s_k s_{k+1}\rangle) + \frac{1}{2}(1+\beta)[(1-\gamma)(\langle s_i\rangle + \langle s_k\rangle) + \gamma(\langle s_{i-1}s_k\rangle + \langle s_{i+1}s_k\rangle + \langle s_i s_{k-1}\rangle + \langle s_i s_{k+1}\rangle)] \qquad (i \neq k) \quad (26)$$

and the Keller model

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle s_i\rangle = -k_2\langle s_i\rangle + (k_2-k_1)(\langle s_{i-1}s_i\rangle + \langle s_i s_{i+1}\rangle) + (2k_1-k_0-k_2)\langle s_{i-1}s_i s_{i+1}\rangle \tag{27}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle s_i s_k\rangle = -2k_2\langle s_i s_k\rangle + (k_2-k_1)(\langle s_{i-1}s_i s_k\rangle + \langle s_i s_{i+1}s_k\rangle + \langle s_i s_{k-1}s_k\rangle + \langle s_i s_k s_{k+1}\rangle)$$
$$+(2k_1-k_0-k_2)(\langle s_{i-1}s_i s_{i+1}s_k\rangle + \langle s_i s_{k-1}s_k s_{k+1}\rangle) \qquad (i\neq k). \tag{28}$$

It is worth noting that these sets of equations are not formally closed, because correlators on the right-hand side of the equations have higher order than those on the left-hand side. For the Glauber model the closed equations hierarchy can be obtained in two limiting cases, corresponding either to zero or infinite magnetic field

$$\text{(a) } H=0,\beta=0 \qquad \text{(b) } H=\infty,\beta=-1. \tag{29}$$

It is noteworthy that case (b) was not considered either in Glauber's original paper [24], or in its following generalizations. We shall not consider it specially, because it reduces to the Keller model at the following values of its kinetic parameters

$$k_1=\alpha \qquad k_0=\alpha(1-\gamma) \qquad k_2=\alpha(1+\gamma). \tag{30}$$

It is possible to obtain the closed set of equations for one- and two-point correlators in the Keller model due to its shielding property (8) and its consequences [30]

$$P(UA^n) = P(UAA)(1-\theta)^{n-2} \qquad \theta = 1-\exp(-k_0 t) \qquad (n\geqslant 2). \tag{31}$$

In its original paper [30] the proof of theorem (8) was based on the general theory of Markovian processes with local interactions [34]. The alternative method of proof of statistical independence property (8), based on direct analysis of master equation (9), is presented in the appendix. Let us now demonstrate the truncation of the equation hierarchy for correlation functions of the first two orders (27) and (28) using this shielding property.

It is easy to note that according to (31) the three-point correlator on the right-hand side of equation (27) can be expressed in terms of a two-point correlator

$$\langle s_{i-1}s_i s_{i+1}\rangle = \langle s_i s_{i+1}\rangle(1-\theta). \tag{32}$$

The equation for this two-point correlator can be found from (28) at $k=i+1$. The right-hand side of the last equation contains besides $\langle s_{i-1}s_i s_{i+1}\rangle$ only identical correlator $\langle s_i s_{i+1}s_{i+2}\rangle$, which can be expressed according to (32) in terms of the two-point correlation functions. Thus, using expression (32) we obtain the closed set of two equations for correlators $\langle s_i\rangle$ and $\langle s_i s_{i+1}\rangle$. Taking into account the fact that we consider only translational invariant solutions of the master equations (9) (because Mityushin's theorem (8) holds only for these ones) the mentioned correlators $P(A)$ and $P(AA)$ do not depend on index i. Turning to the equation for a two-point correlator (28), we note that due to uniformity and isotropy of the one-dimensional system under consideration the two-point correlation function will depend only on the absolute value of the difference $n=|k-i|$ coordinates of lattice sites. The case of $n=1$ was considered above. At $n>1$ the highest order of correlators on the right-hand side of equation (28) will be equal to three, because all the four-point correlators can be eliminated via expressions

$$\begin{aligned}\langle s_{i-1}s_i s_{i+1}s_k\rangle &= \langle s_i s_{i+1}s_k\rangle(1-\theta) = P(A^3X^{n-2}A)\\ &= P(A^2X^{n-2}A)(1-\theta) = P(AX^{n-2}A^2)(1-\theta) = P(AX^{n-2}A^3)\\ &= \langle s_i s_{k-1}s_k\rangle(1-\theta) = \langle s_i s_{k-1}s_k s_{k+1}\rangle\end{aligned} \tag{33}$$

which are evident from (31). Hereinafter the symbol X represents either or both symbols, A, B. In turn, deriving the equations for three-point correlators (33) one finds them unclosed

since right-hand sides of these equations will contain four- and five-point correlators. These latter can be expressed through the former ones via equations

$$\langle s_{i-1}s_is_{i+1}s_ks_{k+1}\rangle = \langle s_is_{i+1}s_ks_{k+1}\rangle(1-\theta) = P(A^3X^{n-2}A^2) = P(A^2X^{n-2}A^2)(1-\theta)$$
$$= P(A^2X^{n-2}A^3) = \langle s_{i-1}s_is_{k-1}s_k\rangle(1-\theta) = \langle s_{i-1}s_is_{k-1}s_ks_{k+1}\rangle. \tag{34}$$

The equations for the above-mentioned four-point correlators are closed due to property (31). Thus we have the set of three linear differential equations for correlation functions $P(AX^{n-1}A)$, $P(AX^{n-1}AA)$ and $P(AAX^{n-1}AA)$ with time-dependent coefficients [28].

The equations for correlators (17) of an arbitrary order can be obtained by taking a term-by-term derivatives of both parts of equation (20) (in the case of the Keller model $\hat{D}_j^- \equiv 0$), with respect to its corresponding fields

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle s_{i_1}s_{i_2}\dots s_{i_n}\rangle = -nk_2\langle s_{i_1}s_{i_2}\dots s_{i_n}\rangle + (k_2-k_1)\sum_{k=1}^{n}(\langle s_{i_1}s_{i_2}\dots s_{i_k-1}s_{i_k}\dots s_{i_n}\rangle$$
$$+\langle s_{i_1}s_{i_2}\dots s_{i_k}s_{i_k+1}\dots s_{i_n}\rangle) + (2k_1-k_0-k_2)\sum_{k=1}^{n}\langle s_{i_1}s_{i_2}\dots s_{i_k-1}s_{i_k}s_{i_k+1}\dots s_{i_n}\rangle$$
$$i_1 \neq i_2 \neq \dots \neq i_n. \tag{35}$$

Taking into account the translational invariance of the considered system, we define the $(n+1)$-point correlation function as follows

$$P({}_1\boldsymbol{f}_n) = P(AX^{f_1}AX^{f_2}\dots AX^{f_n}A) = \langle s_{i_0}s_{i_1}\dots s_{i_n}\rangle \tag{36}$$

where $f_k = i_k - i_{k-1} - 1$, $f_k \geqslant 0, k = 1,\dots,n$. This function is the probability of sequence

$$U_n^{\alpha\beta}(\boldsymbol{f}) \equiv A^\alpha X^{f_1}AX^{f_2}\dots AX^{f_n}A^\beta = \sum_{\{U\}} A^\alpha U_{f_1}AU_{f_2}\dots AU_{f_n}A^\beta \tag{37}$$

of $(n+1)$ symbols A, separated by distances $f_1,\dots,f_n$ from each other at $\alpha,\beta = 1$. The sum in (37) is taken over all possible sets $\{U_{f_i}\}$ of sequences $U_{f_1}, U_{f_2},\dots,U_{f_n}$, comprised, correspondingly from $f_1, f_2,\dots,f_n$ symbols. The equation for the correlator (36) follows immediately from (35)

$$(1-\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}P({}_1\boldsymbol{f}_n) = \sum_{j=1}^{n+1}(1-\delta(f_{j-1},0))(1-\delta(f_j,0))\Big\{(r-q-1)P({}_1\boldsymbol{f}_n)$$
$$+\left(\frac{q-2r}{2}\right)[P({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1},0,{}_j\boldsymbol{f}_n) + P({}_1\boldsymbol{f}_{j-1},0,{}_j\boldsymbol{f}_n-\boldsymbol{e}_j)]$$
$$+rP({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1},0,0_j,\boldsymbol{f}_n-\boldsymbol{e}_j)\Big\} + \sum_{j=1}^{n}\sum_{k=j}^{n}T(j,k) \tag{38}$$

where the following designations are used

$$q = 2(k-1) \qquad r = 2k-k'-1 \qquad k = k_1/k_0 \qquad k' = k_2/k_0$$
$$T(j,k) = \phi(j,k)\Big\{(j-k-q-2)P({}_1\boldsymbol{f}_{j-1},{}_j0_k,{}_{k+1}\boldsymbol{f}_n)$$
$$+\frac{q}{2}(P({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1},0,{}_j0_k,{}_{k+1}\boldsymbol{f}_n) + P({}_1\boldsymbol{f}_{j-1},{}_j0_k,0,{}_{k+1}\boldsymbol{f}_n-\boldsymbol{e}_{k+1}))\Big\}$$
$$\phi(j,k) = (1-\delta(f_{j-1},0))\left(\prod_{\mu=j}^{k}\delta(f_\mu,0)\right)(1-\delta(f_{k+1},0)) \tag{39}$$

and for compactness of formulae we formally denote

$$P({}_1\boldsymbol{f}_0, {}_j0_k, {}_{k+1}\boldsymbol{f}_n) = P({}_j0_k, {}_{k+1}\boldsymbol{f}_n) = P({}_1\boldsymbol{f}_n)\prod_{\mu=1}^{k}\delta(f_\mu, 0)$$

$$P({}_1\boldsymbol{f}_0, {}_j0_n, {}_{n+1}\boldsymbol{f}_n) = P({}_1\boldsymbol{f}_{j-1}, {}_j0_n) = P({}_1\boldsymbol{f}_n)\prod_{\mu=j}^{n}\delta(f_\mu, 0)$$

$$P({}_1\boldsymbol{f}_0, {}_00_k, {}_{n+1}\boldsymbol{f}_n) = P({}_00_n) = P({}_1\boldsymbol{f}_n)\prod_{\mu=1}^{n}\delta(f_\mu, 0)$$

$$P({}_1\boldsymbol{f}_{j-1}, {}_j0_k, {}_{k+1}\boldsymbol{f}_n) = P({}_1\boldsymbol{f}_n)\prod_{\mu=j}^{k}\delta(f_\mu, 0) \qquad f_0 = 1, \quad f_{n+1} = 1 \tag{40}$$

and $\boldsymbol{e}_j$ is a vector with jth component equal to 1, and all others are equal to zero. The correlator $P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0, {}_j\boldsymbol{f}_n)$ represents the probability of finding the sequence formed from $U_n^{11}(\boldsymbol{f})$ by adding one A symbol to the left from the jth A symbol. In the same manner function $P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0, 0, {}_j\boldsymbol{f}_n - \boldsymbol{e}_j)$ represents the probability of sequence formed from $U_n^{11}(\boldsymbol{f})$ by adding to it two A symbols, one to the left and one to the right from jth A symbol. The shielding property (8) of the Keller model enables us to write down these correlators as follows

$$P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0, {}_j\boldsymbol{f}_n) = [P(AA)]^{-1}P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0)P(0, {}_j\boldsymbol{f}_n)$$

$$P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0, 0, {}_j\boldsymbol{f}_n - \boldsymbol{e}_j) = (1-\theta)[P(AA)]^{-1}P({}_1\boldsymbol{f}_{j-1} - \boldsymbol{e}_{j-1}, 0)P(0, {}_j\boldsymbol{f}_n - \boldsymbol{e}_j) \tag{41}$$

where the probability of finding the AA dyad is given by the expression [27, 28]

$$P(AA) = (1-\theta)^{q+2}\exp(q\theta). \tag{42}$$

Although the relationships (41) allow us to lower the order of the majority of correlators on the right-hand side of equation (38), however, the hierarchy of equations (38) is not formally closed because its right-hand side contains correlators $P(0, {}_1\boldsymbol{f}_n)$ and $P({}_1\boldsymbol{f}_n, 0)$. The order of these correlators is one unit higher than order of correlator $P({}_1\boldsymbol{f}_n)$ on the left-hand side of equation (38). The mentioned correlation function describe the probability of sequences $U_n^{21}(\boldsymbol{f})$ and $U_n^{12}(\boldsymbol{f})$ (37), respectively. In its turn the right-hand side of the equations for $P(0, {}_1\boldsymbol{f}_n)$ and $P({}_1\boldsymbol{f}_n, 0)$ contain correlators $P(0, {}_1\boldsymbol{f}_n, 0)$, which represent the probability of finding the sequence $U_n^{22}(\boldsymbol{f})$ (37). Finally, the hierarchy for correlators $P(0, {}_1\boldsymbol{f}_n, 0)$ turns out to be closed in the manner similar to the considered case of two-point correlator. Entering the notation

$$P({}_1\boldsymbol{f}_n) = P_{11}({}_1\boldsymbol{f}_n) \qquad P(0, {}_1\boldsymbol{f}_n) = P_{21}({}_1\boldsymbol{f}_n) \qquad P({}_1\boldsymbol{f}_n, 0) = P_{12}({}_1\boldsymbol{f}_n)$$
$$P(0, {}_1\boldsymbol{f}_n, 0) = P_{22}({}_1\boldsymbol{f}_n) \tag{43}$$

we write down the final form of the closed set of equations for correlators (43)

$$(1-\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}P_{\alpha\beta}({}_1\boldsymbol{f}_n) = P_{\alpha\beta}({}_1\boldsymbol{f}_n)\{(1-\delta(f_1,0))\eta_1(\alpha) + (1-\delta(f_n,0))\eta_1(\beta)\}$$
$$+\eta_2(\alpha)(1-\delta(f_1,0))P_{2\beta}({}_1\boldsymbol{f}_n) + \eta_2(\beta)(1-\delta(f_n,0))P_{\alpha 2}({}_1\boldsymbol{f}_n)$$
$$+\eta_3(\alpha)(1-\delta(f_1,0))P_{2\beta}({}_1\boldsymbol{f}_n - \boldsymbol{e}_1) + \eta_3(\beta)(1-\delta(f_n,0))P_{\alpha 2}({}_1\boldsymbol{f}_n - \boldsymbol{e}_n)$$

$$+\sum_{j=2}^{n}(1-\delta(f_{j-1},0))(1-\delta(f_j,0))\Big\{(r-q-1)P_{\alpha\beta}({}_1\boldsymbol{f}_n)$$
$$+[P(AA)]^{-1}\Big[\left(\frac{q-2r}{2}\right)[P_{\alpha 2}({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1})P_{2\beta}({}_j\boldsymbol{f}_n)$$
$$+P_{\alpha 2}({}_1\boldsymbol{f}_{j-1})P_{2\beta}({}_j\boldsymbol{f}_n-\boldsymbol{e}_j)]+r(1-\theta)P_{\alpha 2}({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1})P_{2\beta}({}_j\boldsymbol{f}_n-\boldsymbol{e}_j)\Big]\Big\}$$
$$+[P(AA)]^{-1}\sum_{j=1}^{n}\sum_{k=j}^{n}Q_{\alpha\beta}(j,k) \tag{44}$$

where the following designations are used

$$Q_{\alpha\beta}(j,k)=\phi(j,k)(1-\theta)^{k-j}\Big\{d_{\alpha\beta}(j,k)P_{\alpha 2}({}_1\boldsymbol{f}_{j-1})P_{2\beta}({}_{k+1}\boldsymbol{f}_n)$$
$$+\frac{q}{2}(1-\theta)(P_{\alpha 2}({}_1\boldsymbol{f}_{j-1}-\boldsymbol{e}_{j-1})P_{2\beta}({}_{k+1}\boldsymbol{f}_n)+P_{\alpha 2}({}_1\boldsymbol{f}_{j-1})P_{2\beta}({}_{k+1}\boldsymbol{f}_n-\boldsymbol{e}_{k+1}))\Big\}$$
$$\eta_1(\rho)=(2-\rho)r-q-\rho+\frac{q}{2}(1-\theta)(\rho-1)$$
$$\eta_2(\rho)=\frac{1}{2}(q-2r)(2-\rho)$$
$$\eta_3(\rho)=\frac{1}{2}(q-2r)(1-\theta)^{\rho-1}+r(1-\theta)$$
$$d_{\alpha\beta}(j,k)=j-k-q-2+(1-\alpha)\delta(j,1)+(1-\beta)\delta(k,n) \tag{45}$$

and the extensions of definition (36) introduced as follows

$$P_{\alpha 2}({}_1\boldsymbol{f}_0)=P_{\alpha 2}({}_1\boldsymbol{f}_0-\boldsymbol{e}_0)=(1-\theta)^{\alpha-1}P(AA)$$
$$P_{2\beta}({}_{n+1}\boldsymbol{f}_n)=P_{2\beta}({}_{n+1}\boldsymbol{f}_n-\boldsymbol{e}_{n+1})=(1-\theta)^{\beta-1}P(AA).$$

To obtain the analytical solution for equation (44) it is convenient to construct the generating functions as follows

$$G_{\alpha\beta}({}_1\boldsymbol{x}_n)=\sum_{\boldsymbol{f}}P_{\alpha\beta}({}_1\boldsymbol{f}_n)\prod_{k=1}^{n}x_k^{f_k}\qquad(\alpha,\beta=1,2). \tag{46}$$

The functions G_{11} are of major importance for the statistical thermodynamics of polymers, because they determine (in momentum space) the coefficients of the Landau expansion of the free energy of the macromolecule solution formed by the cooperative chemical reaction under the scheme (1) [36]. To obtain the equations for the generating functions (46) one has to multiply both sides of equation (44) by $x_1^{f_1}x_2^{f_2}\ldots x_n^{f_n}$ and take the sum over all values of variables $f_1, f_2, \ldots, f_n$

$$(1-\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}G_{\alpha\beta}({}_1\boldsymbol{x}_n)=\{\eta_1(\alpha)+\eta_1(\beta)+(n-1)(r-q-1)\}G_{\alpha\beta}({}_1\boldsymbol{x}_n)$$
$$+\{\eta_2(\alpha)+\eta_3(\alpha)x_1\}G_{2\beta}({}_1\boldsymbol{x}_n)+\{\eta_2(\beta)+\eta_3(\beta)x_n\}G_{\alpha 2}({}_1\boldsymbol{x}_n)$$
$$-\{\eta_2(\alpha)(1-\theta)+\eta_1(\alpha)(1-\theta)^{\alpha-1}\}G_{2\beta}({}_2\boldsymbol{x}_n)$$
$$-\{\eta_2(\beta)(1-\theta)+\eta_1(\beta)(1-\theta)^{\beta-1}\}G_{\alpha 2}({}_1\boldsymbol{x}_{n-1})$$
$$+[P(AA)]^{-1}\Big\{\sum_{j=2}^{n}F_{\alpha\beta}+\sum_{j=1}^{n}\sum_{k=j}^{n}R_{\alpha\beta}(j,k)\Big\}$$

$$F_{\alpha\beta} = \rho(x_{j-1}, x_j)G_{\alpha 2}({}_1\boldsymbol{x}_{j-1})G_{2\beta}({}_j\boldsymbol{x}_n) + \lambda(x_{j-1})G_{\alpha 2}({}_1\boldsymbol{x}_{j-1})G_{2\beta}({}_{j+1}\boldsymbol{x}_n)$$
$$+\lambda(x_j)G_{\alpha 2}({}_1\boldsymbol{x}_{j-2})G_{2\beta}({}_j\boldsymbol{x}_n) + (r-q-1)(1-\theta)G_{\alpha 2}({}_1\boldsymbol{x}_{j-2})G_{2\beta}({}_{j+1}\boldsymbol{x}_n)$$
$$R_{\alpha\beta}(j,k) = (1-\delta(x_{j-1},0))(1-\delta(x_{k+1},0))(1-\theta)^{k-j}$$
$$\times\left[d_{\alpha\beta}(j,k) + \frac{q}{2}(1-\theta)(x_{j-1}+x_{k+1})\right]G_{\alpha 2}({}_1\boldsymbol{x}_{j-1})G_{2\beta}({}_{k+1}\boldsymbol{x}_n) \tag{47}$$

where besides those presented in (45) the following designations are used

$$\rho(a,b) = \tfrac{1}{2}(q-2r)(a+b) + r(1-\theta)ab$$
$$\lambda(a) = q - r + 1 - \tfrac{1}{2}(q-2r)(1-\theta)a$$

and formal extensions of definition (46) introduced as follows

$$G_{\alpha 2}({}_1\boldsymbol{x}_0) = P(AA)(1-\theta)^{\alpha-1} \qquad G_{2\beta}({}_{n+1}\boldsymbol{x}_n) = P(AA)(1-\theta)^{\beta-1}$$
$$x_0 = x_{n+1} = 1. \tag{48}$$

Because at $\theta = 0$ initial infinite sequences consist of only A symbols the initial condition for generating function (46) is as follows

$$G_{\alpha\beta}({}_1\boldsymbol{x}_n) = \prod_{k=1}^{n}\left[\frac{1}{(1-x_k)}\right].$$

It is essential that equations (47) are linear with respect to functions $G_{\alpha\beta}({}_1\boldsymbol{x}_n)$, because all nonlinear terms contain the generating functions of correlators of lower order than those on the left-hand side of (47). This circumstance makes it possible to find solutions for the generating functions of the correlators of an arbitrary order n and therefore correlation functions, with knowledge of all the generating functions of correlators of lower orders. Thus the set of equations (47) allows exact analytical solution in quadratures. As an example we present the set of equations for the generating functions of the three-point correlators $G_{11}, G_{12} = G_{21}, G_{22}$

$$(1-\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}G_{\alpha\beta}({}_1\boldsymbol{x}_2) = [\eta_1(\alpha) + \eta_1(\beta) + (r-q-1)]G_{\alpha\beta}({}_1\boldsymbol{x}_2)$$
$$+[\eta_2(\alpha) + \eta_3(\alpha)x_1]G_{2\beta}({}_1\boldsymbol{x}_2) + [\eta_2(\beta) + \eta_3(\beta)x_2]G_{\alpha 2}({}_1\boldsymbol{x}_2)$$
$$+w(\alpha, x_2)G_{2\beta}({}_2\boldsymbol{x}_2) + w(\beta, x_1)G_{\alpha 2}({}_1\boldsymbol{x}_1)$$
$$+[P(AA)]^{-1}\rho(x_1,x_2)G_{\alpha 2}({}_1\boldsymbol{x}_1)G_{2\beta}({}_2\boldsymbol{x}_2) + P(AA)(1-\theta)^{\alpha+\beta-1}$$
$$\times[r-2q-2-\alpha-\beta+q(1-\theta)] \qquad (\alpha,\beta = 1,2) \tag{49}$$

where besides those presented in (45) and (48) the following designations are used

$$w(\mu,z) = (1-\theta)^{\mu-1}\left\{\lambda(z) + (1-\delta(z,0))[-q-1-\mu+\frac{q}{2}(1-\theta)(1+z)] - \eta_1(\mu)\right\}$$
$$-(1-\theta)\eta_2(\mu). \tag{50}$$

4. The domain length distribution of the identically oriented spins

In this section we consider in the framework of the Keller model, the problem of finding the probabilities of B-clusters, i.e. contiguous sequences of symbols B framed by A symbols

$$P(AB^nA) \qquad n \geqslant 0. \tag{51}$$

Although the probabilities of the contiguous sequences of A symbols can be obtained exactly in the general case [27], the solution for the probabilities of finding the B-clusters has not

been found at the present time. Different approximations have been used for this problem's solution: the 'B-approximation' [28], is based on an arbitrary assumption of the statistical independence of any sequences separated by the AB dyad. Using this approximation, whose area of application remains unknown, authors [28] have obtained the closed set of nonlinear equations for the probabilities of finding B-clusters and presented their numerical simulations at different values of kinetic parameters. Another approach was suggested by Evans *et al* [37]. In this framework one has to express the probability $P(AB^nA)$ in terms of correlators (36) using the stoichiometric relations, and then write down the exact sets of equations for these correlators, whose number dramatically increases as n grows. Performing this procedure, Nord *et al* [37] found probabilities $P(AB^n)A$ for $n \leqslant 11$ by solving numerically the hundreds of differential equations.

To find the probabilities of $P(AB^nA)$ we propose an original approach. First, we extend the definition of B-clusters distinguishing them in number of the A symbols which frame contiguous sequence of B-symbols. Thus we shall consider the generalized B-clusters $A^\alpha B^n A^\beta$, where indices α and β may take values 1 and 2. We demonstrate that the equations for correlators' generating function (47) can be used to obtain a *closed* set consisting of partial differential equations of first order for generating functions of probabilities of the generalized B-clusters. The derivation of this set of equations starts with the stoichiometric identity which can be easily proved by induction:

$$P(UB^nV) = P(UX^nV) - \sum_{\alpha=0}^{n-1} P(UB^\alpha AX^{n-\alpha-1}V) \tag{52}$$

where U and V are arbitrary sequences. Choosing in (52) $U = V = A$, we obtain

$$P(AB^nA) = P(AX^nA) - \sum_{\alpha=0}^{n-1} P(AB^\alpha AX^{n-\alpha-1}A). \tag{53}$$

Using the equality (52) with $U = A$, $V = AX^{n-\alpha-1}A$, we can write down

$$P(AB^nA) = P(AX^nA) - \sum_{\alpha=0}^{n-1} P(AB^\alpha AX^{n-\alpha-1}A) + \sum_{\alpha=0}^{n-1}\sum_{\beta=0}^{\alpha-1} P(AB^\beta AX^{\alpha-\beta-1}AX^{n-\alpha-1}A). \tag{54}$$

The sequential use of this procedure leads to the formula

$$P(AB^nA) \equiv P_{11}^B(n) = \sum_{s=0}^{n}(-1)^s \sum_{f_1=0}^{n-s} \cdots \sum_{f_{s+1}=0}^{n-s} \delta\left(n - s - \sum_{\lambda=1}^{s+1} f_\lambda\right) P_{11}({}_1\boldsymbol{f}_{s+1}) \tag{55}$$

where the probabilities of finding B-clusters are linearly expressed in terms of the correlators (36) and (43). Now we define the following generating functions

$$G_{\alpha\beta}(y;\boldsymbol{x}) = \sum_{n=0}^{\infty} y^n G_{\alpha\beta}({}_1\boldsymbol{x}_{n+1}) \qquad \alpha\beta = 1, 2. \tag{56}$$

Using the relationship

$$G_{\alpha\beta}^B(x) = G_{\alpha\beta}(-x; x_1 = x, x_2 = x, \ldots, x_n = x, \ldots) \tag{57}$$

we express in terms of (56) the generating functions of the probabilities of generalized B-clusters

$$G_{\alpha\beta}^B(x) = \sum_{n=0}^{\infty} x^n P_{\alpha\beta}^B(n). \tag{58}$$

To obtain the relation (57) relating generating functions (56) to (58), one has to multiply both sides of expression (55) by x^n and carry out the sum over all $n \geqslant 0$.

For the functions

$$g_{\alpha\beta}(y,x) = G_{\alpha\beta}(-y; x_1 = x, x_2 = x, \ldots, x_n = x, \ldots) \tag{59}$$

which are equal to generating functions of the probabilities of generalized B-clusters (58) at $y = x$, the following set of the partial differential equations has been derived

$$\begin{aligned}\left[(1-\theta)\frac{\partial}{\partial\theta} + (q-r+1)\frac{\partial}{\partial y}\right] g_{\alpha\beta}(y,x) &= g_{\alpha\beta}(y,x)[2(r-q-1) - (\alpha+\beta-2)a(\theta)] \\ &+ b(\theta)[g_{2\beta}(y,x)(2-\alpha) + g_{\alpha 2}(y,x)(2-\beta)] \\ &+ \left[\frac{1}{P(AA)}\right] c(\theta) g_{\alpha 2}(y,x) g_{2\beta}(y,x) + P(AA)(1-\theta)^{\alpha+\beta-2} \\ &\times [q - r + r\delta_{\alpha\beta}(\alpha+\beta-3) + r(1-\theta)(4-\alpha-\beta-y)]\end{aligned} \tag{60}$$

where the following designations are used

$$\begin{aligned}a(\theta) &= r + 1 - (1-\theta)\left[\frac{q}{2}(1+x) - (q-r)y\right] + ry(y-x)(1-\theta)^2 \\ b(\theta) &= \frac{1}{2}(q-2r)(1+x-2y) + r(1-\theta)(1-y)(x-y) \\ c(\theta) &= y(y-x)[q - 2r - r(y-x)(1-\theta)].\end{aligned} \tag{61}$$

The set of equations (60) can be derived by multiplying equations (47) term by term by $(-y)^n$ and carrying the sum over all possible values of n. When the solution of equation set (60) is obtained, it is possible to find the required generating function of the probabilities of generalized B-clusters using the relationship

$$G^B(x) \equiv G^B_{11}(x) = g_{11}(x,x). \tag{62}$$

The equation set (60) can be solved sequentially. At first one has to find the solution of the equation for $g_{22}(y,x)$, and then substitute it in the equation for $g_{12}(y,x)$, whose solution, in turn, is inserted into the equation for $g_{11}(y,x)$. This procedure forces us to find the solution of the nonlinear problem at the first step. If we succeed in solving this problem then finding the functions $g_{12}(y,x)$ and $g_{22}(y,x)$ will reduce to quadratures.

As usual, to solve the partial differential equation set we use the method of characteristics [38]. Along the characteristics the equation for the function $g_{22}(y,x)$ comprises the well known Riccatti equation, which enables the exact solution in the special case of the simplified Keller model, when its parameters k_0, k_1, k_2 in arithmetic progression. In the case when r (39) is equal to zero we have found the partial solution of the Riccatti equation. This enables us to find its general solution and to obtain generating functions of the probabilities of generalized B-clusters in an explicit form

$$g_{\alpha\beta}(y,x) = (1-\theta)^{\alpha+\beta-3} P(AA) \frac{\Phi(y,x)}{y(1+\Phi(y,x))} \tag{63}$$

where the following notation is used

$$\Phi(y,x) = y(1-\theta)^{q+1}\exp(qx\theta)\left(\frac{1}{1-x} + q\int_0^\theta \mathrm{d}z(1-z)^{-q-1}\exp(-qxz)\right). \tag{64}$$

It is worth noting that expression (63) can be derived in another way based on the property of statistical independence (8) and its consequence (31), which in the case of $r = 0$ takes the form [30]

$$P(UAV) = \frac{P(UA)P(AV)}{P(A)} \qquad P(UA^n) = P(UA)(1-\theta)^{n-1} \qquad n \geqslant 1 \tag{65}$$

where $P(A) = (1-\theta)^{q+1}\exp(q\theta)$ [27, 28]. The stoichiometric identity (53), taking into account condition (65), is written as follows

$$P(AB^nA) = P(AX^nA) - [P(A)]^{-1}\sum_{\alpha=0}^{n-1} P(AB^\alpha A)P(AX^{n-\alpha-1}A). \tag{66}$$

Multiplying both sides of (65) by x^n and taking the sum over $n \geqslant 0$, we obtain a simple expression

$$G_{11}^B(x) = \frac{G_{11}(x)}{1 + x[P(A)]^{-1}G_{11}(x)} \qquad G_{11}(x) \equiv G_{11}({}_1x_1) = x^{-1}P(A)\Phi(x,x) \tag{67}$$

connecting $G_{11}^B(x)$ (62) with the generating function $G_{11}({}_1x_1)$ of the two-point correlators $P(AX^nA)$. It is known [22, 29] that in the case of the simplified model, correlators $P(AX^nA) \approx (q\theta)^n/(n!)$, as $n \to \theta$, i.e. this demonstrates decay sharper than exponential. The asymptotical decay of the probability $P(AB^nA)$ is determined by the singular points of the generating function (63) and (67). At positive values of $q \ll 1$ we obtain $P(AB^nA) \approx \theta^n$ as $n \to \infty$. At large values of q the probability $P(AB^nA)$ asymptotically decays exponentially (as $n \to \infty$); $P(AB^nA) \approx \theta^n$ as $\theta \to 1$ and if $\theta \to 0$ then $P(AB^nA)$ decays as $(q\theta)^n$ [37].

It is possible to find the explicit form of the generating functions of the probabilities of generalized B-clusters in another partial case at $r - q - 1 = 0$, when equation (60) is reduced to a set of ordinary differential equations. In this case the factor at partial derivative with respect to y vanishes so after setting $y = x$ in equations (60) we obtain the linear differential equation set for functions $g_{\alpha\beta}(x,x)$. Integrating the equation for $g_{22}(x,x)$, $g_{12}(x,x)$, $g_{11}(x,x)$ subsequently, we get

$$\begin{aligned} G^B(x) = g_{11}(x,x) &= P(AA) + \frac{4x(1-x)}{[q-(q+2)x]^2}[P(AA)-1] \\ &\quad + x\left[1 + \frac{2(1-x)[4-(q+2)^2(1-x)]}{[q-(q+2)x]^2}\right] \\ &\quad \times \int_0^\theta \mathrm{d}z(1-z)^{q+2}\exp(qz) + \frac{4(q+2)x(1-x)}{[q-(q+2)x]^2} I(0,\theta\, x) \\ &\quad + x\int_0^\theta \mathrm{d}z(1-z)^{-q}\exp(-(q+2)xz)[I(z,\theta,x)]^2 \\ I(z,\theta,x) &= \frac{1}{2}(q+2)(1-x)\int_z^\theta \mathrm{d}t(1-t)^{q+1}\exp\left\{\frac{1}{2}[q+(q+2)x]t\right\}. \end{aligned} \tag{68}$$

When $q = 0$ it is possible to integrate the set of equations (68) exactly and obtain

$$\begin{aligned} G^B(x) &= \frac{1}{2}(1+(1-\theta)^2) + \frac{1}{x}\left(\theta - \theta^2 + \frac{\theta^3}{3}\right) - \frac{1}{x^2}\left(\theta - \frac{\theta^2}{2}\right) \\ &\quad + \frac{1}{2}\left(\frac{1-x}{x}\right)^2\left[\exp(2x\theta)\left(1-\theta+\frac{1}{x}\right)^2 - \left(\frac{1+x}{x}\right)^2\right]. \end{aligned} \tag{69}$$

Expanding (69) as a series in the powers of x we get

$$\begin{aligned} P(AB^nA) &= \frac{1}{2}(1-\theta)^2\delta_{n,0} + \frac{2^{n+1}\theta^n}{(n+2)!} \\ &\quad \times\left[\frac{(n+1)(n+2)}{4}(1-\theta)^2 + n\theta(1-\theta) + \frac{n}{n+4}\theta^4\right]. \end{aligned} \tag{70}$$

Let us note that the probabilities of finding B-clusters and sequences of the contiguous symbols B (so called B-tuplets) are connected by the simple stoichiometric relationship; $P(AB^nA) = P(B^n) - 2P(B^{n+1}) + P(B^{n+2}), n \geqslant 1$, where $P(B^n)$ denotes the probability of the corresponding tuplet. This relationship allows us to express the generating function

$$g^B(x) = \sum_{n=1}^{\infty} P(B^n)x^n \tag{71}$$

in terms of generating function (69)

$$g^B(x) = \frac{x^2}{(x-1)^2}\left[G^B(x) - 1 - \frac{1}{x}[1 + P(A)]\right]. \tag{72}$$

Substituting (69) into (72) we obtain

$$g^B(x) = \frac{1}{2}\left[(1-\theta)^2 - 1 + \exp(2x\theta)\left(1 - \theta + \frac{1}{x}\right)^2 - \left(1 + \frac{1}{x}\right)^2\right]. \tag{73}$$

Expanding (73) as a power series leads to the formula

$$P(B^n) = \frac{2^{n+1}\theta^n}{(n+2)!}\left[\frac{(n+1)(n+2)}{4}(1-\theta)^2 + (n+2)\theta(1-\theta) + \theta^2\right] \tag{74}$$

which was obtained in [39] by a different method. It is noteworthy, that when $r = 0$ and $q = -1$, i.e. $k' = 0, k = 1/2$, both discussed cases coincide. Therefore, we can use (63) and (64) to obtain

$$G^B(x) = \frac{1}{x}\exp(-\theta)[1 - (1-x)\exp(x\theta)] \qquad P(AB^nA) = \frac{\theta^n}{n!}\left[1 - \frac{\theta}{n+1}\right]\exp(-\theta). \tag{75}$$

Analysis of (68) shows that

$$P(AB^nA) \approx (q+2)^n\frac{\theta^n}{n!} \tag{76}$$

as $n \to \infty$, in accordance with the results obtained in [39].

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Appendix

In order to obtain the simple proof of the Mityushin theorem (8), we use the approach suggested in [22, 40] for determining the probability

$$P(A^n) \equiv P_n(t) \tag{A1}$$

to find the sequence of n symbols A, in the framework of the Keller model. The authors of [22, 27], having written the exact set of equations for $P_n(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t}P_n(t) = -[2k_1 + (n-2)k_0]P_n(t) + 2(k_1 - k_0)P_{n+1}(t) \qquad n \geqslant 2 \tag{A2}$$

found that its solution, subject to the initial condition $P_n(0) = 1$, is

$$P_n(t) = P_2(t)\exp[-(n-2)k_0 t] \qquad n \geqslant 2 \tag{A3}$$

which enabled them to reduce the infinite equations hierarchy (A2) to one easily solved equation for $P(AA)$. We generalize this approach to consider the probability of finding the sequences $A^\alpha U_m A^\beta$

$$P(A^\alpha U_m A^\beta) \equiv P_{\alpha,\beta}(U_m; t) \tag{A4}$$

where (U_m) is an arbitrary sequence comprised of m symbols. Indices α, β meet the following inequalities

$$(1)\ \alpha \geqslant 0, \beta \geqslant 2 \qquad (2)\ \alpha \geqslant 2, \beta \geqslant 0 \tag{A5}$$

meaning that there are not less than two A symbols framing the U_m sequence. Without loss of generality let us restrict our further consideration to the first case of (A5). The evolution of function $P_{\alpha,\beta}(U_m; t)$ is governed by the following equation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}P_{\alpha,\beta}(U_m; t) &= [(\delta_{\alpha 0} - 1)\phi_1(U, 1, \alpha) - k_1 - (\beta - 2)k_0 - k_1\delta_U^m(B) - k_0\delta_U^m(A)]P_{\alpha,\beta}(U_m; t) \\ &\quad -(\delta_{\alpha 0} - 1)\phi_2(U, 1, \alpha)P_{\alpha+1,\beta}(U_m; t) + (k_1 - k_0)P_{\alpha,\beta+1}(U_m; t) \\ &\quad -\delta_{\alpha 0}[\delta_U^1(A) - \delta_U^1(B)]\{[k_2\delta_U^2(B) + k_1\delta_U^2(A)]P_{\alpha+1,\beta}(U_{m-1}; t) \\ &\quad -z_U^2 P_{\alpha+2,\beta}(U_{m-1}; t)\} - \sum_{j=1}^{m}\Lambda_{j,\alpha}^{+}P_{\alpha,\beta}(U_m; t) + \sum_{j=1}^{m}\Lambda_{j,\alpha}^{-}P_{\alpha,\beta}(U_m^{(j)}; t)\end{aligned} \tag{A6}$$

where the following notation is used

$$z_U^i = (k_2 - k_1)\delta_U^i(B) + (k_1 - k_0)\delta_U^i(A)$$

$$\Lambda_{j,\alpha}^{\pm} = \Lambda_j^{\pm}(1 - \delta_{\alpha 0}\delta_{j1})$$

$$\phi_1(U, i, \nu) = [k_1 + (\nu - 2)k_0 + k_1\delta_U^i(B) + k_0\delta_U^i(A) + \delta_{\nu 1}(k_0 - k_1 + z_U^i)]$$

$$\phi_2(U, i, \nu) = (k_1 - k_0)(1 - \delta_{\nu 1}) + \delta_{\nu 1}z_U^i. \tag{A7}$$

Equation (A6) is derived from master equation (9) with regard to (A3). Herein the sequence $U_m^{(j)}$ is formed from sequence U_m by substitution of the jth symbol for the opposite one $(A \leftrightarrow B)$. The symbol $\delta_u^i(A)$ is equal to 1 only if the ith symbol of (U_m) sequence is A, otherwise $\delta_u^i(A)$ is equal to 0. In the same manner, the symbol $\delta_U^i(B)$ is not equal to zero only if the ith place of the sequence U_m is occupied by B. Taking into account that initially all spins have orientation opposite to the magnetic field, which corresponds to an infinite initial sequence of A symbols, then $P_{\alpha,\beta}(U_m; 0) = 1$ for all α, β and U_m. Thus, the solution of equation (A6) for all sequences U_m satisfying the above initial condition, takes the form

$$P_{\alpha,\beta}(U_m; t) = \begin{cases} P_{2,2}(U_m; t)\exp[-(\alpha + \beta - 4)k_0 t] & \alpha, \beta \geqslant 2 \\ [8pt]P_{\alpha,2}(U_m; t)\exp[-(\beta - 2)k_0 t] & \alpha = 0, 1, \quad \beta \geqslant 2 \end{cases} \tag{A8}$$

which makes it possible to reduce the infinite hierarchy equation (A6) to a set of a finite number of equations for the functions $P_{\alpha,\beta}(U_m; t)$ for all sequences (U_m) at the following

indice values: $\alpha = 0, 1, 2, \beta = 2$. The described procedure is useful when we prove the Mityushin theorem. In order to do this we present the function

$$R_{\alpha,\beta}(U_m, V_l; t) = P(A^\alpha U_m A A V_l A^\beta) P(AA) - P(A^\alpha U_m AA) P(AA V_l A^\beta) \tag{A9}$$

specified for any non-negative values of indices α, β and for pairs of arbitrary sequences (U_m) and (V_l), consisting of m and l symbols A and B, respectively. The equation for the description of $R_{\alpha,\beta}(U_m, V_l; t)$ time evolution is

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} R_{\alpha,\beta}(U_m, V_l; t) = \Bigg[& (\delta_{\alpha 0} - 1)\phi_1(U, 1, \alpha) + (\delta_{\beta 0} - 1)\phi_1(V, l, \beta) - k_1[\delta_U^m(B) + \delta_V^1(B)] \\
& - k_0[\delta_U^m(A) + \delta_V^1(A)] + 2(k_1 - k_0)\exp(-k_0 t) - \sum_{j=1}^{m} \Lambda_{j,\alpha}^{+} - \sum_{j=1}^{l} \Lambda_{j,\beta}^{+} \Bigg] \\
& \times R_{\alpha,\beta}(U_m, V_l; t) - (\delta_{\alpha 0} - 1)\phi_2(U, 1, \alpha) R_{\alpha+1,\beta}(U_m, V_l; t) \\
& - (\delta_{\beta 0} - 1)\phi_2(V, l, \beta) R_{\alpha,\beta+1}(U_m, V_l; t) - \delta_{\alpha 0}[\delta_U^1(A) - \delta_U^1(B)] \\
& \times \{[k_2 \delta_U^2(B) + k_1 \delta_U^2(A)] R_{\alpha+1,\beta}(U_{m-1}, V_l; t) - z_U^2 R_{\alpha+2,\beta}(U_{m-1}, V_l; t)\} \\
& - \delta_{\beta 0}[\delta_V^l(A) - \delta_V^l(B)]\{[k_2 \delta_V^{l-1}(B) + k_1 \delta_V^{l-1}(A)] R_{\alpha,\beta+1}(U_m, V_{l-1}; t) \\
& - z_V^{l-1} R_{\alpha,\beta+2}(U_m, V_{l-1}; t)\} \\
& + \sum_{j=1}^{m} \Lambda_{j,\alpha}^{-} R_{\alpha,\beta}(U_m^{(j)}, V_l; t) + \sum_{j=1}^{l} \Lambda_{j,\beta}^{-} R_{\alpha,\beta}(U_m, V_l^{(j)}; t)
\end{aligned} \tag{A10}$$

where in addition to the notation presented in (A7), the following notations is used

$$\Lambda_{j,\beta}^{\pm} = \Lambda_j^{\pm}(1 - \delta_{\beta 0}\delta_{jl}) \tag{A11}$$

as derived from master equation (9) with regard to (A3) and (A8). The sequences $U_m^{(j)}$ and $V_l^{(j)}$ are formed correspondingly from the sequences U_m and V_l by substitution of the jth symbol for the opposite one ($A \leftrightarrow B$). The symbol $\delta_U^i(A)$ has the same meaning as $\delta_u^i(A)$ provided sequence (U_m) is replaced by V_l. In the same manner the symbol $\delta_V^i(A)$ is not equal to zero only if the ith place of sequence V_l is occupied by A. It is evident, taking into account the fact that at initial time $U_m = A^m$, $V_l = A^l$, that the function $R_{\alpha,\beta}$, $\alpha, \beta \geqslant 0$, (A9) is equal to zero at $t = 0$. Similarly from (A8) we shall find the solution of equation (A10) satisfying the mentioned initial condition for all the sequences U_m and V_l as follows

$$R_{\alpha,\beta}(U_m; t) = \begin{cases} R_{2,2}(U_m; t)\exp[-(\alpha + \beta - 4)k_0 t] & \alpha, \beta \geqslant 2 \\ [6pt] R_{\alpha,2}(U_m; t)\exp[-(\beta - 2)k_0 t] & \alpha = 0, 1, \quad \beta \geqslant 2 \\ [6pt] R_{2,\beta}(U_m; t)\exp[-(\alpha - 2)k_0 t] & \alpha \geqslant 2, \quad \beta = 0, 1. \end{cases} \tag{A12}$$

This substitution allows us to obtain the closed sets of equations for the functions $R_{\alpha,\beta}(U_m, V_l; t)$, given at manifolds of all the sequences $\{U_m\}$ and $\{V_l\}$ at the indice values $\alpha, \beta = 0, 1, 2$. These sets have the following structure: the right-hand side of the equation for $R_{0,0}$ contains functions $R_{1,0}$, $R_{0,1}$, $R_{2,0}$ and $R_{2,0}$. The right-hand side of the equations for functions $R_{0,1}$ and $R_{1,0}$ contains functions $R_{2,0}$, $R_{1,1}$, $R_{2,1}$ and $R_{2,0}$, $R_{1,1}$, $R_{1,2}$ correspondingly. The right-hand side of the equations for functions $R_{2,0}$ and $R_{2,0}$ contains corresponding functions $R_{2,1}$, $R_{2,2}$ and $R_{1,2}$, $R_{2,2}$. The right-hand side of the equations

for functions $R_{1,1}$, contains functions $R_{2,1}$ and $R_{1,2}$, and their equations contain on the right-hand side functions $R_{2,2}$. At last, the set of equations for functions $R_{2,2}$ is closed:

$$\frac{\mathrm{d}}{\mathrm{d}t}R_{2,2}(U_m, V_l; t) = -R_{2,2}(U_m, V_l; t)\Bigg[4k_1 + 2(k_1 - k_0)\exp(-k_0 t) + k_1[\delta_U^1(B) + \delta_U^m(B) + \delta_V^1(B) + \delta_V^l(B)] + k_0[\delta_U^1(A) + \delta_U^m(A) + \delta_V^1(A) + \delta_V^l(A)] + \sum_{j=1}^{m}\Lambda_j^+ + \sum_{j=1}^{l}\Lambda_j^+\Bigg] + \sum_{j=1}^{m}\Lambda_j^- R_{2,2}(U_m^{(j)}, V_l; t) + \sum_{j=1}^{l}\Lambda_j^- R_{2,2}(U_m, V_l^{(j)}; t). \tag{A13}$$

It is clear from (A13) that if the function $R_{2,2}(U_m, V_l; 0) = 0$, it will remain equal to zero at all times. This statement is evident because the linear homogeneous finite set of ordinary differential equations with zero initial conditions has only trivial solutions. This last circumstance allows us to obtain a linear uniform set of equations for functions $R_{1,2}$ and $R_{2,1}$, which also has only a trivial solution at zero initial conditions. In the same way, it is not difficult to demonstrate that at zero initial conditions all the other functions $R_{\alpha,\beta}, \alpha, \beta = 0, 1, 2$ will be equal to zero, and among them the function $R_{0,0}$. According to (A9) the last result ends the alternative derivation of theorem (8), proved for the first time by Mityushin [30].

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