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ONE EXACTLY SOLVABLE MODEL OF CHEMICALLY REACTIVE SYSTEM ON 1D PARTIALLY FILLED LATTICE

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It is well known that one-dimensional (1D) models can be an effective tool for solving many problems in statistical mechanics. For instance a particular attention in such areas as chemical reactions, random walks and aggregation problems has been paid to the role of dimensionality. We study the effects of low dimensional constrains of model reactive systems. We present an exactly solvable model of fluctuational dynamics in bimoleculary reactive, partially filled, 1D perfect lattice. A rigorous expressions have been obtained for the probability distribution function, average numbers of particles, mean square fluctuations, configurational entropy and statistical sum. The previous data for Ising model of 1D nonreactive lattice gas adsorption have been completed by getting a rigorous expression for configurational statistical sum. We found that in the case of vacancied chemically reactive lattice, like in the case of exclusion statistics , distribution function has a chiral form, expressed in terms of Jacobi polynomials or Gauss confluent functions. It is shown that the nonlinearity of the reaction radically change the expected mean-field behavior. We show considered system is nonergodic with respect to chemical dynamics, and has a steady state, with a not a mean-field ratio of the average numbers of particles, which approached asymptotically. Obtained results also contrastly display coupling between microscopic processes and collective behavior as described by the macrovariables

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1. INTRODUCTION

One-dimensional models are known to be an effective tool for solving a variety of problems in statistical mechanics. In particular, large attention in such areas as chemical reactions, random walks and aggregation problems (but not only) is devoted to the role of dimensionality in the dynamical evolution. It has been shown [1, 2], that restricting space to low dimension can cause deviations from the mean field behavior, depending on the type of the nonlinearity involved. In this systems deviations from mean field (MF) behavior might be expected due to reduced effective mobility of the reactants. Along this line we perform here an explicit calculation of the distribution function of 1D bimolecularly, chemically reactive lattice which include the random vacancies by means of conditional probability method. The 1D lattice gas adsorption model will be considered first, to obtain a rigorous expression for corresponding configurational statistical sum. An explicit expression for distribution function in the case of chemically reactive adsorbed gas is expressed in form of Jacobi polynomials. This chiral form of distribution function, which is typical for the systems with an exclusion statistics is shown to appear also in the case 1D lattice adsorbed reactive gas, (where the vacancies distribution is random.)

2. BIMOLECULARY REACTIVE TOTALLY FILLED LATTICE

Consider bimoleculary reactive system $A+B \Leftrightarrow 2X$ in one dimension. We stipulate, that particles of type A, can change their sort into X, whenever they feel the presence of X particles. And similarly for X particles. The simplest reaction model consist of particles A and X occupying the sites of one-dimensional lattice, one particle per lattice site, with either periodic or fixed boundary condition. We first assume that these are no vacant sites on the lattice. We start with a one-dimensional lattice of size M. As initial condition we consider a uniform configuration containing only X particles. Let us call the number of deferent ways of putting N_A particles A in 1D lattice of size M as distribution function, denoted by $g_M(N_A)$. Because in the considered model (which is ergodic) all possible configurations are allowed. Then $g_M(N_A)$ would be equal to combinational factor $\binom{M}{N_A}$. Performing the normalization one has

$$g_M\left(N_A\right)=\binom{M}{N_A}/\left(2^M-1\right). \qquad (1)$$

Thus, the average number of A particles in a chain of size M, under the arbitrary boundary conditions can be estimated as

$$\langle N_A \rangle = \sum_{N_A=0}^{M-1} N_A \binom{M}{N_A} / \left(2^M - 1\right). \qquad (2)$$

Making normalization

$$g_M\left(N_A\right) = \binom{M}{N_A} / \sum_{N_A=0}^{M-1} \binom{M}{N_A},$$

we leave one state should not be occupied by *A* particles, because of dynamic (totally filled lattice with only *A* particles is a "frozen'', i.e. nonergodic state). And similarly for $\langle N_X \rangle$. Note, that obviously, we have a sum rule : $N_X + N_A = M$, and thus $\langle N_X \rangle + \langle N_A \rangle = M$. Form (2) it is follows that the ratio $r = \dfrac{\langle N_A \rangle}{\langle N_X \rangle}$

$$r = 1 - \frac{1}{2^M - 1} \to 1 \qquad (3)$$
$$as \qquad M \to \infty.$$

Thus, this quantity attains its mean-field value $r = 1$. In addition to this known result [4] we are now in the position to perform a calculations of the mean system fluctuations of the numbers of given particles $\langle N_A^2 \rangle$, $\langle N_X^2 \rangle$ of given sorts which occur due to chemical reaction. Namely, we have

$$\langle N_A^2 \rangle = \frac{\sum_{N_A=0}^{M-1} N_A^2 \binom{M}{N_A}}{2^M - 1} = \frac{M^2}{4}\left(1 - \frac{1}{2^M - 1}\right)^2 \to \frac{M^2}{4}. \qquad (4)$$

One can compute a covariance matrix of the fluctuations around the mean particle numbers on the form (2), (4)

$$\left\langle \left(\Delta N_A\right)^2 \right\rangle = \langle N_A^2 \rangle - \langle N_A \rangle^2 =$$
$$= \frac{M}{4}\left[\frac{1 - \left(M+1\right) \times 2^{-M}}{\left(1 - 2^{-M}\right)^2}\right] \to \frac{M}{4} \qquad (5)$$
$$as \qquad M \to \infty.$$

On the same way, one can perform also correlation function of the fluctuations of the numbers of deferent particles $\langle \Delta N_A \Delta N_X \rangle$. Namely, taking into account Eqs. (4) and (2), we obtain

$$\langle \Delta N_X \Delta N_A \rangle = \langle N_A^2 \rangle - \langle N_A \rangle^2 =$$
$$= -\frac{M}{4}\left[\frac{1 - \left(M+1\right) \times 2^{-M}}{\left(1 - 2^{-M}\right)^2}\right] \to -\frac{M}{4} \qquad (6)$$
$$as \qquad M \to \infty.$$

In Eq.(6), the negative sign means that because of bimolecular character of the reaction, if particle of sort *A* appears, then particle of sort *X* disappears from the lattice.

Thus it is clear that the bimolecularly reactive 1D lattice shows mean-field behavior already in one dimension (at least as far as the steady state properties are concerned). This system is ergodic over all the state space except for the state which consist entirely of *A* particles. This unique configuration is frozen and cannot be reached from any other configuration with the Morkovian evolution rules adopted. In the classification of the states familiar from Markov chains those frozen state qualified as a closed class consisting a single adsorbing state.

The mean square fluctuations in 1D totally filled bimolecularly reacted perfect lattice, as well as correlations of fluctuations of the numbers of particle behave normal and not anomalous. In the next paragraph we go to study partially filled lattice expecting the deviations from given above scenario. As it will be shown, along this line an exact results could be obtained.

3. EXACTLY SOLVABLE MODEL FOR 1D LATTICE GAS ADSORPTION

In this section we consider the classical problem of gas adsorption in 1D perfect lattice, first in the case, in which individual sites (or subsystems) were independent of each other and then when interactions between the nearest neighbor sites exist. Second neighbor and higher interactions are important in some cases but, here, we shall confine ourselves to particular models without intersite interactions or with nearest-neighbor interactions only because especially these models can be solved exactly. In the development of classical theory of Ising lattices, we focus our consideration on the rigorous treatment of statistical mechanics of considered systems, like, for instance, mean square fluctuations, configurational entropy. In the case of adsorption in the 1D lattice gas with the nearest neighbor interactions we show, that in addition to [3] the rigorous expression for the statistical sum in terms of Jacobi polynomials can be obtained.

Let 1D lattice of size *M* contained *L* particles of one kind, say, *X* and *M-L* vacancies. Thus all

X-particles are distributed randomly among *N* sites. We introducing three auxiliary variables; N_{XX} the number of nearest neighbor pairs (NNP) occupied simultaneously by *X* particles, N_{XO} the number of NNP of which only one is occupied by *X* particles, and N_{OO} the number of NNP both of which are vacant. Then the following relations among them can be easily established [3]:

$$\begin{aligned} 2N_{XX} + N_{XO} &= 2L, \\ 2N_{OO} + N_{XO} &= 2(M - L). \end{aligned} \tag{7}$$

Eq.(7) shows that of these three variables only one can be chosen independently, say N_{xx}.

The number of deferent configurations of *X* particles with only N_{xx} pairs in a lattice of size *M* with a *M-L* vacancies $G_{MN}(N_{xx})$ one can express rigorously, as follows

$$g_{M,L}(N_{XX}) = \binom{L}{N_{XX}}\binom{M-L}{L-N_{XX}}. \tag{8}$$

Obviously, we have for a total number of configurations with given *L* and *M*

$$\sum_{N_{XX}=0}^{L} g_{M,L}(N_{XX}) = \sum_{N_{XX}=0}^{L}\binom{L}{N_{XX}}\binom{M-L}{L-N_{XX}} = \binom{M}{L}. \tag{9}$$

With the help of Eqs. (8) and (9), one can perform the rigorous calculations of the "fluctuational dynamics" of 1D lattice gas adsorption. Namely, for the average number of $N_{XX} - \langle N_{XX}\rangle$, and for the mean-square fluctuations of

$$N_{XX} - \left\langle (\Delta N_{XX})^2 \right\rangle - \langle N_{XX}\rangle^2$$

we obtain:

$$\langle N_{XX}\rangle = \sum_{N_{XX}=0}^{L} N_{XX}\binom{L}{N_{XX}}\binom{M-L}{L-N_{XX}} \Big/ \binom{M}{L} = \frac{L^2}{M}, \tag{10}$$

$$\begin{aligned} \left\langle (\Delta N_{XX})^2 \right\rangle &= \sum_{N_{XX}=0}^{L} N_{xx}^2 \binom{L}{N_{XX}}\binom{M-L}{L-N_{XX}} \Big/ \binom{M}{L} \\ &= \frac{L^2}{M}\left(1 - \frac{L}{M}\right)^2. \end{aligned} \tag{11}$$

Eqs.(10) and (11) show that the mean square fluctuations of N_{xx}, related to the system size *M* has a maxima under the value of filling fraction $L = \frac{M}{2}$:

$$\frac{\left\langle (\Delta N_{XX})^2 \right\rangle}{M} = \left(\frac{L}{M}\right)^2\left(1 - \frac{L}{M}\right)^2. \tag{12}$$

One can observe here the reminiscence of "phase transition" between the gas, liquid and solid phases in the case of a system which consists of distinguished clumps. Note, that this is of course not a real phase transition in terms of regular density, as it will be shown latter. This phase transition is impossible in 1D case. The maximum value of $\frac{\left\langle (\Delta N_{xx})^2 \right\rangle}{M}$ achieved under the condition that $\frac{L}{M} = 1$ is equal to 1/16.

Performing simultaneously calculations of the configurational entropy *S*, given by $S = k_B \ln g_{M,L}(N_{xx})$, one has

$$S = k_B \ln\binom{L}{N_{xx}}\binom{M-L}{L-N_{XX}}. \tag{13}$$

Using the Stirling formula, we find that expression (13) has a maximum under the value of $N_{XX} = \frac{L^2}{M}$, which is exactly equal to the average number of $N_{XX} - \langle N_{XX}\rangle$. Comparing (10), (11) and (13) we see that the average density of nearest-neighbors pairs $\langle N_{XX}\rangle / M$ mononically increases as a parabolic law, but the relative mean square fluctuations and the entropy of displacement (configurational entropy) has a maximum. Namely, the maximum in the mean-square fluctuations have observed in the case that the half of lattice sites are occupied, and thus characterized by the mean value $\langle N_{XX}\rangle$ equal to $\langle N_{XX}\rangle = \frac{L^2}{M} = \frac{M}{4}$. At the same time, the entropy of displacement, given by Eq.(13), after substitution $N_{XX}^{\circ} = \langle N_{XX}\rangle = \frac{L^2}{M}$ reached their maximum value, but it is simple to show that *S* has no maximum as a function of density $\frac{L}{M}$. Thus, the point $L = \frac{M}{2}$ is not a point of real phase transition, because under the given value of $\langle N_{XX}\rangle = \frac{L^2}{M}$, entropy *S* has a maximum value under the any

appropriate value of density $\frac{L}{M}$ (M is fixed). Note that when $M \to \infty$ (a sufficiently large system), and $\frac{L}{M}$ -constant, entropy S has no maximum at all for any values of $\frac{L}{M}$. Thus above described property of the considered model is occurred for the finite sized systems only.

Consider now the same model, as described above, when the nearest-neighbor interactions between the X particles within N_{XX} pairs are taken into account on a simplest way. Namely, rewriting the expression for the statistical sum of Izing model [3] within the framework of our model we obtain the following expression

$$Z = e^{L\varepsilon/k_BT} \sum_{N_{XX}=0}^{L} \binom{L}{N_{XX}} \binom{M-L}{L-N_{XX}} \left(e^{2\varepsilon/k_BT}\right)^{N_{XX}}. \quad (14)$$

The summation in the Eq.(14) have been performed approximately by means of maximum term method, giving rise to the estimation of the certain statistical mechanical values, like configurational energy and heat capacity, for instance [3]. We found that the sum (14) can be calculated explicitly, which allow us to conclude about the real exact character of considered model. Namely, performing sum (14) [5], we have

$$Z(\varepsilon) = \theta(M-2L)\left\{\left(2sh\left(\frac{\varepsilon}{k_BT}\right)\right)^{L} P_L^{(M-2L,0)}\coth\left(\frac{\varepsilon}{k_BT}\right)\right\} + \theta(2L-M)e^{(M-2L)\varepsilon/k_BT}\left\{\left(2sh\left(\frac{\varepsilon}{k_BT}\right)\right)^{M-L} P_{M-L}^{(2L-M,0)}\coth\left(\frac{\varepsilon}{k_BT}\right)\right\} \quad (15)$$

where $P_n^m(x)$ are the Jacobi polynomials. Taking the limit $\varepsilon \to 0$ in (15) and using the properties of Jacobi polynomials [5], one has as expected

$$\lim_{\varepsilon\to 0}\left(Z(\varepsilon)\right) = \theta(M-2L)\binom{M}{L} + \theta(2L-M)\binom{M}{M-L} = \binom{M}{L}. \quad (16)$$

Eq.(15) permits us to perform a rigorous analytical or numerical simulations of statistical thermodynamics of the considered system, which is not a purpose of this paper.

4. BIMOLECULARY REACTIVE LATTICE

We are now in the position to make a hybridization of the two previously considered in Secs. 2 and 3 models, for the bimolecularly reactive, totally filled lattice, and for the 1D lattice gases adsorption, respectively. Consider the possibility of reversible bimolecular reaction type $X + A \to 2X$ in 1D lattice gases adsorption model, described above. The presence of vacancies is expected to change an ergodic character of 1D bimolecularly reactive system (see Sec. 2). Here we are going to obtain an explicit expressions for the respective distribution functions, average number of particles and their mean-square fluctuations. We also address here the question weather exist a steady state in bimolecularly reactive 1D adsorptive lattice gas, and how our system approach this steady state, if so. Clear, that under the above construction, particles A can only be created from the configurations initially involving continuous X particles (note, that again as before we start from homogenous initial configuration, which consist of only X particles). Furthermore, the conditional probability to find N_A number of A particles in whole system which include N_{XX} nearest neighbors pairs occupied simultaneously by X particles is $\binom{N_{XX}}{N_A}\Big/2^{N_{XX}}$ (see Sec. 2). Thus, the total distribution of A particles $G_{M<L}(N_A)$ within 1D partially filled bimolecularly reactive system of size M with M-L vacancies can be expressed as following sum

$$G_{M,L}(N_A) = \sum_{N_{XX}=0}^{L} \binom{N_{XX}}{N_A}\binom{L}{N_{XX}}\binom{M-L}{L-N_{XX}}\Big/2^{N_{XX}}. \quad (17)$$

Eq.(17), after using the following property for the products of binomials,

$$\binom{n+a}{n}\binom{b}{n+a} = \binom{b}{n}\binom{b-n}{a}$$

can be rewritten as

$$G_{M,L}(N_A) = \binom{L}{N_A}\sum_{N_{XX}=0}^{L}\binom{L-N_A}{L-N_{XX}}\binom{M-L}{L-N_{XX}}\frac{1}{2^{N_{XX}}}. \quad (18)$$

Finally, performing the summation in Eq.(18) explicitly [5], we obtain:

$$G_{M,L}\left(N_A\right)=\binom{L}{N_A}\times\left\{\theta\left(2L-M-N_A\right)P_{M-L}^{\left(2L-M-N_A,0\right)}\left(\varepsilon\right)+\theta\left(M-2L+N_A\right)P_{L-N_A}^{\left(M-2L+N_A,0\right)}\left(\varepsilon\right)\right\}. \tag{19}$$

In terms of Gauss confluent function ${}_2F_1\left(\alpha,\beta,\gamma,z\right)$ Eq.(19) can be rewritten as follows:

$$G_{M,L}\left(N_A\right)=\frac{\binom{L}{N_A}}{2^L}\times$$
$$\times\left\{\theta\left(2L-M-N_A\right)\binom{L-N_A}{M-L}{}_2F_1\left(-M+L,L-N_A+1,2L-M-N_A+1;-1\right)+\theta\left(M-2L+N_A\right)\binom{M-L}{L-N_A}{}_2F_1\left(-L+N_A,M-L+1,M-2L+N_A+1;-1\right)\right\}. \tag{20}$$

One can see, that taking the limit $L\to M$ (totally filled lattice) in the rigorous Eqs.(18) and (19) we obtain explicitly the respective expression for the distribution function, given by Eq.(1), thus

$$\lim_{L\to M} g_{M,L}\left(N_A\right)=\binom{M}{N_A}. \tag{21}$$

Obviously, the normalization condition is satisfied by Eqs.(19), (20). In particular, we have:

$$\sum_{N_A=0}^{L} G_{M,L}\left(N_A\right)=\frac{1}{2^L}\sum_{N_A=0}^{L}\binom{L}{N_A}\times\left\{\theta\left(2L-M-N_A\right)P_{M-L}^{\left(2L-M-N_A,0\right)}\left(\varepsilon\right)+\theta\left(M-2L+N_A\right)P_{L-N_A}^{\left(M-2L+N_A,0\right)}\left(\varepsilon\right)\right\}=$$
$$=\left\{\theta\left(M-2L\right)\binom{M}{L}+\theta\left(2L-M\right)\binom{M}{L}\right\}=\binom{M}{L}. \tag{22}$$

From Eqs.(19) and (20) it follows that distribution function has change of their behavior (bifurcation point) at the value of $L=\frac{M}{2}$, which is the reminiscence of the critical behavior of 1D lattice gas adsorption (See Sec. 2). One can perform now the calculations of the average values $\left\langle N_A\right\rangle$, $\left\langle N_X\right\rangle$ and their ratio $r=\frac{\left\langle N_A\right\rangle}{\left\langle N_X\right\rangle}$. By use of definition $\left\langle N_A\right\rangle$, after some transformations, we calculate the respective sum explicitly:

$$\left\langle N_A\right\rangle=\sum_{N_A=0}^{L} N_A\binom{L}{N_A}P_{L-N_A}^{\left(M-2L+N_A,0\right)}\left(\varepsilon\right)\Bigg/\sum_{N_A=0}^{L}\binom{L}{N_A}P_{L-N_A}^{\left(M-2L+N_A,0\right)}\left(\varepsilon\right)=\frac{L^2}{2M}. \tag{23}$$

Here we put for simplicity $L=\frac{M}{2}$. Using Eq.(23) and taking into account the trivial sum rule for our model $L=\left\langle N_A\right\rangle+\left\langle N_X\right\rangle$, we calculated the ratio $r=\frac{\left\langle N_A\right\rangle}{\left\langle N_X\right\rangle}$, namely

$$r=\frac{L}{M}\Bigg/\left(2-\frac{L}{M}\right). \tag{24}$$

Eq.(24) shows that ratio $r=\frac{\left\langle N_A\right\rangle}{\left\langle N_X\right\rangle}$ increased monotonically as a function of density $\frac{L}{M}$ and under the

value of $L=\frac{M}{2}$ approaches 1/3. This is, as expected, quite different from the mean-field value $r_{mf}=1$. Note, that the value *r*, given by Eq.(24) approaches mean-field value 1 in the limit, when $L\to M$ (totally filled lattice without the vacancies). We can conclude now that bimolecularly reactive partially filled 1D lattice, starting from homogeneous initial configuration, asymptotically approaches a steady state in which the ratio *r* takes the value $r<1$ ($r=\frac{1}{3}$ when $L=\frac{M}{2}$). We performed a calculation of the mean-square fluctuations $\left\langle\left(\Delta N_A\right)^2\right\rangle=\left\langle N_A^2\right\rangle-\left\langle N_A\right\rangle^2$, namely, with the help of Eqs.(19) and (20), we obtain

$$\left\langle\left(\Delta N_A\right)^2\right\rangle=\frac{L^2}{2M}\left(1-\frac{L}{M}+\frac{1}{2}\frac{L^2}{M^2}\right). \qquad (25)$$

From Eq.(25) it follows that mean-square fluctuations decreased as a function of density $\frac{L}{M}$. The relative mean-square fluctuations $\frac{\left\langle\left(\Delta N_A\right)^2\right\rangle}{M}$ behaves as square law from the density, approaching the value 1/4 (which is exactly equal to the limit of totally filled lattice, See Sec. 1) in the limit $L\to M$. For the dilute lattice, when $L<\frac{M}{2}$, the mean-square fluctuations are much smaller then in the case of totally filled lattice. As expected, the presence of vacancies plays a role of restrictor for the development of chemical fluctuations, which developed only within the *X* particle islands. We present also the useful formula for the ratio $\frac{\left\langle\left(\Delta N_A\right)^2\right\rangle}{\left\langle N_A\right\rangle}$, which is related with respective static structure factor $S(k)$ under the value of wave vector k equal to 0

$$\frac{\left\langle\left(\Delta N_A\right)^2\right\rangle}{\left\langle N_A\right\rangle}=1-\frac{L}{M}+\frac{L^2}{2M^2}. \qquad (26)$$

Comparing the result described above with the conclusions made in Sec. 2, we see an exact correspondence between them if one adopt simply $\left\langle N_A\right\rangle=\left\langle N_{XX}\right\rangle/2$. This isomorphism, however, dropped when one goes to express the mean square fluctuations (compare Eq.(11), and Eq.(25)). We would not present here the precise calculations of average values and mean-square fluctuations in the case of $\frac{1}{2}<\frac{L}{M}<1$. It could be done without principal difficulties with the help of rigorous expressions for the distribution function $g_{M,L}\left(N_A\right)$, given by Eq.(19) and Eq.(20). Note only, that in the limit of $L\to M$ we obtain again famous results for totally filled 1D lattice we would get again the familiar results obtained in the Sec. 2,3.

5. SUMMARY

We have developed a 1D model of chemically reactive lattice which include the vacancies. It is shown that even in one dimension bimolecularly reactive totally filled lattice mimics a mean-field scenario of fluctuational chemical dynamics, which is rather surprising. From another side in the reactive lattice with vacancies, the nonergodic scenario of the behavior of chemical fluctuations occurs. An important advantage of considered model and given approach is that one obtains an explicit expressions either for distribution functions (which gives the probability to find a given particle configuration) and average number of particles, or mean-square fluctuations, configuration sum and entropy. We found that in the case of vacancied chemically reactive lattice, like in the case of exclusion statistics [7,8], distribution function has a chiral form, expressed in terms of Jacobi polynomials or Gauss confluent functions. We conclude that in spite their simplicity 1D reactive lattices able to exhibit complex not a mean-field, and nonergodic behavior. This property should be taken into account, for instance, in the description of cooperative adsorption of the products on the surfaces, or band formation in the polymers [9].

REFERENCES

1. Nicolis *G.,* Prigogine I. S*elf-organization in Non-equilibrium systems.* New York: Wiley Interscience, 1977.
2. Privman V.(Ed.) *Non-equilibrium Statistical Mechanics in 1D*. Cambridge: Cambridge University Press, 1997.
3. Hill T. *An introduction to statistical thermodynamics*. New York: Dover Publ., 1986.
4. Provata A., Turner J., Nicolis G. *Journ. Stat. Phys*, 1993, vol. 70, p. 1195.
5. Prudnicov A., Brychkov Yu., Marichev O. *Integrals and series. Vol.1.: Elementary functions. Vol.2.: Special functions*. New York: Gordon and Breach S.P., 1986.

6. Marro J., Dickman R. *Non-equilibrium phase transitions in Lattice models*. Cambridge: Cambridge University Press, 1999.
7. Hikami K. *Excusion statistics and chiral partition function. Physics and combinatorics.* Singapore: World Scientific, 2002. (Ed.:A.Kirilov)
8. Gerasymov O.I,Khudyntsev N.N.Condensed Matter Physics, 1999, Vol. 2, No. 1(17), p. 75.
9. Bowker M. *The basis and applications of Heterogeneous Catalysis*. Oxford: Oxford University Press, 1998.

ТОЧНО-РОЗВЯЗУВАНА МОДЕЛЬ ХИМІЧНО РЕАГУЮЧОЇ СИСТЕМИ НА ОДНОВИМІРНІЙ ЧАСТКОВО ЗАПОВНЕНІЙ ГРАТЦІ

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Розглянута модель флуктуаційної динаміки двох-компонентної реагуючої суміші на одновимірній гратці із вакансіями,яка припускає точні розв'язки. Отримані аналітичні вирази для ймовірнісних функцій розподілу,середніх чисел заповнення та їх середньоквадратичних флуктуацій,конфігураційної ентропії та статистичної суми. Модель Ізинга не реагуючої заповненої гратки доповнена отриманим точним виразом для статистичної суми на випадок наявності вакансій. Наочно продемонстрована не ергодичність розглянутої системи,яка характеризується відмінними від висновків моделі середнього поля співвідношеннями між середніми кількостями реагентів у асимптотичних квазістаціонарних станах..

Ключові слова : реагуючі одновимірні гратки, флуктуаційна динаміка,ймовірнісні функції розподілу,ергодичність,статистична механіка реагуючих граток із вакансіями

ТОЧНО-РЕШАЕМАЯ МОДЕЛЬ ХИМИЧЕСКИ РЕАГИРУЮЩЕЙ СИСТЕМЫ НА ОДНОМЕРНОЙ ЧАСТИЧНО ЗАПОЛНЕНОЙ РЕШЕТКЕ

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Рассмотрена модель флуктуационной динамики двух-компонентной химически реагирующей системы на одномерной решетке с вакансиями, которая допускает точное решение. Получены аналитические выражения для вероятностных функций распределения, средних чисел заполнения и их среднеквадратичных флуктуаций, конфигурационной энтропии и статистической суммы. Модель Изинга нереагирующей заполненной решетки дополнена полученным точным выражением для статистической суммы на случай наличия вакансий. Наглядно продемонстрирована неэргодичность рассмотренной системы, которая характеризуется отличными от предсказанных теорией среднего поля соотношениями средних чисел реагентов в асимптотически квази-стационарных состояниях.

Ключевые слова: реагирующие одномерные решетки, флуктуационная динамика, вероятностные функции распределения, эргодичность, статистическая механика реагирующих решеток с вакансиями

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