PACS: 05.20.Dd

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KINETIC EQUATIONS FOR THE PSEUDOSPIN MODEL WITH BARRIERS

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Received January 26, 2011

A new formalization of Glauber method is developed and applied to the pseudospin model with barriers. Kinetic equations are derived for this model and numeric solutions in simplest approximations are obtained. Relaxation and kinetic properties of the model are shown to depend on the barrier value as well on the heating-cooling rate. Heating-cooling cycles reveal hysteresis. The relaxation times are determined by the temperature and the barrier value. The relaxation time for the structural order parameter S_z possesses two vertical asymptotes: the first one caused by phase transition, and the second one determined by slowing kinetics at low temperatures.

Keywords: structural disorder, kinetic equations, Ising model, pseudospin model, phase transitions

Introduction

The pseudospin model can be used for a wide class of the objects which represent structural disorder and order-disorder transitions. These are Jahn–Teller crystals, hydrogen bonded crystals, molecular crystals, binary alloys, lattice gas and lattice model of fluid. A lot of papers have been published about this approach since pioneer works of J.S. Slater [1] and P.G. De Gennes [2]. Unfortunately, this model regards only two states at the bottoms of the potential minima and ignores all others. It's really correct as an approximation at the temperatures $kT << U_0$, where U_0 is the value of the energy barrier between the minima, but it excludes possibility of description of the kinetic properties and such phenomena as pretransition slowing of kinetics and metastable glass-like frozen disorder, because the states of the over-barrier motion are essential in these cases. In order to include over-barrier states to the pseudospin framework, we developed the Ising model with barriers [3]. The main results of this work are: three-component pseu-

dospin $\hat{S}_{zi} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ (instead of usual two-component one), where $S_{zi} = 0$ corresponds to the states of the over-barrier motion, and the effective Hamiltonian:

$$\hat{H}_{\text{eff}} = -\frac{1}{2}\sum_{i \neq j} J_{ij}\hat{S}_{zi}\hat{S}_{zj} - T\ln\left(\frac{z_1}{z_0}\right)\sum_i \hat{S}_{zi}^2 - TN\ln z_0, \qquad (1)$$

where $z_+ = z_- \equiv z_1 = \int_0^1 \exp\left(-\frac{\varepsilon}{\theta}\right) g(\varepsilon)\mathrm{d}\varepsilon$, $z_0 = \int_1^\infty \exp\left(-\frac{\varepsilon}{\theta}\right) g(\varepsilon)\mathrm{d}\varepsilon$ are partial statistical integrals taken over the states within the potential wells and over the states of the cross-well motion respectively, $\varepsilon = \frac{E}{U_0}$ is the reduced energy, U_0 is the energy barrier between the minima, E is the energy, g(ε) is the density of states, $t = \frac{kT}{U_0}$ is the reduced temperature, J_{ij} are the pair interaction constants, T is the absolute temperature, N is the number of lattice sites. Let's notice that we are currently considering the classical mechanics case, so all matrix operators commute with each other and should be regarded just as pseudospin variables which can take values from the set of their eigenvalues. We have chosen such representation because of benefits of matrix representation and in order to have a good start for extending the results to the quantum mechanics case. This model was shown by means of computer simulations really to reveal pretransition kinetics slowing and glass-like metastable state of the frozen disorder [3]. By the way, these results are in accordance with frustration-volumetric theory of glass by A.S. Bakai [4], where glassy state is also regarded as a metastable phase, but not as an unstable very slowly evolving one.

Further investigations were performed on the four-sublattice model in order to apply the results to interpretation of the Mössbauer investigations of the Jahn–Teller crystal of $Cu(H_2O)_6{\cdot}SiF_6$ [5,6]. The state of metastable disorder and the equilibrium phase transition for a four-sublattice model have been studied in this work. These results were used for the theoretical explanation of the statics–dynamics transformation observed in the disordered phase of this crystal when the structural phase transition point is approached [7]. The next step of these investigations is studying of kinetic properties.

So, the aim of this paper is obtaining of corresponding kinetic equation from the model (1). The basic approach was founded by Glauber [8]. But our case differs from the original by two means: a) multicomponent pseudospin; b) transfer rules: direct jumps between wells are forbidden because of classical character of

our model, only over-barrier – well transfers and vice versa are allowed. In order to fit these conditions, we have to reformulate Glauber approach. It should be noticed that the same approach was used by Vaks with coworkers in their investigations of kinetic properties of alloys [9–12].

There are five steps, which we firstly illustrate on traditional two-component model and then apply to our model with barriers.

1. Ising model

1. We start from the master equation in a general form:

$$\frac{\mathrm{d}\, p\left(\{S\}\right)}{\mathrm{d}\,\tau} = \sum_j \left[-w_j\left(S_{zj}\right) p\left(\left\{S\middle|S_{zj}\right\}\right) + w_j\left(-S_{zj}\right) p\left(\left\{S\middle|-S_{zj}\right\}\right)\right],$$

where $\{S\}$ is a certain configuration of pseudospin values at each site $\{\ldots S_{z\,i}, \ldots, S_{z\,j}, \ldots\}$, $w_j(S_{z\,j}), w_j(-S_{z\,j})$ are the transition probabilities for the changes $-S_{z\,j} \to S_{z\,j}$, $S_{z\,j} \to -S_{z\,j}$ respectively at the site j, $p(\{S|S_{z\,j}\}), p(\{S|-S_{z\,j}\})$ are the probabilities of the pseudospin values $S_{z\,j}, -S_{z\,j}$ respectively at the site j in the given configuration $\{S\}$.

2. Demand of detailed balance principle leads to a definite form of the transition probabilities:

$$-w_j(S_{z\,j}) p_0(\{S|S_{z\,j}\}) + w_j(-S_{z\,j}) p_0(\{S|-S_{z\,j}\}) = 0, \Rightarrow$$

$$\Rightarrow w_j(S_{z\,j}) \sim p_0(\{S|-S_{z\,j}\}) \sim \exp(-\beta h_j S_{z\,j}),$$

where $\beta = 1/kT$, $h_j = \sum_{j \neq i} J_{j\,i} S_{z\,i}$ – molecular field at the site j.

3. Operators $\hat{S}_z, \hat{1}$ form the basis of the matrix algebra, and all functions of them are expressed through the linear combinations of this basis:

$$\hat{S}_z^2 = \hat{1}, \exp(aS_z) = \cosh a + \hat{S}_z \sinh a = \cosh a(\hat{1} + \hat{S}_z \tanh a).$$

4. Using statements 2 and 3, one can express the transfer probabilities (τ_0 is a phenomenological constant):

$$w_j\left(S_{zj} \to S'_{zj}\right) = \frac{1}{2\tau_0}\left(1 - S'_{zj} \tanh \beta h_j\right).$$

5. Using 4, one can calculate the mean values and finally obtain the well known kinetic equation:

$$\frac{\mathrm{d}\left\langle S_{zl}\right\rangle}{\mathrm{d}\,\tau} = \sum_{\{S\}} S_{zl} \frac{\mathrm{d}\, p\left(\{S\}\right)}{\mathrm{d}\,\mathrm{t}} = -\frac{1}{\mathrm{t}_0}\left(\left\langle S_{zl}\right\rangle - \left\langle \tanh \mathrm{b} h_j \right\rangle\right).$$

2. Ising model with barrier

We can generalize now this approach on Ising model with barriers [3].

1. Master equation:

$$\frac{\mathrm{d}\, p\left(\{S\}\right)}{\mathrm{d}\,\tau} = \sum_{j}\sum_{S'_{zj}}\left[-w_j\left(S_{zj}\to S'_{zj}\right)p\left(\{S\}\right)+w_j\left(S'_{zj}\to S_{zj}\right)p\left(\{S'\}\right)\right]$$

where $w_j\left(S_{zj}\to S'_{zj}\right)$ is a probability of a transition from the spin value S_{zj} to the spin value S'_{zj} at the site j.

2. Demand of the detailed balance principle:

$$\sum_{S'_j\neq S_j}\left[-w_j(S_j\to S'_j)p_0(\{S\})+w_j(S'_j\to S_j)p_0(\{S'\})\right]=0$$

$$\Downarrow$$

$$w_j(S_j\to S'_j)\sim p_0(\{S'\})\sim\exp\left(\beta h_j S'_{z\,j}+\beta h(S'_{z\,j})^2\right),$$

where $h_j=\sum_{j\neq i}J_{ji}S_{zi}$ is the molecular field at the site j, $h=T\ln\left(\frac{z_1}{z_0}\right)$ is the effective energy barrier.

3. Rules of the matrix algebra: basis $\hat{S}_z, \hat{S}_z^2, \hat{1}$, operations: $\left(\hat{S}_z^2\right)^2=\hat{S}_z^2,\ \hat{S}_z\cdot\hat{S}_z^2=\hat{S}_z$.

4. Form of the matrix of transfer probabilities:

$$w_{S\,S'}(j)=\frac{1}{2\tau_{S\,S'}}\left[1+S'_{z\,j}\exp(\beta h)\sinh(\beta h_j)+(S'_{z\,j})^2\left(\exp(\beta h)\cosh(\beta h_j)-1\right)\right],$$

where phenomenological matrix $\frac{1}{\tau_{SS'}}$ defines accordingly transfer rules:

$$\frac{1}{\tau_{S\,S'}}=\begin{pmatrix}0 & \frac{1}{\tau_+} & 0\\ \frac{1}{\tau_+} & 0 & \frac{1}{\tau_-}\\ 0 & \frac{1}{\tau_-} & 0\end{pmatrix},$$ zero values of non-diagonal elements do satisfy our transfer rules here; finally one obtains:

$$w_{SS'}(j)=\frac{1}{2}\begin{pmatrix}0 & \frac{1}{\tau_+} & 0\\ \frac{e_+}{\tau_+} & 0 & \frac{e_-}{\tau_-}\\ 0 & \frac{1}{\tau_-} & 0\end{pmatrix},$$ where $e_+=\exp\beta(h+h_j), e_-=\exp\beta(h-h_j)$.

5. Calculating the mean values with $w_{SS'}(j)$ from statement 4 yields:

$$\begin{aligned}
\frac{\mathrm{d}\left\langle S_{z\,l}\right\rangle}{\mathrm{d}t} &= \sum_{\{S\}} S_{z\,l}\frac{dp(\{S\})}{\mathrm{d}t} = \\
&= \sum_{\{S\}} S_{z\,l}\sum_{j}\sum_{S'}\left[-w_{S\,S'}(j)p(\{S\})+w_{S'\,S}(j)p(\{S'\})\right] = \\
&= \sum_{\{S\}}\sum_{S_l'} w_{S_l\,S_l'}(-S_l+S_l')p(\{S\}) = \\
&= -\frac{1}{2}\left\langle\left(\frac{1}{\tau_+}+\frac{1}{\tau_-}\right)S_{z\,l}\right\rangle-\frac{1}{2}\left\langle\left(\frac{1}{\tau_+}-\frac{1}{\tau_-}\right)S_{z\,l}^2\right\rangle+\left\langle\left(\frac{e_+}{\tau_+}-\frac{e_-}{\tau_-}\right)\left(1-S_{z\,l}^2\right)\right\rangle,
\end{aligned} \tag{1}$$

$$\begin{aligned}
\frac{\mathrm{d}\left\langle S_{z\,l}^2\right\rangle}{\mathrm{d}\tau} &= \sum_{\{S\}} S_{z\,l}^2\frac{dp(\{S\})}{\mathrm{d}\tau} = \\
&= \sum_{\{S\}} S_{z\,l}^2\sum_{j}\sum_{S'}\left[-w_{S\,S'}(j)p(\{S\})+w_{S'\,S}(j)p(\{S'\})\right] = \\
&= \sum_{\{S\}}\sum_{S_l'} w_{S_l\,S_l'}(-S_{z\,l}^2+S_{z\,l}'^2)p(\{S\}) = \\
&= -\frac{1}{2}\left\langle\left(\frac{1}{\tau_+}+\frac{1}{\tau_-}\right)S_{z\,l}^2\right\rangle-\frac{1}{2}\left\langle\left(\frac{1}{\tau_+}-\frac{1}{\tau_-}\right)S_{z\,l}\right\rangle+\left\langle\left(\frac{e_+}{\tau_+}+\frac{e_-}{\tau_-}\right)\left(1-S_{z\,l}^2\right)\right\rangle.
\end{aligned}$$

As a result, in the molecular field approximation and assuming $\tau_- = \tau_+ \equiv \tau_0$, we obtain the kinetic equations:

$$\left.\begin{aligned}
\frac{\partial\left\langle S_{zi}\right\rangle}{\partial\tau} &= -\frac{1}{\tau_0}\left(\left\langle S_{zi}\right\rangle-2\exp(\beta h)\sinh(\beta h_i)\left(1-\left\langle S_{zi}^2\right\rangle\right)\right)\\
\frac{\partial\left\langle S_{zi}^2\right\rangle}{\partial\tau} &= -\frac{1}{\tau_0}\left(\left\langle S_{zi}^2\right\rangle-2\exp(\beta h)\cosh(\beta h_i)\left(1-\left\langle S_{zi}^2\right\rangle\right)\right)
\end{aligned}\right\}, \tag{2}$$

where τ is a time in relative units, $t = kT/U_0$ is the reduced temperature.

Let's consider the limit passage. At the big barrier limit we have $\beta h >> 1$, hence $\left\langle S_{zi}^2\right\rangle \approx 1-\dfrac{\exp(-\beta h)}{2\cosh(\beta h_i)}$ and $\dfrac{\partial\left\langle S_{zi}\right\rangle}{\partial\tau} = -\dfrac{1}{\tau_0}\left(\left\langle S_{zi}\right\rangle-\tanh(\beta h_i)\right)$, that is the well known Glauber result for the two-component model. So, the correspondence principle is valid in this case.

3. Three-component model with barrier

Static behaviour of this model was investigated in our previous works [5,6]. The structure parameter is represented by the vector matrix

$$\hat{\mathbf{Q}} \equiv (\hat{\mathrm{Q}}_3, \hat{\mathrm{Q}}_2) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathbf{Q}_x & 0 & 0 \\ 0 & 0 & \mathbf{Q}_y & 0 \\ 0 & 0 & 0 & \mathbf{Q}_z \end{pmatrix}, \tag{3}$$

and over-barrier motion is described by the matrix

$$\hat{\mathbf{Q}}^{\mathbf{2}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{4}$$

where

$$\left.\begin{aligned} \mathbf{Q}_\mathbf{x} &= (-\frac{1}{2}, \frac{\sqrt{3}}{2}) \\ \mathbf{Q}_\mathbf{y} &= (-\frac{1}{2}, -\frac{\sqrt{3}}{2}) \\ \mathbf{Q}_\mathbf{z} &= (1, 0) \end{aligned}\right\} \tag{5}$$

are three equivalent minima in the 2*d* space of the normal modes $(\mathrm{Q}_3, \mathrm{Q}_2)$, as it is illustrated in Fig. 1.

Passing through 5 steps described above, one can obtain the following kinetic equations for this model:

$$\left.\begin{aligned} \frac{\mathrm{d}\left\langle \mathrm{Q}_{j3} \right\rangle}{\mathrm{d}\,\tau} &= -\frac{1}{\tau_0}\left\langle \mathrm{Q}_{j3} \right\rangle + \frac{1}{2\tau_0}(-e_{j\,x} - e_{j\,y} + 2e_{j\,z})e_u(1 - \left\langle \mathrm{Q}_j^2 \right\rangle) \\ \frac{\mathrm{d}\left\langle \mathrm{Q}_{j2} \right\rangle}{\mathrm{d}\,\tau} &= -\frac{1}{\tau_0}\left\langle \mathrm{Q}_{j2} \right\rangle + \frac{\sqrt{3}}{2\tau_0}(e_{j\,x} - e_{j\,y})e_u(1 - \left\langle \mathrm{Q}_j^2 \right\rangle) \\ \frac{d\left\langle \mathrm{Q}_j^2 \right\rangle}{\mathrm{d}\,\tau} &= -\frac{1}{\tau_0}\left\langle \mathrm{Q}_j^2 \right\rangle + \frac{1}{2\tau_0}(e_{j\,x} + e_{j\,y} + e_{j\,z})e_u(1 - \left\langle \mathrm{Q}_j^2 \right\rangle) \end{aligned}\right\}, \tag{6}$$

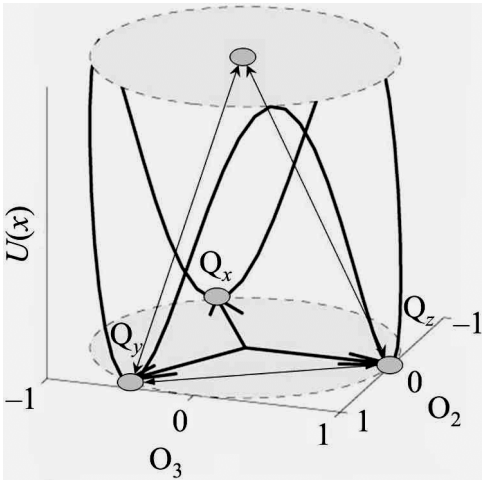

Fig. 1. Three-minima model potential $U(\varphi)$

where

$$\left.\begin{aligned} e_{\mathrm{j\,x}} &= \exp(\beta \mathbf{h}_j \mathbf{Q}_x) \\ e_{\mathrm{j\,y}} &= \exp(\beta \mathbf{h}_j \mathbf{Q}_y) \\ e_{\mathrm{j\,z}} &= \exp(\beta \mathbf{h}_j \mathbf{Q}_z) \\ e_{\mathrm{u}} &= \exp(\beta h) \end{aligned}\right\},$$

$\mathbf{h}_j = v_j \mathbf{Q}_j$ is the molecular field at the site j, v_j is the pair interaction constant, $h = T \ln\left(\frac{z_1}{z_0}\right)$ is the effective energy barrier with partial statistical integrals z_0, z_1 the same as for (1), but taken over three-minima potential (Fig. 1).

4. Numeric results for Ising model with barrier

So, we have a toy – why not to play with it for a while? Results obtained from (2) are represented below.

1. *Relaxation* below phase transition temperature is shown in Fig. 2,*a* and relaxation above the critical point is depictured in Fig. 2,*b*. In Fig. 2,*a,* we start from the fully disordered static state $\left\langle S_{z\,j} \right\rangle = 0, \left\langle S_{z\,j}^2 \right\rangle = 1$ and can observe how it evolves to the ordered state which is stable at this temperature. Some unusual (but expected) feature is unfreezing of over-barrier motions during this process (temporal decrease of $\left\langle S_{z\,j}^2 \right\rangle$). In Fig. 2,*b* we start from the fully ordered static state $\left\langle S_{z\,j} \right\rangle = \left\langle S_{z\,j}^2 \right\rangle = 1$ and can observe relaxation to the stable disordered state and regular unfreezing of dynamics expressed in regular decrease of $\left\langle S_{z\,j}^2 \right\rangle$.

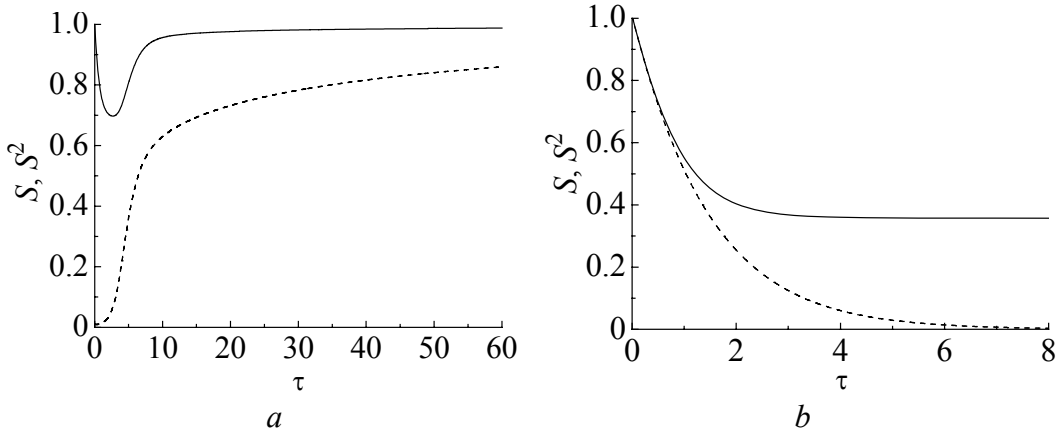

Fig. 2. Relaxation of $\left\langle S_{zj} \right\rangle$ (dashed line) and $\left\langle S_{zj}^2 \right\rangle$ (solid line) at t = 1 below the critical poind (*a*) and at t = 3 above the critical point (*b*) (reduced pair interaction $j = \frac{J}{U_0} = 5$, t_c = 2.2), τ is time measured in relative units

2. *Kinetic behaviour* is shown in Fig. 3. These results are obtained from the kinetic equations (2) under condition that temperature linearly depends on time. On heating, we start from the fully disordered state, same as in Fig. 2,*a*. One can observe evolution of this state to the ordered one firstly (increasing $\langle S_{z\,j} \rangle$), and then – to the fully disordered state (decreasing $\langle S_{z\,j} \rangle$ to 0). Then, cooling from the last state leads again to the static state: $\langle S_{z\,j}^2 \rangle = 1$ (frozen over-barrier states), but some long range order remains frozen, what is indicated by non-zero $\langle S_{z\,j} \rangle$. So that, we can see a hysteresis without any additional assumptions but kinetic equations (2) as is. These processes are also accompanied with unfreezing-freezing of the over-barrier motions which can be traced by the temperature dependence of $\langle S_{z\,j}^2 \rangle$.

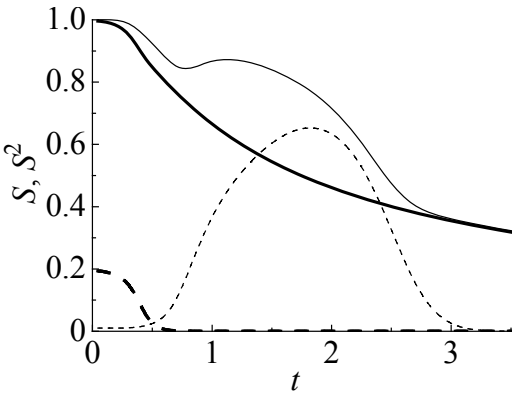

Fig. 3. Kinetic properties of $\langle S_{zj} \rangle$ (dashed lines) and $\langle S_{zj}^2 \rangle$ (solid lines) (the reduced pair interaction $j = \dfrac{J}{U_0} = 5$, t_c = 2.2) at heating (thin lines), $\dfrac{\mathrm{d}t}{\mathrm{d}\tau} = 0.1$ and at cooling (bold lines) $\dfrac{\mathrm{d}t}{\mathrm{d}\tau} = -0.1$; t is the reduced temperature

3. *Relaxation time* for $\langle S_{z\,j} \rangle$ is shown in Fig. 4,*a* and relaxation time for $\langle S_{z\,j}^2 \rangle$ is shown in Fig. 4,*b*. The relaxation time for the structural order parameter $\langle S_{z\,j} \rangle$ possesses two vertical asymptotes: the first one caused by phase transition, as usual, but the second one reveals slowing kinetics at low temperatures caused by

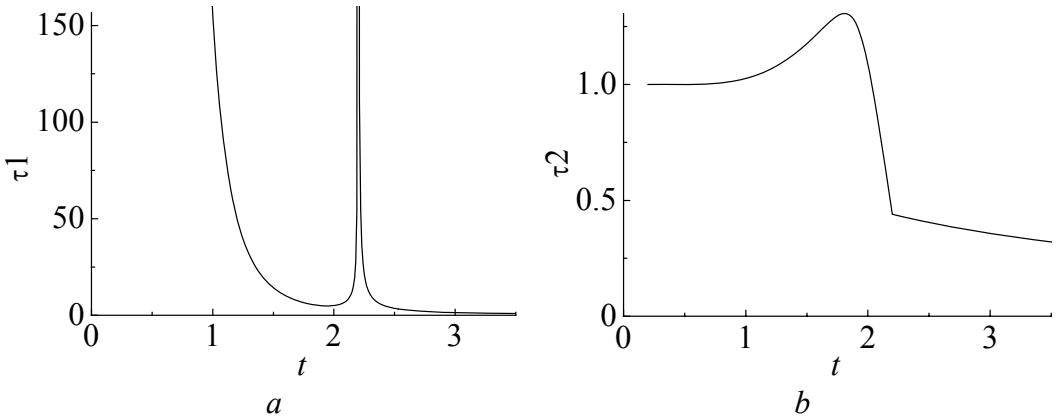

Fig. 4. Relaxation time for $\langle S_{zj} \rangle$ (*a*) and $\langle S_{zj}^2 \rangle$ (*b*) in relative units versus temperature *t* (the reduced pair interaction $j = \dfrac{J}{U_0} = 5$, $t_c = 2.2$)

the energy barrier. The relaxation time for the «dynamics» parameter $\left\langle S_{z\,j}^2 \right\rangle$ indicates the phase transition too, but not so dramatically: it undergoes only the discontinuity of its first derivative at the critical point.

In contrast with computer modelling results [3], we did not consider here a metastable glass-like state because we investigate here only the simplest spatially homogeneous structure, but the glassy state needs to take into account spatial dependence of parameters $\left\langle S_{z\,j} \right\rangle, \left\langle S_{z\,j}^2 \right\rangle$ in order to describe short range order which is essential for this state. We are planning to include inhomogeneous states just as the next step of these investigations.

5. Conclusions

We explored our numeric solutions in a wide range of parameters, so it allows us to make the following conclusions.

1. A new formalization of Glauber method is developed and is applied to the pseudospin model with barriers.

2. Kinetic equations have been derived for this model and numeric solutions in the simplest approximations have been obtained.

3. Relaxation and kinetic properties of the model has been shown to depend on the barrier value as well on heating-cooling rate.

4. Heating-cooling cycles reveal hysteresis.

5. The relaxation times are determined by the temperature and the barrier value.

6. The relaxation time for the structural order parameter $\left\langle S_{zj} \right\rangle$ possesses two vertical asymptotes: the first one caused by phase transition, and the second one determined by slowing kinetics at low temperatures.

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КІНЕТИЧНІ РІВНЯННЯ ДЛЯ ПСЕВДОСПІНОВОЇ МОДЕЛІ З БАР'ЄРАМИ

Розроблено нове формулювання методу Глаубера, яке застосовано до псевдоспінової моделі з бар'єрами. Отримано кінетичні рівняння для цієї моделі, а також чисельні рішення у найпростіших наближеннях. Показано, що релаксація й кінетичні властивості моделі залежать від енергетичного бар'єру й швидкості нагрівання–охолодження. Цикли нагрівання–охолодження виявляють гістерезіс. Часи релаксації визначаються температурою та величиною енергетичного бар'єру. Час релаксації для структурного параметра порядку S_z має дві вертикальні асимптоти: перша обумовлена фазовим переходом, друга – уповільненням кінетики за низьких температур.

Ключові слова: структурний безлад, кінетичні рівняння, модель Ізинга, псевдоспінова модель, фазові перетворення

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КИНЕТИЧЕСКИЕ УРАВНЕНИЯ ДЛЯ ПСЕВДОСПИНОВОЙ МОДЕЛИ С БАРЬЕРАМИ

Разработана новая формулировка метода Глаубера, дано ее приложение к псевдоспиновой модели с барьерами. Получены кинетические уравнения для этой модели, а также численные решения в простейших приближениях. Показано, что релаксация и кинетические свойства модели зависят от энергетического барьера и скорости нагрева–охлаждения. Циклы нагрева–охлаждения обнаруживают гистерезис. Времена релаксации определяются температурой и величиной энергетического барьера. Время релакации для структурного параметра порядка S_z обладает двумя вертикальными асимптотами: первая обусловлена фазовым переходом, вторая – замедлением кинетики при низких температурах.

Ключевые слова: структурный беспорядок, кинетические уравнения, модель Изинга, псевдоспиновая модель, фазовые переходы

Рис. 1. Трехминимумный модельный потенциал $U(\varphi)$

Рис. 2. Релаксация $\left\langle S_{zj} \right\rangle$ (штриховая линия) и $\left\langle S_{zj}^2 \right\rangle$ (сплошная) при t = 1 ниже критической точки (*a*) и при t = 3 выше критической точки (*b*) (приведенная константа парного взаимодействия $j = \dfrac{J}{U_0} = 5$, t_c = 2.2), t – время в относительных единицах

Рис. 3. Кинетические свойства $\left\langle S_{zj} \right\rangle$ (штриховые линии) и $\left\langle S_{zj}^2 \right\rangle$ (сплошные) (приведенная константа парного взаимодействия $j = \dfrac{J}{U_0} = 5,\ t_c = 2.2$) при нагревании (тонкие линии), $\dfrac{\mathrm{d}t}{\mathrm{d}\tau} = 0.1$ и охлаждении (жирные линии), $\dfrac{\mathrm{d}t}{\mathrm{d}\tau} = -0.1$; t – приведенная температура

Рис. 4. Время релаксации для $\left\langle S_{zj} \right\rangle$ (*a*) и $\left\langle S_{zj}^2 \right\rangle$ (*b*) в относительных единицах в зависимости от приведенной температуры t (приведенная константа парного взаимодействия $j = \dfrac{J}{U_0} = 5,\ t_c = 2.2$)