Systematic perturbation approach for a dynamical scaling law in a kinetically constrained spin model

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Abstract. The dynamical behaviours of a kinetically constrained spin model (Fredrickson–Andersen model) on a Bethe lattice are investigated by a perturbation analysis that provides exact final states above the nonergodic transition point. It is observed that the time-dependent solutions of the derived dynamical systems obtained by the perturbation analysis become systematically closer to the results obtained by Monte Carlo simulations as the order of the perturbation series is increased. This systematic perturbation analysis also clarifies the existence of a dynamical scaling law, which provides an implication for a universal relation between a size scale and a timescale near the nonergodic transition.

Keywords: percolation problems (theory), dynamical processes (theory), stochastic processes (theory), slow relaxation and glassy dynamics

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1. Introduction

Recently, soft materials such as colloidal and granular systems have attracted considerable interest owing to their rich behaviours. For instance, such systems can be in a supercooled state under conditions of low temperature and high density [1]. Under such conditions, a characteristic time acts as a function of system parameters such as temperature or density, and often obeys a non-Arrhenius law, which substantially influences the properties of the materials. Understanding the mechanism of such anomalous dynamical behaviours in many-body systems is important in the field of statistical physics.

The kinetically constrained spin model (KCSM) is a simple model that follows the non-Arrhenius law [2]–[4]. Thus far, it has been rigorously proved that the characteristic times in some kinds of KCSM on finite-dimensional lattices show super-Arrhenius type and Vogel–Fulcher type behaviours [5, 6]. Furthermore, in the case of a KCSM on a Bethe lattice, another non-Arrhenius type behaviour of the characteristic time has been found by Monte Carlo simulations [7]. From a static aspect, this non-Arrhenius type behaviour is due to a nonergodic transition corresponding to k-core percolation; this transition is not a thermodynamic phase transition. Concretely, at this percolation point, the characteristic time diverges with a power-law (non-Arrhenius law); this divergence is supposedly controlled by a mode-coupling equation [7].

The above mentioned mode-coupling equations are also believed to be related with the anomalous dynamical behaviours of colloidal or granular systems. A related conjecture is that a finite-dimensional system mimics a nonergodic transition described by a mode-coupling equation in a mean field sense although it is not a true nonergodic transition but a strong finite-size effect [1]. In the case of the KCSM, it has been rigorously proved

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that the nonergodic transition observed specifically in the KCSM on a Bethe lattice does not occur in the model on a finite-dimensional lattice although there are strong finite-size effects arising from the nonergodic transition on the Bethe lattice \cite{8, 9}.

This leads us to consider whether the mechanisms of the appearance of such strong finite-size effects for different finite-dimensional systems have common features. In order to resolve this problem, it is necessary to find a relationship between the KCSM and mode-coupling equations. However, the mode-coupling equation describing the nonergodic transition has not been derived yet for the KCSM on Bethe lattices; there have been some related studies on the derivations of mode-coupling equations for the KCSM \cite{10}–\cite{14}.

In this paper, as a preliminary step to understand such a relationship, we attempt to clarify the dynamical aspect of the universality class of the nonergodic transition observed in the Fredrickson–Andersen model (a KCSM) on a Bethe lattice. Concretely, we derive approximately dynamical systems from this model using a perturbation analysis which provides exact final states as stationary solutions above the nonergodic transition. We find that the universal class of the nonergodic transition cannot be captured by each dynamical system only at any order of the perturbation. Nevertheless, we find that the differences between the time-dependent solutions of the derived dynamical systems and the results obtained by Monte Carlo (MC) simulations are systematically reduced on a perturbation series. Furthermore, we find that this systematic perturbation analysis clarifies the existence of a dynamical scaling law, which provides an implication for a universal relation between a size scale and a timescale near the nonergodic transition.

2. Model

Let us consider a regular random graph consisting of \( N \in \mathbb{N} \) sites, each of which connects to \( c \in \mathbb{N} \) sites chosen randomly, where \( \mathbb{N} \) is the set of natural numbers. Then \( G(c, N) \) is defined as a set of such regular random graphs. For the spin variable \( \sigma_i \in \{-1, 1\} \) defined on each site \( i \in \{1, \ldots, N\} \) in a graph \( G \in G(c, N) \), the Hamiltonian we consider is

\[
H(\sigma) = \frac{1}{2} \sum_{i=1}^{N} \sigma_i, \tag{1}
\]

where we express \( \sigma \equiv (\sigma_i)_{i=1}^{N} \) collectively. Here, as a preliminary step to define the dynamics of the system, let us consider a transition rate \( r(\sigma, F_i \sigma) \) from \( \sigma \) to \( F_i \sigma \), which satisfies the detailed balance condition. Here \( F_i \) is the spin flip operator such that \( F_i \sigma = (\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N) \). Let \( B_i \) be a set of sites connected to site \( i \). Next, we consider the following dynamical rule. If the number of upward spins on the sites in set \( B_i \) is more than or equal to \( k \in \mathbb{N} \), the spin on site \( i \) does not flip absolutely; otherwise, the spin on site \( i \) flips at a transition rate \( r(\sigma, F_i \sigma) \). In other words, under this rule, the transition rate \( T(\sigma \to F_i \sigma) \) from \( \sigma \) to \( F_i \sigma \) is expressed by \( r(\sigma, F_i \sigma) \Theta(2k - c - \sum_{j \in B_i} \sigma_j) \), where \( \Theta(x) = 1 \) for \( x > 0 \), otherwise 0. We define the situation of a spin \( \sigma_i \) with \( \Theta(2k - c - \sum_{j \in B_i} \sigma_j) = 0 \) as ‘kinetically constrained’ or simply ‘constrained’. The master equation for the probability \( P(\sigma, t) \) that the spin configuration at time \( t \) is \( \sigma \) is

\[
\partial_t P(\sigma, t) = \sum_{i=1}^{N} [T(F_i \sigma \to \sigma)P(F_i \sigma, t) - T(\sigma \to F_i \sigma)P(\sigma, t)]. \tag{2}
\]
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In this paper, we consider the case

\[ r(\sigma, F, \sigma) = \min \left( 1, \exp \left( \frac{H(\sigma) - H(F, \sigma)}{T} \right) \right). \]  

(3)

Under this constrained dynamical rule, it may be confirmed that the canonical distribution is a stationary distribution. Further, in equilibrium, the magnetization per site is \( m_{eq}(T) = \tanh(1/2T) \), and the energy density is \(-\tanh(1/2T)/2\). Therefore, there are no thermodynamic phase transitions in the system. In this paper, MC simulations are performed by the following rule. First, a site \( i \) is randomly chosen. Next, the spin on site \( i \) flips with the probability \( T(\sigma \rightarrow F_i \sigma) \). This step is repeated and time \( t = 1 \) is defined by \( N \) repeated steps. It is plausible that in the thermodynamic limit, this MC simulation is the same as the dynamics of the system described by equation (2).

Here we briefly review the static aspect of a nonergodic transition in the system caused by the constrained dynamics, which is discussed in the previous study [7]. Suppose that a spin \( \sigma_i \) is constrained. If this constraint is permanent, we define the situation of the spin \( \sigma_i \) as 'frozen'. Here, let us consider a Cayley tree, which has the same local structures as those of the random graph, ignoring the effects of the loop length \( O(\log N) \). Let \( g \in \{1, 2, \ldots, g_{\text{max}}\} \) be a generation of a Cayley tree where \( g = 1 \) is assigned to the root. Let us consider the probability \( Q_g \) that a spin at the \( g \)th generation obtained under equilibrium conditions dependent on \( T \) is frozen and upward without considering the state of spin at the \((g-1)\)th generation. From the tree structure of the graph, we can obtain the relation

\[ Q_{g-1} = F(Q_g), \]  

(4)

\[ F(Q_g) = p(T) \sum_{n=k}^{c-1} \binom{c-1}{n} Q_g^n (1 - Q_g)^{c-1-n}, \]  

(5)

where \( p(T) \equiv 1/(1 + \exp(-1/T)) \). It should be noted that by solving recursion equation (5) for given values of \( Q_{g_{\text{max}}} \), \( Q_g \) for \( g \ll g_{\text{max}} \) becomes a solution \( Q(h) \) satisfying \( Q(T) = F(Q(T)) \). When \( c = 4 \) and \( k = 3 \), \( Q(T) \) is zero for sufficiently high temperatures. However, when the temperature is decreased, \( Q(T) \) can suddenly take a finite value at finite temperature \( T_c = 0.480 \), as shown in the left-hand side of figure 1. This singular point is the \( k \)-core percolation point, below which the system is nonergodic. Using the quantity \( Q(T) \), the fraction \( \phi \) of frozen spins is described as

\[ \phi(T) = p(T) \sum_{n=k}^{c} \binom{c}{n} Q(T)^n (1 - Q(T))^{c-n} \]

\[ + (1 - p(T)) \sum_{n=k}^{c} \binom{c}{n} (Q'(T))^n (1 - Q'(T))^{c-n}, \]  

(6)

where \( Q'(T) = p(T) \sum_{n=k}^{c-1} \binom{c-1}{n} Q(T)^n (1 - Q(T))^{c-1-n} \). In this model, it has been known that for \( 2 < k < c \) this type of nonergodic transition occurs at \( T = T_c \) with \( 0 < T_c < \infty \). For \( k = c \), \( T_c \) is zero, and for \( k \leq 2 \), \( T_c \) is \( \infty \). The schematic phase diagram is shown in the right-hand side of figure 1.

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3. Simple analysis of the dynamics

Although master equation (2) provides the complete information about the system, it is very difficult to extract useful information on the system from (2) because the system has $2^N$ states, which is quite a large number when $N$ is large. To avoid this difficulty, we consider describing the system by $N_{\text{eff}} \in \mathbb{N}$ number of variables and derive approximately a dynamical system closed by the set of the variables, where $N_{\text{eff}}$ remains finite when $N \to \infty$. For simplicity, we consider the relaxation behaviours of the system for the initial condition $\hat{m}(0) = -1$ where $\hat{m}(t) \equiv \sum_{i=1}^{N} \sigma_i / N$. It should be noted that the spin configuration for $\hat{m}(0) = -1$ has no constrained spins. In the following analysis, we fix a graph $\mathcal{G} \in \mathcal{G}(c, N)$ for sufficiently large $N$ without considering ensembles for $\mathcal{G}(c, N)$. In other words, the following analysis can be applicable to almost all graphs $\mathcal{G} \in \mathcal{G}(c, N)$ in the thermodynamic limit.

As a first step to derive an effective dynamical system, let $P_i(\sigma; t)$ be the probability that $\sigma_i$ takes $\sigma$ at time $t$ and $P_i((\sigma_j')|\sigma'; t)$ be the probability that the spin configuration on the sites in set $B_i$ is $(\sigma_j')_{j \in B_i}$ provided that $\sigma_i$ takes $\sigma'$ at time $t$. Then, we have the following exact evolution equation:

$$
\partial_t P_i(\sigma; t) = \sum_{(\sigma_j')} \Theta \left( 2k - c - \sum_{j' \in B_i} \sigma_{j'} \right) \times 
\left[ -r_\sigma P_i(\sigma; t) P_i((\sigma_j')|\sigma; t) + r_{-\sigma} P_i(-\sigma; t) P_i((\sigma_j')|\sigma; t) \right].
$$

where we define $r_\sigma \equiv \min(1, \exp(-\sigma/T))$. Here we assume that the value of $P_i((\sigma_j')|\sigma)$ does not depend on the chosen site $i$. This assumption may be plausible because at least, in this case, inhomogeneous properties of the system arising from the effects of loops of the random graph $\mathcal{G}$ may be negligible in the thermodynamic limit. This assumption corresponds to the assumption that $P_i((\sigma_j')|\sigma)$ is the same as the conditional probability $P((\sigma_j')|\sigma; t)$ that if a site with spin variable $\sigma$ is randomly chosen, the spin configuration
of its nearest neighbour sites is \((\sigma'_j)\). With this assumption, equation (7) is rewritten as
\[
\partial_t \rho_\sigma(t) = \sum_{(\sigma'_j)} \Theta \left( 2k - c - \sum_{j' \in B_\sigma} \sigma'_j \right) [-r_\sigma \rho_\sigma(t) P((\sigma'_j)|\sigma;t) + r_{-\sigma} \rho_{-\sigma}(t) P((\sigma'_j)|-\sigma;t)],
\]
where \(B_\sigma\) is a set of sites connected to a site with spin variable \(\sigma\) and \(\rho_\sigma \equiv \sum_{i=1}^N P_i(\sigma)/N\). It is plausible that \(\rho_\sigma\) is identical to \(\sum_i \delta(\sigma - \sigma_i)/N\) in the thermodynamic limit \(N \to \infty\). That is, the magnetization is expressed as
\[
m(t) = \sum_\sigma \sigma \rho_\sigma(t).
\]

Next, we use the approximation that the spin variables on individual sites are independent of each other, which is exact for equilibrium spin configurations. That is, we rewrite \(P((\sigma'_j)|\sigma;t)\) as
\[
P((\sigma'_j)|\sigma;t) = \prod_{j \in B_\sigma} \rho_{\sigma_j}(t).
\]
Further, we can obtain a simpler expression as follows:
\[
\sum_{(\sigma'_j)} \Theta \left( c - 2k - \sum_{j' \in B_\sigma} \sigma'_j \right) \prod_{j \in B_\sigma} \rho_{\sigma_j}(t) = \sum_{l=f}^c \binom{c}{l} \rho_{l-1}(t) \rho_{l+1}(t)^{c-l},
\]
where we define \(f \equiv c - k + 1\). Equations (7), (9), and (10) lead to a closed dynamical system in terms of \(\rho^{(0)} \equiv (\rho_\sigma)_{\sigma}^0\):
\[
\partial_t \rho^{(0)} = G^{(0)}(\rho^{(0)}).
\]

It should be noted that stationary solutions of dynamical system (11) provide the exact final states above the nonergodic transition point. However, the behaviours of the system at intermediate timescales are very different from the MC simulations, as seen in figure 2. This means that approximation (9) fails to capture the heterogeneous spin configurations responsible for the dynamics in intermediate timescales. In this paper, we use the fourth-order Runge–Kutta method to obtain solutions of dynamical systems with the time discretization \(dt = 10^{-2}\).

Here, let us consider a persistent time \(\tau_p(i)\) of a site \(i\), which is the time span for a spin to flip at site \(i\). Next, let us focus on the target site \(i\) in the set \(C_i\) of sites on which constrained spins are connected to each other. Clearly, \(\tau_p(i)\) strongly depends on the entire spin configuration of sites in set \(C_i\) because the spins from an edge site in set \(C_i\) must be flipped in order to flip the target spin \(\sigma_i\). Furthermore, the spin configuration on the sites in set \(C_i\) is heterogeneous in terms of the spin direction if it is prepared from the equilibrium spin configurations. This suggests that in order to detect growing relaxation times of the system with respect to the persistent time, it is necessary to obtain information on the heterogeneous configurations of the connected constrained spins.

4. Perturbation analysis of the dynamics

From the results in section 3, heterogeneous spin configurations seem to play important roles in the growing relaxation times of the system. Therefore, in order to continue our analysis, we attempt to apply the information on the surrounding spin configurations of a target site perturbatively to effective variables by increasing the value of \(N_{\text{eff}}\). Such a method has been previously applied to some systems and was successful in determining some nontrivial dynamical properties [15, 16].

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4.1. First layer

We attempt to apply the information on the first ‘layer’ of surrounding spin configurations of a target site to effective variables. To this end, we suppose \( w_i \in \{1, \ldots, c\} \) as the number of downward spins on sites in set \( B_i \). With this representation, site \( i \) is characterized by \( (\sigma_i, w_i) \). Here, let \( P_i(\sigma, w; t) \) be the probability that \( (\sigma_i, w_i) \) takes \( (\sigma, w) \) and \( P_{ij}(\sigma, w|\sigma', w'; t) \) be the conditional probability that \( (\sigma_i, w_i) \) takes \( (\sigma, w) \) provided that \( (\sigma_j, w_j) \) takes \( (\sigma', w') \). Of course, a trivial relation \( \sum_{\sigma} \sum_{w} P_i(\sigma, w; t) = 1 \) holds. Using these expressions, we have the following exact evolution equation:

\[
\partial_t P_i(\sigma, w; t) = (-r_\sigma P_i(\sigma, w; t) + r_\sigma P_i(\sigma, w; t)) \Theta(w - f) \\
+ \sum_{j \in B_i} \sum_{\sigma'} \sum_{w = f} c r_{\sigma'} P_j(\sigma', w'; t) \\
\times (P_{ij}(\sigma, w + \sigma'|\sigma', w'; t) - P_{ij}(\sigma, w|\sigma', w'; t)),
\]

where \( f \) is defined as \( c - k + 1 \) and \( \Theta(x) = 1 \) for \( x \geq 0 \), otherwise 0.

Here, we assume that the value of \( P_{ij}(\sigma, w|\sigma', w') \) does not depend on the chosen sites \( i \) and \( j \) if two sites \( i \) and \( j \) are chosen among the pairs of sites which have the same distance. This assumption may be plausible because at least, in this case, the inhomogeneous properties of the system arising from the effects of loops of the random graph \( \mathcal{G} \) may be negligible in the thermodynamic limit. This assumption corresponds to the assumption that \( P_{ij}(\sigma, w|\sigma', w'; t) \) with \( j \in B_i \) is the same as the conditional probability \( P_{i1}(\sigma, w|\sigma', w'; t) \) that after a site characterized by \( (\sigma', w') \) is randomly chosen, then one of its nearest neighbour sites, when randomly chosen, is characterized by \( (\sigma, w) \).
Here, let us define
\[
P_{c1}(w|\sigma', w'; \tau) \equiv \frac{P_{c1}(\sigma, w|\sigma', w'; t)}{P_{c1}(\sigma|\sigma', w'; t)},
\]
where \(P_{c1}(\sigma|\sigma', w'; t)\) is defined in a similar way to \(P_{c1}(\sigma, w|\sigma', w'; t)\). In fact, we can obtain
\[
P_{c1}(\sigma|\sigma', w'; t) = \frac{1}{c} C_{\sigma}(w'),
\]
\[
C_{\sigma}(w') = \begin{cases} 
  c - w' & (\sigma = 1) \\
  w' & (\sigma = -1).
\end{cases}
\]
Therefore,
\[
\partial_t \rho_{\sigma, w}(t) = \left( \sum_{\sigma'} \sum_{w'=f} r_{\sigma'}\rho_{\sigma',w'}(t) C_{\sigma}(w')(P_{c1}(w + \sigma'|\sigma', w'; t) - P_{c1}(w|\sigma', w'; t)) \right)
\]
\[
+ \sum_{\sigma'} \sum_{w'=f} r_{\sigma'}\rho_{\sigma',w'}(t) C_{\sigma}(w') (P_{c1}(w|\sigma', w'; t) - P_{c1}(w|\sigma', w'; t)),
\]
where \(\rho_{\sigma, w} = \sum_{i=1}^{N} P_i(\sigma, w)/N\). It is plausible that \(\rho_{\sigma, w}\) corresponds to \(\sum_{i=1}^{N} \delta(\sigma - \sigma_i)\delta(w - w_i)/N\) in the thermodynamic limit \(N \to \infty\). That is, the magnetization is expressed as
\[
m(t) = \sum_{\sigma} \sum_{w=0}^{c} \sigma \rho_{\sigma, w}(t).\]
Here, in order to obtain a closed description in terms of \(\rho^{(1)} \equiv (\rho_{\sigma, w})_{\sigma, w}\), we use the following approximation:
\[
P_{c1}(w|\sigma', w'; t) = P_{c1}^{\sigma}(w|\sigma'; t),
\]
which is exact for equilibrium states. Hence, we can obtain
\[
P_{c1}^{\sigma}(w - 1; t) = \frac{w\rho_{\sigma, w}(t)}{\sum_{w=0}^{c} w\rho_{\sigma, w}(t)},
\]
\[
P_{c1}^{\sigma}(w + 1; t) = \frac{(c - w)\rho_{\sigma, w}(t)}{\sum_{w=0}^{c} (c - w)\rho_{\sigma, w}(t)}.
\]
Equations (16)–(19) lead to a closed dynamical system in terms of \(\rho^{(1)}\) as follows:
\[
\partial_t \rho^{(1)} = G^{(1)}(\rho^{(1)}).
\]

The stationary solutions of dynamical system (20) also provide the exact final states above the nonergodic transition point. The dynamical behaviours of dynamical system (20) are closer to the MC simulations than those of dynamical system (11). However, as seen in figure 3, the behaviours of dynamical system (20) also gradually deviate from the MC simulations if the temperature approaches the transition point \(T_c\). This deviation indicates that approximation (17) does not determine the behaviours at low temperatures.
does not depend on the chosen sites. Provided that \(P\) where \(j\) is plausible because at least, in this case, the inhomogeneous properties of the system arising the same relationship for their distances in the chosen sequence. These assumptions are from the effects of loops of the random graph.

Figure 3. Time-dependent magnetization \(\sum_\sigma \sum_{\ell=0}^c \sigma \rho_{\sigma,\ell}\) described by (20) and \(\tilde{m}\) by the MC simulations with \(N = 10^6\) for \(c = 4, k = 3\).

4.2. Second layer

We attempt to apply the information on the second ‘layer’ of the surrounding spin configurations of a target site to effective variables. Here, to include such effects, we consider the following characterization of a site. First, let \(l_i \in \{1, \ldots, c\}\) be the number of downward-constrained spins on sites in set \(B_i\). Second, let \(u_i \in \{1, \ldots, c\}\) be the number of upward-constrained spins and \(v_i \in \{1, \ldots, c\}\) be the number of downward constrained spins on the sites in set \(B_i\). Thus, a site \(i\) is characterized by \((\sigma_i, l_i, u_i, v_i)\).

With these expressions, let \(P_l(\sigma, l, u, v; t)\) be the probability that \((\sigma_i, l_i, u_i, v_i)\) takes \((\sigma, l, u, v)\). In addition, let \(P_{ij}(\sigma, l, u, v|\sigma', l', u', v'; t)\) be the conditional probability that \((\sigma_i, l_i, u_i, v_i)\) takes \((\sigma, l, u, v)\) provided that \((\sigma_j, l_j, u_j, v_j)\) takes \((\sigma', l', u', v')\), and let \(P_{i_1i_2i_3}((\sigma_1, l_1, u_1, v_1), (\sigma_2, l_2, u_2, v_2)|\sigma_3, l_3, u_3, v_3; t)\) be the conditional probability that \((\sigma_{i_1}, l_{i_1}, u_{i_1}, v_{i_1})\) and \((\sigma_{i_2}, l_{i_2}, u_{i_2}, v_{i_2})\) take \((\sigma_1, l_1, u_1, v_1)\) and \((\sigma_2, l_2, u_2, v_2)\) respectively, provided that \((\sigma_{i_1}, l_{i_1}, u_{i_1}, v_{i_1})\) takes \((\sigma_3, l_3, u_3, v_3)\).

As in the previous sections, we assume that the value of \(P_{ij}(\sigma, l, u, v|\sigma', l', u', v')\) does not depend on the chosen sites \(i, j\) if two sites \(i, j\) are chosen among the pairs of sites which have the same distance. In addition, we assume that the value of \(P_{i_1i_2i_3}((\sigma_1, l_1, u_1, v_1), (\sigma_2, l_2, u_2, v_2)|\sigma_3, l_3, u_3, v_3)\) does not depend on the chosen sites \(i_1, i_2, i_3\) if three sites \(i_1, i_2\) and \(i_3\) are chosen among the sets of three sites which have the same relationship for their distances in the chosen sequence. These assumptions are plausible because at least, in this case, the inhomogeneous properties of the system arising from the effects of loops of the random graph \(G\) may be negligible in the thermodynamic limit. This assumption corresponds to the assumption that \(P_{ij}(\sigma, l, u, v|\sigma', l', u', v')\) where \(j \in B_i\) is the same as \(P_{i_1}(\sigma, l, u, v|\sigma', l', u', v')\) and to the assumption that \(P_{i_1i_2i_3}((\sigma_1, l_1, u_1, v_1), (\sigma_2, l_2, u_2, v_2)|\sigma_3, l_3, u_3, v_3)\) where \(i_2 \in B_{i_1}, i_3 \in B_{i_2}(i_3 \neq i_1)\).
is the conditional probability $P_{c2}((\sigma_1, l_1, u_1, v_1), (\sigma_2, l_2, u_2, v_2)|\sigma_3, l_3, u_3, v_3)$ that a site characterized by $(\sigma_3, l_3, u_3, v_3)$ is randomly chosen first, after which one of two connected sites, which is connected to the first chosen site, is randomly chosen, then among the two connected sites the far site from the first chosen site is characterized by $(\sigma_1, l_1, u_1, v_1)$, and the near site is characterized by $(\sigma_2, l_2, u_2, v_2)$.

Further, we define

$$P_{c1}^{l, \sigma}(u, v|\sigma', l', u', v') \equiv \frac{P_{c1}(\sigma, l, u, v|\sigma', l', u', v')}{P_{c1}(\sigma, l'|\sigma', l', u', v')}.$$  \hspace{1cm} (21)

Using this representation, we also define

$$P_{c2}^{l, \sigma_1}(l_1, u_1, v_1|(\sigma_2, l_2, u_2, v_2), (\sigma_3, l_3, u_3, v_3)) \equiv \frac{P_{c2}(\sigma_1, l_1, u_1, v_1)|\sigma_2, l_2, u_2, v_2, \sigma_3, l_3, u_3, v_3)}{P_{c2}(\sigma_1, l_1)|(\sigma_2, l_2, u_2, v_2), (\sigma_3, l_3, u_3, v_3)} \times P_{c2}^{l, \sigma_2}(u_2, v_2|\sigma_3, l_3, u_3, v_3)P_{c1}(\sigma_2, l_2|\sigma_3, l_3, u_3, v_3).$$ \hspace{1cm} (22)

In fact, we can obtain

$$P_{c1}(\sigma, l|\sigma', l', u', v') = \frac{1}{c} C_{\sigma, l}(l', u', v'),$$

$$C_{\sigma, l}(l', u', v') = \begin{cases} 
  u' & (\sigma = 1, l < f) \\
  v' & (\sigma = -1, l < f) \\
  l' - v' & (\sigma = -1, l \geq f) \\
  c - l' - u' & (\sigma = 1, l \geq f),
\end{cases}$$ \hspace{1cm} (23)

$$P_{c2}(\sigma_1, l_1|(\sigma_2, l_2, u_2, v_2), (\sigma_3, l_3, u_3, v_3)) = \frac{1}{c - 1} C_{\sigma_1, l_1}(l_2, u_2, v_2, \sigma_3, l_3),$$

$$C_{\sigma_1, l_1}(l_2, u_2, v_2, \sigma_3, l_3) = \begin{cases} 
  u_2 - \delta(\sigma_3 - \sigma_1)\Theta(f - l_3) & (\sigma_1 = 1, l_1 < f) \\
  v_2 - \delta(\sigma_3 - \sigma_1)\Theta(f - l_3) & (\sigma_1 = -1, l_1 < f) \\
  l_2 - v_2 - \delta(\sigma_3 - \sigma_1)\Theta(l_3 - f) & (\sigma_1 = -1, l_1 \geq f) \\
  c - l_2 - u_2 - \delta(\sigma_3 - \sigma_1)\Theta(l_3 - f) & (\sigma_1 = 1, l_1 \geq f).
\end{cases}$$ \hspace{1cm} (24)

Using these expressions, we can write the evolution equation as follows:

$$\partial_l \rho_{\sigma, l, u, v} = (-r_\sigma \rho_{\sigma, l, u, v} + r_{-\sigma} \rho_{-\sigma, l, u, v})\Theta(l - f)$$

$$+ \sum_{\sigma'} \sum_{l' = f}^{c - l} \sum_{u' = 0}^{l'} \sum_{v' = 0}^{l'} r_{\sigma'} \rho_{\sigma', l', u', v'} C_{\sigma, l}^{l'}(l', u', v')$$

$$\times [P_{c1}^{l, \sigma} (u, v|\sigma', l', u', v') - P_{c1}^{l, \sigma} (l, u|\sigma', l', u', v')]$$

$$+ \sum_{\sigma'} \sum_{l'' = f}^{c - f + 1} \sum_{u'' = 0}^{l''} \sum_{v'' = 0}^{l''} r_{+1} \rho_{+1, l''} C_{\sigma', l''}(l'', u'', v'')$$

$$\times \sum_{\sigma} \sum_{u'' = 0}^{l''} \sum_{v'' = 0}^{l''} P_{c1}^{l - 1, \sigma} (u'', v''|+1, l'', u'', v'' ) C_{\sigma, l}(l', u', v', +1, l'')$$

$$\times [P_{c2}^{l, \sigma} (u + \delta(\sigma' + 1), v + \delta(\sigma' - 1)|\sigma', f - 1, u', v'), (+1, l'', u'', v'')]$$
Systematic perturbation approach for a dynamical scaling law in a kinetically constrained spin model

\[ - P_{c1}^{l \sigma}(u, v|\{(\sigma', f - 1, u', v'), (\sigma'', l'', u'', v''\})] + \sum_{c_l=0}^{c-1} \sum_{v''=0}^{v''} r_{-l-1, v''} C_{\sigma'}(l'', u'', v'') \]

\[ \times \sum_{c_{l'}=0}^{c-l'} \sum_{l''=0}^{l''} P_{c1}^{l' \sigma}(u', v'| - 1, l'', u'', v'') C_{\sigma,l}(l', u', v', -1, l'') \]

\[ \times \left[ P_{c2}^{l \sigma}(u + \delta(\sigma' + 1), v + \delta(\sigma' - 1))(\sigma', f, u', v'), (-1, l', u'', v'') \right] - P_{c2}^{l \sigma}(u, v|\{(\sigma', f, u', v'), (-1, l', u'', v''\}]) \]

where \( \rho_{\sigma, luv} \equiv \sum_{i=1}^{N} P_{\sigma, i, l, u, v; t}/N \). It is plausible that \( \rho_{\sigma, luv} \) corresponds to \( \sum_{i=1}^{N} \delta(c - c_{i}) \delta(l - l_{i}) \delta(u - u_{i}) \delta(v - v_{i})/N \) in the thermodynamic limit \( N \to \infty \). Using this, the magnetization is expressed as \( m(t) = \sum_{\sigma} \sum_{l=0}^{c-l} \sum_{u=0}^{u} \sum_{v=0}^{v} \rho_{\sigma, luv}(t) \). In order to obtain a closed dynamical system in terms of \( \rho^{(2)} \equiv (\rho_{\sigma, luv})_{\sigma, luv} \), we use the following approximations:

\[ P_{c2}^{l \sigma}(u_{1}, v_{1}|(\sigma_{2}, l_{2}, u_{2}, v_{2}), (\sigma_{3}, l_{3}, u_{3}, v_{3})) = P_{c1}^{l \sigma}(u_{1}, v_{1}|\sigma_{2}, l_{2} \geq f), \]

\[ P_{c1}^{l \sigma}(u, v|\sigma', l', u', v') = P_{c1}^{l \sigma}(u, v|\sigma', l' \geq f), \]

which are exact for equilibrium states. In fact, we can obtain the concrete expression of \( P_{c1}^{l \sigma}(u, v|\sigma', l' \geq f) \) as follows:

\[ P_{c1}^{l \sigma}(u, v|1, l' \geq f) = (c - l - u) \rho_{\sigma, luv}/ \sum_{l' \geq f, uv} (c - l - u) \rho_{\sigma, luv}, \]

\[ P_{c1}^{l \sigma}(u, v|1, l' < f) = u \rho_{\sigma, luv}/ \sum_{l' \geq f, uv} u \rho_{\sigma, luv}, \]

\[ P_{c1}^{l \sigma}(u, v|-1, l' \geq f) = (l - v) \rho_{\sigma, luv}/ \sum_{l' \geq f, uv} (l - v) \rho_{\sigma, luv}, \]

\[ P_{c1}^{l \sigma}(u, v|1, l' < f) = v \rho_{\sigma, luv}/ \sum_{l' \geq f, uv} v \rho_{\sigma, luv}, \]

where \( \sum_{l \geq f, uv} = \sum_{c_l=f}^{c-l} \sum_{u=0}^{u} \sum_{v=0}^{v} \) and \( \sum_{l < f, uv} = \sum_{l=0}^{f-1} \sum_{u=0}^{c-l} \sum_{v=0}^{v} \). That is, equations (25)–(31) lead to a closed dynamical system in terms of \( \rho^{(2)} \) as follows:

\[ \partial_{t} \rho^{(2)} = G^{(2)}(\rho^{(2)}). \]

The stationary solutions of dynamical system (32) also provide exact final states of the system above the nonergodic transition point. Further, the solutions of dynamical system (32) are closer to the MC simulations than those of the previous two descriptions. However, similar to the previous descriptions, the solutions gradually deviate from the MC simulations for lower temperatures, as seen in figure 4.

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5. On a perturbation series

5.1. Systematic improvement of the solutions

We consider the manner of changes in the solutions of the derived dynamical systems on a perturbation series. It is noteworthy that the differences between the MC simulations and the time-dependent solutions of the derived dynamical systems are systematically reduced with the increase in the number $n$ of $\rho^{(n)}$, as observed in the left-hand side of figure 5.

The MC simulations show that under the initial condition that all spins are downward, the magnetization behaves as $\hat{m}(t) \approx m_{\text{eq}}(T) \exp(-t/\tau)$ in the long time limit, as shown in the right-hand side of figure 5. As shown in figure 6, a rough estimation of $\tau$ indicates the behaviour $\tau \approx \epsilon^{-\zeta}$, where $\zeta \approx 3$ and $\epsilon \equiv (T/T_c - 1)$. In fact, the value around $\zeta \approx 3$ has been already confirmed for the persistent time in a previous study [7].
Let us consider the relaxation time $\tau_n(T)$ of the dynamical systems defined as $|\lambda^{(n)}|^{-1}$, where $\lambda^{(n)}$ is the maximum eigenvalue, except for trivial zero, of matrix $M^{(n)}$ obtained by linearizing $G^{(n)}$ at a stationary solution $\rho^{(n)}_{\text{st}} \equiv \lim_{t \to \infty} \rho^{(n)}(t)$ with $\hat{m}(0) = -1$. $\tau_n(T)$ does not show the power-law behaviour $\epsilon^{-\zeta}$, as seen in figure 6, although when $\epsilon$ is slightly below 1, $\tau_n(T)$ behaves as $\epsilon^{-\zeta_n}$ with $\zeta_n < \zeta_{n+1} < \zeta$, and $\tau_n(T_c)$ is finite. Thus, higher order analyses will be needed to capture the power-law behaviour $\epsilon^{-\zeta}$.

5.2. Systematic construction of higher order perturbations

In this section, we consider a perturbation analysis that is of a higher order than those discussed thus far. Let us reiterate the way to characterize a site discussed in section 4.1. In the analysis, in order to define the effective state of a target site $i$, we use information of sites in set $B_i$. We regard the way of such a characterization of site $i$ as the first order characterization. Next, let us reiterate the way to characterize a site discussed in section 4.2. In the analysis, in order to define the effective state of a target site $i$, we use information on sites in set $B_i$ and set $B_j$ with $j \in B_i$. In other words, site $i$ is characterized by the number of sites in set $B_i$, where each site in set $B_i$ is characterized by the information on the first order characterization. We regard such a characterization of site $i$ as the second order characterization.

Using this second order characterization, we can characterize the sites in set $B_i$ except for the information on the branch directed to site $i$. Next, site $i$ is characterized by the number of sites in set $B_i$, where each site in set $B_i$ is characterized by the above characterization. This procedure defines third order characterization of site $i$. In the same way, we can define arbitrary $n$th order characterization iteratively.

Further, essentially the same approximation as those used in the first order and second order perturbation analyses can be applicable to $n$th order perturbation analysis, which
provides the exact final states of the system as stationary solutions above the transition point. With this procedure, in principle, we can compute the relaxation time \( \tau_n(T) \) described by the dynamical system for all \( n \) orders. In this perturbation series, the formal ‘small’ parameter can be regarded as the distance between which sites are used for defining the effective states of a target site. It should be noted that the concrete value of \( n \) does not have any significance other than in the sequence, and \( \infty \)-order perturbation analysis may provide the original master equation in the thermodynamic limit by the definition.

5.3. A dynamical scaling law in maximum eigenvalues at \( T_c \)

The systematic improvement of the solutions described by the derived dynamical systems on a perturbation series and the systematic construction of a higher order perturbation series motivate us to consider some scaling relation between order \( n \) in the perturbation series and relaxation time (the inverse of the maximum eigenvalue) \( \tau_n(T) \). The first question raised here is how large an \( n \) causes the divergence of \( \tau_n(T_c) \) as \( \lim_{n \to n_c} \tau_n(T_c) \to \infty \). On the basis of the consideration that the size of connected constrained sites with the heterogeneous spin configuration resulting in the maximum relaxation time can be infinite for equilibrium spin configurations at \( T = T_c \), we can expect \( n_c = \infty \). Explicitly, using a function \( F \) dependent on \((c,k)\), we express \( \tau_n(T_c) = F(n,c,k) \) where \( F(n,c,k) \to \infty \) with \( n \to \infty \).

As shown in figure 6, since \( \tau_0 \) seems to be out of the scaling region even if some scaling relation exists, we focus on \( \tau_1(T_c) \) and \( \tau_2(T_c) \) for various parameters \((c,k)\). Let us recall that this perturbation analysis includes the effects of larger connected constrained spins if order \( n \) is increased. Therefore, it may be plausible that the accessible correlation sizes by the perturbation analysis with order \( n \) are increased as order \( n \) is increased. On the basis of this consideration, first, we assume that \( R(c,k;\alpha)n^\alpha \) expresses the accessible correlation sizes by the perturbation analysis with order \( n \), where \( R \) and \( \alpha \) are certain constants. It should be noted that the determination of \( \alpha \) needs the information about the nature of correlation sizes in the system, which is discussed in section 5.4. Furthermore, we also assume that \( \tau_n \) has power-law forms in the accessible correlation sizes in the system. Therefore, if we set a value of \( \alpha \), the above assumptions lead to the exponents of the power-law forms. That is, we assume the following form:

\[
\tau_n(T_c) = F_\alpha (R(c,k;\alpha)n^\alpha, c, k), \tag{33}
\]

where \( R(c,k;\alpha) \) are fitting parameters, and \( F_\alpha(x,c,k) = Cx^{z_\alpha} \). Surprisingly, as seen in figure 7, we can find that there are values of \( R \) for arbitrary values of \( \alpha \) such that \( F_\alpha(x,c,k) \) is independent of \( c \) within the numerical analysis. This result indicates that the assumption for the power-law dependences of \( \tau_n \) on order \( n \) is plausible. Concretely, \( \alpha z_\alpha(k;\alpha) \simeq z'(k) (z'(3) \simeq 2.15, z'(4) \simeq 2.4) \). In the following, we present some conjectures related to the nature of correlation sizes in the system.

5.4. Conjectures arising from dynamical scaling law (33)

The law (33) implies that there exists a characteristic size \( \mathcal{N} \) obeying the dynamical scaling law \( \tau(T) \simeq \mathcal{N}(T)^z \) where \( \tau(T) \) has already been defined through the relaxation of the magnetization. In fact, we already know a candidate of \( \mathcal{N}(T) \), which is called the minimal rearrangement size defined as the minimum number of flipped spins on the
surrounding sites of a target spin in order to flip the target spin [17,18]. The previous study has shown that the size scale shows a power-law behaviour such as $\epsilon^{-\nu(c,k)}$ near the nonergodic transition in the FA model [18].

Here, we mention the meaning of the parameter $\alpha$. Rough numerical simulations indicate that we need to set $\alpha = \alpha_{\text{mrs}} \simeq 1.1$ in order to identify $z_*$ as $z$. In this context, $\alpha_{\text{mrs}}$ can be regarded as the quantity connecting the perturbation order $n$ to the accessible minimal rearrangement size by the perturbation analysis with order $n$. In other words, if we obtain an exact value of $\alpha_{\text{mrs}}$ such that $\alpha_{\text{mrs}} z = z'$ in a certain case of $(c,k) = (c',k')$, the values of $z(= z'/\alpha_{\text{mrs}})$ in any cases $(c,k) \neq (c',k')$ can be derived by the perturbation analysis presented above, because the analysis provides $z'$ in any cases of $(c,k)$, in principle.

The result for $z_*$ leads to the conjecture that $z$ also does not depend on the value of $c$ with the same value of $k$. This means that the universality classes of nonergodic transitions in the kinetically constrained spin model are classified by the value of the constraint parameter $k$, and the quantity characterizing the universality is not $\zeta$ or $\nu$ but $z$, where $\zeta$ and $\nu$ depend on the value of $c$. Actually, we have performed MC simulations in order to confirm the above conjecture. Although we have found signs supporting the above conjecture, we could not obtain plausible results due to the finite-size effects and the limitation of the maximum step of time. It is an important future study to confirm the conjecture by MC simulations.

6. Concluding remarks

In this study, we have constructed a systematic perturbation analysis for the dynamics of the FA model on a Bethe lattice. This systematic perturbation analysis clarifies the
existence of a dynamical scaling law, which provides an implication for a universal relation between a size scale and a timescale near the nonergodic transition.

Here, we discuss the relevance of our results to the previous studies. Actually it has been conjectured that the persistent time found by MC simulations can be described by a mode-coupling equation [7]. This statement is not inconsistent with \( n_c = \infty \) because mode-coupling equations are \( \infty \)-dimensional differential equations. In addition, a fact supporting the relevance of the model to a mode-coupling equation has been stated in the literature on the analysis of the minimum size rearrangement [17]. In addition to the previous results, the results obtained in this paper provide another plausible conjecture for the properties of the nonergodic transition. That is, the nonergodic transitions have a weak universality. This means that the critical exponents \( \zeta, \nu \) for time and size depend on the value of \( c \), but the dynamical critical exponent \( z \) does not depend on the value of \( c \) with the same value of \( k \). A similar statement has been made in a previous study of the dynamical transition in the \( p \)-spin glass model on the Bethe lattice [19]. The study states that \( z \) does not depend on the quantity \( \gamma \) related to the connectivity of the graph, which plays the similar role to that of \( c \) in this paper. However, the study does not mention the dependence of \( z \) on the value of \( p \), which may play a similar role to that of \( k \) in this paper. The results in this paper indicate that \( z \) depends on the value of \( p \). The confirmation of this conjecture for the dynamical transition in the \( p \)-spin glass model is an important future study.

Another aspect of this weak universality appears in the comparison to the case of a ferromagnetic Ising model on a Bethe lattice. In a previous study, the critical exponent could be obtained using the dynamical system closed by a finite number of effective variables, which was derived by a similar approximation method to that of this paper [15]. Therefore, the universality class of the nonergodic transition in the KCSM is quantitatively and qualitatively different from that of the ferromagnet–paramagnet transition in some spin models including, at least, the Ising model. Here, the word ‘qualitatively’ means that the differences are located in not only the values of the critical exponents and the existence of the dynamical system closed by a finite number of variables capturing the critical exponent.

Finally, we discuss the relationship between the nonergodic transitions discussed in this paper and the related phase transitions in other systems [20]. In fact, the decimation dynamics of a random graph in the thermodynamic limit exhibits a saddle-node bifurcation at the \( k \)-core percolation point [21, 22]. Furthermore, a random-field Ising model with zero-temperature Glauber dynamics in the thermodynamic limit at a spinodal transition has been reported to correspond to the \( k \)-core percolation, which is also a saddle-node bifurcation on Bethe lattices [24, 25]. It should be noted that dynamical behaviours near these transitions corresponding to the saddle-node bifurcation are extremely different from the dynamics near the nonergodic transition in the FA model although they are \( k \)-core percolations from the static viewpoint. This difference may be related to the existence of a no-passing property in the system [23]. That is, the FA model does not have a no-passing property whereas the other systems do. This consideration leads to the conjecture that the nonergodic transition in other kinetically constrained spin models such as Kob–Andersen models belong to universality classes that are different from that of the saddle-node bifurcation; Such models do not have the no-passing property [3, 9]. Finally, we mention a previous study that suggests a relationship between the static properties of the
jamming transition and the $k$-core percolation [26, 27]. Since such a system showing the jamming transition does not have the no-passing property, finding a relationship between the macroscopic dynamical behaviours near the jamming transition and the KCSM is also an interesting topic for future studies.

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