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Analytical Approximations for the Hierarchically Constrained Kinetic Ising Chain

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The hierarchically constrained kinetic Ising model in one dimension is reviewed, and the results of several analytical approaches to the model are presented. Two standard approximation schemes, an effective-medium approximation and a mode-coupling approximation, are shown to fail. A new class of approximations, termed cluster approximations, is better suited for the model. It yields good results for the spin autocorrelation function, and also elucidates important general properties of the model—its connection with defect-diffusion models and the asymptotic long-time behavior of the autocorrelation function.

KEY WORDS: Ising models; kinetic constraint; effective-medium approximation; mode-coupling approximation; cluster approximation; long-time behavior.

1. INTRODUCTION

In ref. 1 the present authors have introduced a hierarchically constrained kinetic Ising model. The model consists of a semi-infinite Ising chain with an asymmetric constraint allowing a spin to flip only when its right neighbor is in the up-spin state. The constraint is purely kinetic. There is no interaction energy between different spins. The asymmetric kinetic constraint introduces dynamic correlations, and represents a simple realization of "hierarchically constrained dynamics" in the sense proposed by Abrahams *et al.*[2]

We calculate the normalized spin autocorrelation function $\phi(t)$, which we often simply call the relaxation function, from the decay of the orientation $\langle \sigma_0 \rangle_t$ of the spin at the origin, which initially is prepared in the

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up-spin state. For the discussion of the basic equations we refer to ref. 1. Here we only give the transition rate for the flip of spin i,

$$w_i(\sigma_0, \sigma_1, \ldots) = (\Gamma/4)[1 + (1-2c)\sigma_i](\sigma_{i+1} + 1)$$

where $c = (1 + (\langle \sigma \rangle_{eq})/2$, $\sigma = \pm 1$, from which the master equation for single-spin-flip dynamics[3] is obtained. The inverse of the attempt rate Γ is often chosen as the unit of time, such that Γ can be dropped.

First results for the relaxation function of finite and infinite chains are given in ref. 1. Here we present the results of several analytical approaches. In Section 2 of this paper we apply two standard approximation methods to our model. First we use an effective-medium approximation, then we derive a mode-coupling approximation. In Section 3 a new approximation method, the cluster approximation, is derived. Results for different orders of the approximation are calculated and discussed in detail. It turns out that for our model there exists a close connection between the cluster approximation and defect-diffusion models.[4,5] Using the result of a renormalization method presented in ref. 6, we are able to give an estimate for the asymptotic long-time behavior of the relaxation function for $c \to 0$.

2. TWO STANDARD APPROXIMATION SCHEMES

2.1. An Effective-Medium Approximation (EMA)

The normalized spin autocorrelation function

$$\phi(t) = \frac{\langle \Delta\sigma_0(t)\, \Delta\sigma_0(0) \rangle_{eq}}{4c(1-c)} \tag{1}$$

where $\Delta\sigma = \sigma - \langle \sigma \rangle$, $\langle \sigma \rangle = 2c - 1$, is derived from the decay of the orientation $\langle \sigma_0 \rangle_t$ of the spin at the origin, which is prepared in the up direction at $t = 0$. The coupling of spin 0 to its right neighbor at site 1 is accurately taken into account, while spin 1 is treated as belonging to an effective medium, in which spins flip independently with a frequency-dependent flip rate $\Gamma(s)$. The main results of this approximation were presented in ref. 1. Here we give some additional results, in particular the asymptotic behavior of $\phi(t)$ at long times.

The frequency-dependent flip rate $\Gamma_1(s)$ was obtained as[1]

$$\Gamma_1(s) = c - \tfrac{1}{2}\{s + 1 - [(s+1)^2 - 4c(1-c)]^{1/2}\} \tag{2}$$

The inverse Laplace transform of

$$\tilde{\gamma}(s) \equiv c - \Gamma_1(s) \tag{3}$$

is found to be given by

$$\gamma(t) = [c(1-c)]^{1/2} \frac{\exp(-t)}{t} I_1(2[c(1-c)t]^{1/2}) \tag{4}$$

where $I_1(x)$ is a modified Bessel function. For t ranging from 0 to ∞, $\gamma(t)$ decreases monotonically from $c(1-c)$ to 0. The rate equation for the time-dependent probability $p(t)$ that a spin of the effective medium, like spin 1, points in the up direction reads

$$\dot{p}(t) = -c[p(t)-c] + \int_0^t dt'\, \gamma(t-t')[p(t')-c] \tag{5}$$

The second term on the r.h.s. is a memory integral with the kernel $\gamma(t)$. Here $p(t)-c$ is the deviation of the probability p from its equilibrium value.

The Laplace transform $\tilde{\phi}$ of the spin autocorrelation function, given by

$$\tilde{\phi}(s) = [s + \Gamma_1(s)]^{-1} \tag{6}$$

has a branch cut on the negative real s axis between s_1 and s_2, where

$$s_{1,2} = -1 \pm 2[c(1-c)]^{1/2} \tag{7}$$

For $c < 1/2$, it has in addition a simple pole at the origin. Expressing the inverse Laplace transform by the discontinuity of $\tilde{\phi}(s)$ across the branch cut, one obtains

$$\phi(t) = \frac{1-2c}{1-c}\theta\left(\frac{1}{2}-c\right) - \frac{1}{1-c}\int_{s_2}^{s_1} \frac{ds}{2\pi} e^{st} \left[\frac{(s_1-s)(s-s_2)}{s}\right]^{1/2} \tag{8}$$

For $c \neq 1/2$, the asymptotic expansion of the integral for long times yields (see also Section 3.2)

$$\phi(t) - \phi(\infty) \sim \frac{(s_1-s_2)^{1/2}}{4\sqrt{\pi}\,|s_1|} \frac{\exp(-|s_1|\,t)}{t^{3/2}} \tag{9}$$

For $c = 1/2$, the asymptotic behavior is

$$\phi(t) \sim (2/\pi t)^{1/2} \tag{10}$$

The blocking transition at $c = 1/2$, below which $\phi(\infty)$ is nonzero, is an artefact of the approximation. In ref. 1 a detailed argument for the absence of such a transition was given. The argument is supported by our numerically exact calculations for finite chains[1] and by the Monte Carlo

simulations. The asymptotic long-time behavior (9) for $c < 1/2$, however, is of the same form as obtained by more accurate approximations (see Section 3).

2.2. A Mode-Coupling Approximation (MCA)

For the derivation of a mode-coupling approximation the dynamical equations are usually formulated in terms of time-dependent observables rather than probabilities. An observable may be any function of the states of the system. It is more convenient for our model to describe a state by the vector n of site occupation numbers n_i ($n_i = 0$ or 1) than by the spin variables $\sigma_i = \pm 1$. The time dependence of an observable is generated by the adjoint L^+ of the Liouvillian operator defined by the master equation for the model. L^+ is given by

$$L^+ A(\mathbf{n}) = \sum_i w_i(\mathbf{n})[A(\mathbf{n}^{(i)}) - A(\mathbf{n})] \tag{11}$$

where $A(\mathbf{n})$ is any state function. $\mathbf{n}^{(i)}$ is the state obtained from $\mathbf{n}$ by flipping the spin at site i, i.e., by replacing n_i by $1 - n_i$. The transition rate $w_i(\mathbf{n})$ for spin i reads

$$w_i(\mathbf{n}) = [c + (1 - 2c)n_i]n_{i+1} \tag{12}$$

The first factor fulfills the condition of detailed balance. The factor n_{i+1} expresses the kinetic constraint. The time-dependent state function $A_t(\mathbf{n})$ is obtained as

$$A_t = e^{L^+ t} A \tag{13}$$

A mode-coupling approximation is an approximation for a memory function, for which a formal expression can be derived using the projection operator formalism of Mori and Zwanzig.[7] We select the set of orthonormal state functions

$$A_i = \Delta n_i / [c(1 - c)]^{1/2}, \qquad i = \text{integer} \tag{14}$$

where $\Delta n_i = n_i - \langle n_i \rangle = n_i - c$, and define a projection operator P by

$$PA = A_i(A_i, A) \tag{15}$$

after introducing a scalar product

$$(A, B) = \sum_{\mathbf{n}} \rho_0(\mathbf{n})(A(\mathbf{n}))^* B(\mathbf{n}) \tag{16}$$

with the equilibrium probabilities $\rho_0(\mathbf{n})$ of the states $\mathbf{n}$. Eliminating state functions outside the subspace given by (14) by means of the projection operator

$$Q = 1 - P \tag{17}$$

one arrives at an equation of motion for the normalized autocorrelation function of occupation number fluctuations (equivalent to the spin-autocorrelation function)

$$\phi(t) = (A_0, A_{0,t}) \tag{18}$$

which contains a memory term. This equation reads

$$\dot{\phi}(t) + c\phi(t) = \int_0^t dt'\, M(t')\, \phi(t - t') \tag{19}$$

The kernel $M(t)$ of the memory term on the r.h.s. is the memory function. The formal expression for $M(t)$ is

$$M(t) = c(1-c)(A_0 A_1, e^{QL^+ t} A_0 A_1) \tag{20}$$

The standard recipe for a MCA is to drop the projection operator Q in the reduced time evolution operator $\exp(QL^+ t)$ and to factorize the rest. This yields the approximate memory function

$$M(t) \simeq \bar{M}(t) = c(1-c)\phi^2(t) \tag{21}$$

In the factorization we have used the fact that the correlation functions $(A_j, A_{i,t})$ are site-diagonal, which is a consequence of the asymmetry of the kinetic constraint in our model.

Equations (19) and (21) represent the simplest MCA for our model. Two properties of the solution to these equations are easy to derive.

A. A solution $\phi(t)$ which tends to a finite nonzero value for $t \to \infty$ cannot exist for any value of c. This follows by taking the Laplace transform of (19), which yields

$$(s + c)\, \tilde{\phi}(s) = \tilde{\bar{M}}(s)\, \tilde{\phi}(s) + 1 \tag{22}$$

If $\phi(t)$ tended to a finite nonzero value, $\bar{M}(t)$ would, too. This is not compatible with Eq. (22) for $s \to 0$.

B. For $c < \tilde{c}$ the solution $\phi(t)$ is not a monotonically decreasing function of t. A lower bound to $\tilde{c}$ is 1/3. This is proved by showing that the

assumption of monotonic decay leads to a contradiction for $c < 1/3$. First we transform (19) into the integral equation

$$\phi(t) = e^{-ct} + \int_0^t dt'\, e^{-c(t-t')} \int_0^{t'} \bar{M}(t'')\, \phi(t-t'')\, dt'' \tag{23}$$

The iterative solution of this equation contains only positive terms; therefore $\phi(t) \geqslant 0$ for all $t \geqslant 0$. A lower bound to $\phi(t)$ is given by the first term on the r.h.s. of (23). If we assume that $\phi(t)$ is a monotonically decreasing function, we can estimate in Eq. (19)

$$\dot{\phi}(t) \geqslant \phi(t) \left[-c + c(1-c) \int_0^t dt'\, e^{-2ct'} \right] \tag{24}$$

Since the expression on the r.h.s. becomes positive for $t \to \infty$ if $c < 1/3$, the assumption cannot hold for concentrations below this. Numerical integration of Eqs. (19), (21) in fact shows that the concentration $\tilde{c}$ below which the solution goes nonmonotonic is considerably higher. In Fig. 1 we show the numerical solution for several concentrations, indicating the divergence of the MCA solution for $c \lesssim 0.5$.

We only note that properties (A) and (B) also hold if the subspace (14) of state functions is extended to include the two-site functions

$$A_i A_{i+1} \text{ for all integers } i \tag{25}$$

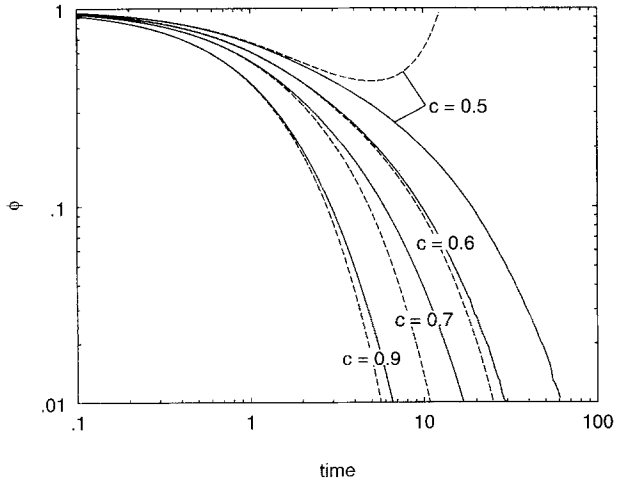

Fig. 1. Mode coupling approximation of $\phi(t)$ (dashed lines) compared with exact solution (full lines; obtained from numerical results for finite chains[1] which are indistinguishable from exact results for the given concentrations and time domain) for various concentrations c.

or both the two- and three-state functions

$$A_i A_{i+1},\ A_i A_{i+1} A_{i+2} \text{ for all integers } i \tag{26}$$

(cf. Sections 2.4 and 2.5 of ref. 8).

Property A is gratifying since our model does not have a sharp blocking transition to a nonergodic phase.[1] Property B, however, is a serious defect. We expect that the spin-autocorrelation function of our model at all up-spin concentrations has no oscillating component and decays to zero monotonically with increasing time. This expectation is borne out both by the results of Monte Carlo simulation and by numerically exact calculations for finite chains.[1] We conclude that straightforward applications of the MCA fail for our model (as they do for related kinetic Ising and lattice-gas models[8,9]). In our opinion the approximation schemes of both MCA and the EMA are too simple to describe the subtle dynamic correlations generated by the kinetic constraints in these models.

3. THE CLUSTER APPROXIMATION

It is one of the main problems in the dynamical theory of Ising models that no generally applicable approximation schemes are known. As seen in the last section, the EMA and the MCA both fail for our model. This being the state of things, we found that it is worthwhile to look for an approximation scheme which better reflects the detailed properties of our model.

For small c most of the spins are down and one could conclude that the first up spin of the chain plus some of its right neighbors is essential for the relaxation of spin 0. Therefore we define a set of variables which explicitly takes account of the "cluster including the first up spin." After an appropriate termination of the corresponding system of equations this leads to a usable approximation for the relaxation function of spin 0.

3.1. The Variable Set

As mentioned above, the first up spin of a chain configuration might contribute essentially to the relaxation of spin 0. This leads us to have a closer look at configurations where for fixed k, $m > 0$, spins $0, 1, \ldots, k-1$ are down, spin k is up, spins $k+1, \ldots, k+m-1$ are in some subconfiguration, and all other spins are not specified. The spin k plus the $m-1$ spins to the right of it is called the *cluster of length m*. For example, the clusters of length $m=2$ are given by $(\uparrow, \downarrow)$ and $(\uparrow, \uparrow)$. Our interest is to find a

system of equations for the probabilities of all clusters of length m, which we define as

$$P_k^{1,j_1,\ldots,j_{m-1}}(t)$$
$$\equiv P(n_0 = n_1 = \cdots = n_{k-1} = 0, n_k = 1, n_{k+1'} = j_1, \ldots, n_{k+m-1} = j_{m-1}; t) \quad (27)$$

As a short-hand form for all probabilities of clusters of length m we shall use the symbol $P_k^{(m)}$.

Below we will calculate the equations of motion for the probabilities of clusters with length m. We shall see that they couple to those with length $m+1$. Therefore we need some approximation scheme to get a closed system of equations for fixed m. There are several possibilities to achieve this:

(a) Factorization of the last cluster element:

$$P_k^{1,j_1,\ldots,j_{m-1},1} \simeq c P_k^{1,j_1,\ldots,j_{m-1}}$$
$$P_k^{1,j_1,\ldots,j_{m-1},0} \simeq (1-c)\, P_k^{1,j_1,\ldots,j_{m-1}} \quad (28)$$

Often we shall call this method *normal factorization.*

(b) Combined factorization of loss and gain term: If a function $P_k^{1,j_1,\ldots,j_{m-1},j_m}$ is found in the loss or gain term of some "reaction pair," both the loss *and* gain terms are factorized as defined in (28).

This possibility is unusual, since it may treat the same function differently according to its "reaction partner." The idea to use this factorization method is motivated by the hope that errors introduced by the factorization of one of the terms are compensated by corresponding errors (with opposite sign) in its reaction partner. We shall see below that this approximation scheme indeed gives better results than possibility (a). Note that compensation only works for clusters with length $m > 1$, because it does not make sense to approximate the function P_k^1 for $m = 1$. For obvious reasons we shall often call this approximation method *compensating factorization.*

We want to solve the initial-value problem where spin 0 is up and all other spins are in equilibrium. In addition, we restrict our attention to the case of an infinite chain—finite chains may be calculated in the same manner, with additional equations for an adequate breakoff.[6] The initial values for our variables are then

$$P_k^{1,j_1,\ldots,j_{m-1}}(t=0) = 0 \qquad k \geqslant 1 \quad (29)$$

For the equilibrium values we get

$$P_k^{1, j_1, \ldots, j_{m-1}}|_{\text{eq}} = (1-c)^k c \prod_{m'=1}^{m-1} [1 - c - (1-2c) j_{m'}] \tag{30}$$

We are interested in the relaxation function $\phi(t)$ of spin 0. To find the connection between $\phi(t)$ and $P_k^{\{m\}}$, we rewrite the equation of motion for $\langle n_0 \rangle_t$ as

$$\begin{aligned} \partial_t \langle n_0 \rangle_t &= \langle (1-n_0) n_1 \rangle - \langle n_1 \rangle + c^2 \\ &= P_1^1(t) - c(1-c) \\ &= \sum_{\{j_{m'}\}} P_1^{1, j_1, \ldots, j_{m-1}}(t) - c(1-c) \end{aligned} \tag{31}$$

where the sum is taken over all subconfigurations of the spins $k+m'$ for $m' = 1, \ldots, m-1$. For the relaxation function $\phi(t) = (\langle n_0 \rangle_t - c)/(1-c)$ we arrive then at

$$\partial_t \phi(t) = \frac{1}{1-c} P_1^1(t) - c \tag{32}$$

or after Laplace transformation

$$\tilde{\phi}(s) = \left[1 - \frac{c}{s} + \frac{1}{1-c} \tilde{P}_1^1(s) \right] \Big/ s \tag{33}$$

where $\tilde{\phi}(s)$ is defined by

$$\tilde{\phi}(s) \equiv \int_0^\infty dt\, e^{-st} \phi(t) \tag{34}$$

and $\tilde{P}_1^{1, \ldots, j_{m-1}}(s)$ is defined correspondingly.

Note that cluster functions $P_k^{(m)}$ with $k = 0$ should *not* be included into our set of variables, because they can be expressed by $P_{k>0}^{(m)}$, and therefore depend on the rest of the set of variables. The reason for this is the choice of our special initial conditions that all spins except spin 0 are in equilibrium. For example, for P_0^{11} we could write

$$P_0^{11} = -\langle (1-n_0) n_1 \rangle + \langle n_1 \rangle = -P_1^1 + c$$

3.2. Clusters of Length 1

As a first application, we perform the cluster approximation for clusters of length $m = 1$. For $k = 1, \ldots$ our main variables are $P_k^1(t)$. In

addition, we get couplings to P_k^{11}, which are factorized by using (28). Writing down the rate equations for all P_k^1, we have

$$\partial_t P_k^1 = -cP_k^1 + (1-c)P_{k-1}^{11} - (1-c)P_k^{11} + cP_{k+1}^1 \tag{35}$$

for $k > 1$. The first and the third term on the r.h.s. are the loss terms. With probability c, spin $k-1$ can flip up. Or, if both spin k and spin $k+1$ are up (taken into account in P_k^{11}), spin k can flip down with probability $(1-c)$. The second and the fourth term are the gain terms and emerge from the reversed processes. With probability $(1-c)$, spin $k-1$ flips down if spin $k-1$ and spin k are both up (taken into account in P_{k-1}^{11}). Or, if spin k is down and spin $k+1$ is up, spin k flips up with probability c.

Equation (35) holds for $k=1$, too, but can be further simplified by using the above relationship between P_0^{11} and P_1^1. This leads to

$$\partial_t P_1^1 = c(1-c) - P_1^1 - (1-c)P_1^{11} + cP_2^1 \tag{36}$$

Then the normal factorization (28) yields the following system of equations:

$$\begin{aligned} \partial_t P_1^1 &= -[1+c(1-c)]P_1^1 + cP_2^1 + c(1-c) \\ \partial_t P_k^1 &= c(1-c)P_{k-1}^1 - c(2-c)P_k^1 + cP_{k+1}^1 \qquad \text{for} \quad k>1 \end{aligned} \tag{37}$$

Taking the Laplace transform with respect to time yields

$$\begin{array}{ccccc} [s+1+c(1-c)]\tilde{P}_1^1 & -c\tilde{P}_2^1 & & & = c(1-c)/s \\ -c(1-c)\tilde{P}_1^1 + [s+c(2-c)]\tilde{P}_2^1 & & -c\tilde{P}_3^1 & & = 0 \\ \ddots & \ddots & \ddots & \vdots & \\ & -c(1-c)\tilde{P}_{k-1}^1 + [s+c(2-c)]\tilde{P}_k^1 & -c\tilde{P}_{k+1}^1 & = 0 & \\ & \ddots & \ddots & \ddots & \vdots \end{array} \tag{38}$$

Equations (38) form a tridiagonal system of equations of a very simple form—nearly all coefficients of the l.h.s. are "diagonally equal" and only the first equation has a nonvanishing r.h.s. Such systems of equations can be transformed into a continued fraction in the following way:[10] Dividing the first of Eqs. (38) by $\tilde{P}_1^1$ yields $\tilde{P}_1^1$ in terms of $\tilde{P}_2^1/\tilde{P}_1^1$. Inserting this expression into (33), we obtain

$$\tilde{\phi}(s) = \frac{1}{s} - \frac{c}{s^2} + \frac{c}{s^2} \frac{1}{s+1+c(1-c)-c\tilde{P}_2^1/\tilde{P}_1^1} \tag{39}$$

Dividing the kth equation ($k>1$) of (38) by $\tilde{P}_k^1$ and solving for $\tilde{P}_k^1/\tilde{P}_{k-1}^1$, we arrive at the recursion relation

$$\frac{\tilde{P}_k^1}{\tilde{P}_{k-1}^1}=\frac{c(1-c)}{s+c(2-c)-c\tilde{P}_{k+1}/\tilde{P}_k^1} \qquad \text{for} \quad k>1 \tag{40}$$

which leads to the continued fraction for $\tilde{\phi}(s)$. The fix point of iteration (40) can easily be calculated. The two solutions are

$$\frac{\tilde{P}_2^1}{\tilde{P}_1^1}=\frac{s+c(2-c)}{2c}\left\{1\pm\left[1-\frac{4c^2(1-c)}{[s+c(2-c)]^2}\right]^{1/2}\right\} \tag{41}$$

Below we shall see that the $(-)$ sign must be chosen for the relaxation function to relax to 0 for $t\to\infty$. This sign corresponds to the *stable* fix point, which is reasonable, since the effect of a small change imposed on the chain at site k', say, should decay (not grow) with increasing distance from k'.

It is instructive to study the expansion of the relaxation function (39) for small s in detail. For $\phi(t)$ to decay to 0 for all c, all coefficients of the negative powers of s should vanish. Second, with the definition of the Laplace transform (34), the coefficient of s^0 is just the mean relaxation time

$$\begin{aligned}\bar{\tau}&\equiv\int_0^\infty \phi(t)\,dt\\ &=\frac{1-c(1-c)}{c^3}\end{aligned} \tag{42}$$

In the last step we used the small-s expansion of (39) together with (41). Since $\bar{\tau}$ is finite for nonzero c, this ensures that $\phi(t)$ decays to 0 for $t\to\infty$. For the $(+)$ sign in (41) this does not work. We see that $\bar{\tau}\sim c^{-3}$ for the smallest concentrations. However, from Monte Carlo simulations it can be seen that $\bar{\tau}\gtrsim 1/c^5$ for small concentrations c. This shows that at least the cluster approximation of first order falls short for the smallest concentrations.

As a third point, we calculate the asymptotic long-time behavior of $\phi(t)$. Watson's lemma[11] states that the behavior of $\phi(t\to\infty)$ is determined by the behavior of $\tilde{\phi}(s)$ in the neighborhood of its rightmost singularity in the complex s plane. $\tilde{\phi}(s)$ has four singularities, which all are real: There is a pole at $s_0=0$, a branch cut between

$$s_{1/2}=-c[2-c\mp 2(1-c)^{1/2}] \tag{43}$$

and another pole at $s_3 = -(1+c)$ which is only present for $c \gtrsim 0.62$. By the above discussion it is clear that $\phi(s)$ is continuous at $s = s_0$. The complex inverse Laplace integral can therefore be written as

$$\phi(t) = \frac{1}{2\pi i} \int_C ds\, \tilde{\phi}(s)\, e^{st} \tag{44}$$

with C denoting the contour around the branch cut between s_1 and s_2. The contribution of the pole at $s = s_3$ is omitted, here, because it does not contribute to the asymptotic behavior. Calculating the discontinuity of $\tilde{\phi}(s)$ across the cut, we find

$$\phi(t) = -\frac{c}{\pi} \int_{s_1}^{s_2} ds\, \frac{(s_1 - s)^{1/2}\,(s - s_2)^{1/2}}{(s + 2 - c^2)^2 + (s_1 - s)(s - s_2)/4}\, e^{st} \tag{45}$$

Since the rightmost singularity is given by $s = s_1$, the use of Watson's lemma yields

$$\phi(t \to \infty) = \frac{1}{2\pi^{1/2} s_1^2 (1-c)^{3/4}\,[c + (1-c)^{1/2}]}\, t^{-3/2} e^{s_1 t} \tag{46}$$

with s_1 given by (43).

As a visualization of the validity of the approximation for different c, we present Fig. 2. For concentrations $c \gtrsim 0.5$ the cluster approximation of

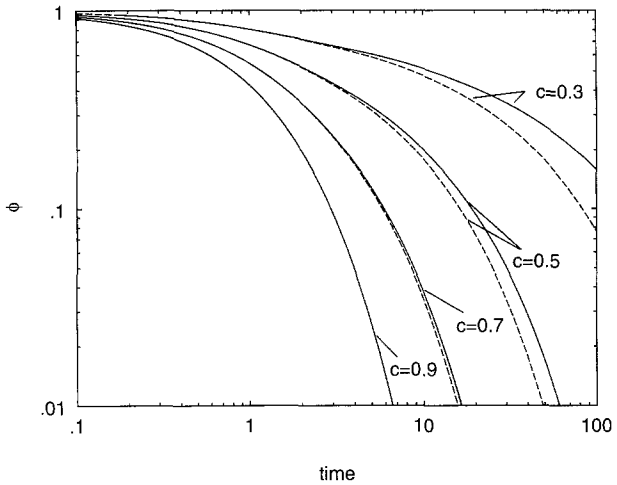

Fig. 2. Double-log plot of $\phi(t)$ for various concentrations c. The dashed lines are obtained from the cluster approximation with $m = 1$. Full lines represent the exact results (obtained from numerical results for finite chains[1] which are indistinguishable from exact results for the given concentrations and time domain).

first order gives good results. For smaller concentrations the approximated relaxation function decreases too fast compared with the exact solution.

3.3. Equivalence of the First Approximation ($m=1$) with a Defect-Diffusion Problem

We first formulate the equations of the $(m=1)$-cluster approximation in terms of a defect-diffusion problem. With Eqs. (37), which are obtained by "normal factorization" for $m=1$, together with Eq. (31), the total probability for finding the first up spin somewhere on the semi-infinite chain $k=0, 1, 2,...$ is conserved, as it should be. This is expressed by the equation

$$\partial_t \left(\langle n_0 \rangle_t + \sum_{k=1}^{\infty} P_k^1(t) \right) = 0 \tag{47}$$

Defining

$$p_k = -\Delta P_k^1, \qquad k \geqslant 1 \tag{48}$$

where

$$\Delta P_k^1 = P_k^1 - P_k^1|_{\text{eq}} \tag{49}$$

with the equilibrium probabilities

$$P_k^1|_{\text{eq}} = c(1-c)^k \tag{50}$$

we find that $\langle \Delta n_0 \rangle_t = \langle n_0 \rangle_t - c$ is given by

$$\langle \Delta n_0 \rangle_t = \sum_{k=1}^{\infty} p_k(t) \tag{51}$$

Initial conditions are

$$p_k(t=0) = P_k^1|_{\text{eq}} = c(1-c)^k \tag{52}$$

corresponding to

$$\langle \Delta n_0 \rangle_{t=0} = 1 - c \tag{53}$$

For $p_k(t)$ the equations

$$\begin{aligned} \partial_t p_1(t) &= [1 + c(1-c)]\, p_1(t) + c p_2(t) \\ \partial_t p_k(t) &= -c(2-c)\, p_k(t) + c(1-c)\, p_{k-1}(t) + c p_{k+1}(t) \qquad k \geqslant 2) \end{aligned} \tag{54}$$

hold. Equation (54b) can be interpreted in terms of hopping of a defect. Let us interpret p_k as the probability for finding the defect at site k. Equation (54b) then describes biased diffusion of the defect with asymmetric hopping rates (for $k \geqslant 1$)

$$\begin{aligned} w_{k \to k+1} &= c(1-c) \\ w_{k+1 \to k} &= c \end{aligned} \tag{55}$$

Equation (54a) is the result of hopping between sites 1 and 2 with hopping rates (55a), (55b) and escape from site 1 to site 0 with escape rate unity. The escape of the defect corresponds to relaxation toward equilibrium at site zero. According to (51), the deviation from equilibrium $\langle \Delta n_0 \rangle_t$ is given by the probability that the defect has not yet escaped. The initial probability distribution for the position of the defect at time $t=0$, which is normalized to the initial value (53), is given by (52).

We now show how the asymptotic result (46) for the relaxation function of the $(m=1)$-cluster approximation can be obtained for small c from the continuum limit of this defect-diffusion problem. In the limit of low concentration $c \ll 1$ this defect-diffusion problem can be considerably simplified and solved by standard methods. First note that for $c \ll 1$ the rate of escape from site 1 to site 0 is much higher than the rate for a jump back from site 1 to site 2. Accordingly, the probability p_1 will be negligibly small (except at very short times). We therefore set

$$p_1(t>0) = 0 \tag{56}$$

which corresponds to replacing Eq. (54a) by an absorbing boundary condition. Second, since the characteristic length of the initial probability distribution is c^{-1}, for $c \ll 1$ a continuum approximation can be applied. Replacing the discrete site probabilities $p_k(t) \equiv p(x_k, t)$ by the continuous probability density $p(x, t)$, we obtain the continuum version of Eq. (54b) as

$$\partial_t p(x, t) = c\, \partial_x^2 p(x, t) + c^2\, \partial_x p(x, t) \tag{57}$$

to lowest order in c. This is a diffusion equation for diffusion with drift in a constant force field. The diffusion coefficient is $D=c$, and the product of mobility B and force F is given by $BF = -c^2$. The force is directed in the negative x direction. In the same approximation, the initial condition becomes

$$p(x \geqslant 1, t=0) = c \exp(-cx) \tag{58}$$

which contains the Boltzmann factor for the potential energy of the defect in that force field. For $c \ll 1$ we introduce only a small error by shifting the boundary from $x=1$ to $x=0$. The boundary condition then is

$$p(x=0,\, t>0)=0 \tag{59}$$

We need to solve Eq. (57) with initial and boundary conditions to obtain

$$\langle \Delta n_0 \rangle_t = \int_0^\infty dx\, p(x,\, t) \tag{60}$$

This is achieved by substituting

$$\begin{aligned} \tau &= c \cdot t \\ p(x,\, t) &= \exp\left[-\frac{c}{2} x - \left(\frac{c}{2}\right)^2 \tau \right] \Psi(x,\, \tau) \end{aligned} \tag{61}$$

which transforms Eq. (57) into the ordinary diffusion equation for $\Psi(x, \tau)$:

$$\partial_\tau \Psi(x,\, \tau) = \partial_x^2 \Psi(x,\, \tau) \tag{62}$$

Using standard methods for the solution of the diffusion equation,[12] we arrive at the result

$$\langle \Delta n_0 \rangle_t = \left[1 + 2\left(\frac{c}{2}\right)^2 \tau \right] \operatorname{erfc}\left(\frac{c}{2}\sqrt{\tau}\right) - \frac{c\sqrt{\tau}}{\sqrt{\pi}} \exp\left[-\left(\frac{c}{2}\right)^2 \tau \right] \tag{63}$$

the asymptotic long-time behavior of which is given by

$$\langle \Delta n_0 \rangle_t \sim \frac{1}{\sqrt{\pi}} \frac{\exp(-c^3 t/4)}{(c/2)^3\, (ct)^{3/2}} \tag{64}$$

3.4. Clusters of Length 2

In the case of clusters of length $m=2$ we have to deal with the variables P_k^{10} and P_k^{11}. The corresponding system of equations is obtained in a similar manner as in Eq. (35):

$$\begin{aligned} \partial_t P_1^{10} &= -P_1^{10} + c(1-c)^2 - cP_1^{101} + (1-c)P_1^{111} \\ \partial_t P_1^{11} &= -P_1^{11} + c^2(1-c) - (1-c)\, P_1^{11} + cP_2^{10} + cP_2^{11} - (1-c)P_1^{111} + cP_1^{101} \\ \partial_t P_k^{10} &= cP_k^{10} + (1-c)P_{k-1}^{110} - cP_k^{101} + (1-c)P_k^{111}, \qquad k>1 \\ \partial_t P_k^{11} &= -cP_k^{11} + (1-c)P_{k-1}^{111} - (1-c)P_k^{11} + cP_{k+1}^{10} + cP_{k+1}^{11} \\ &\quad -(1-c)P_k^{111} + cP_k^{101}, \qquad k>1 \end{aligned} \tag{65}$$

where corresponding loss and gain terms are written in pairs. In the first two of Eqs. (65) the variables $P_0^{110} = c(1-c) - P_1^{10}$ and $P_0^{111} = c^2 - P_1^{11}$ are eliminated as discussed above.

All functions representing clusters of length 3 are to be approximated. This time we will use the "compensating factorization method" [see (b) in Section 3.1]. Performing this factorization and at the same time Laplace-transforming Eq. (65), we get

$$\begin{aligned}
(s+1+c^2)\tilde{P}_1^{10} - c(1-c)\tilde{P}_1^{11} &= c(1-c)^2/s \\
-c^2\tilde{P}_1^{10} + (s+2-c^2)\tilde{P}_1^{11} - c\tilde{P}_2^{10} - c\tilde{P}_2^{11} &= c^2(1-c)/s \\
-(1-c)^2\tilde{P}_{k-1}^{11} + (s+c)\tilde{P}_k^{10} &= 0 \\
-c(1-c)\tilde{P}_{k-1}^{11} + (s+1)\tilde{P}_k^{11} - c\tilde{P}_{k+1}^{10} - c\tilde{P}_{k+1}^{11} &= 0
\end{aligned} \tag{66}$$

We will now cast Eq. (66) into a tridiagonal form which allows the transformation into a continued fraction expansion. As a first step, we change our variables from $\tilde{P}_j^{10}$, $\tilde{P}_j^{11}$ to $\tilde{P}_j^1 = \tilde{P}_j^{10} + \tilde{P}_j^{11}$, $\tilde{P}_k^{11}$ $(j = 1, \ldots)$:

$$\begin{aligned}
(s+1+c^2)\tilde{P}_1^1 - (s+1+c)\tilde{P}_1^{11} &= c(1-c)^2/s \\
-c^2\tilde{P}_1^1 + (s+2)\tilde{P}_1^{11} - c\tilde{P}_2^1 &= c^2(1-c)/s \\
-(1-c)^2\tilde{P}_{k-1}^{11} + (s+c)\tilde{P}_k^1 - (s+c)\tilde{P}_k^{11} &= 0 \\
-c(1-c)\tilde{P}_{k-1}^{11} + (s+1)\tilde{P}_k^{11} - c\tilde{P}_{k+1}^1 &= 0
\end{aligned} \tag{67}$$

By that procedure, we have replaced the two elements $-c\tilde{P}_j^{10} + c\tilde{P}_j^{11}$ by one element. To obtain the desired tridiagonal form we only need to eliminate $\tilde{P}_{k-1}^{11}$ in (67d) using (67c), and get rid of the r.h.s. of (67b) using (67a). We end up with

$$\begin{aligned}
(s+1+c^2)\tilde{P}_1^1 - (s+1+c)\tilde{P}_1^{11} &= c(1-c)^2/s \\
-c(s+1+c)\tilde{P}_1^1 + (s+2-c+c^2)\tilde{P}_1^{11} - c(1-c)\tilde{P}_2^1 &= 0 \\
-(1-c)^2\tilde{P}_{k-1}^{11} + (s+c)\tilde{P}_k^1 - (s+c)\tilde{P}_k^{11} &= 0 \\
-c(s+c)\tilde{P}_k^1 + (s+1-c+c^2)\tilde{P}_k^{11} - c(1-c)\tilde{P}_{k+1}^1 &= 0 \\
\ddots \qquad \ddots \qquad \ddots &\vdots
\end{aligned} \tag{68}$$

In a similar manner as in Section 3.2, a continued fraction expansion of $\tilde{\phi}(s)$ can be derived. It is given by

$$\tilde{\phi}(s) = \frac{1}{s} - \frac{c}{s^2} + \frac{c(1-c)}{s^2} \cfrac{1}{s+1+c^2 - \cfrac{c(s+1+c)^2}{s+2-c(1-c)-c(1-c)\tilde{P}_2^1/\tilde{P}_1^{11}}} \tag{69}$$

with

$$c(1-c)\frac{\tilde{P}_k^1}{\tilde{P}_{k-1}^{11}}=\frac{c(1-c)^3}{s+c-\dfrac{c(s+c)^2}{s+1-c(1-c)-c(1-c)\,\tilde{P}_{k+1}^1/\tilde{P}_k^{11}}} \tag{70}$$

for $k=2,\ldots$. The recursion relation (70) is derived by eliminating $\tilde{P}_k^{11}/\tilde{P}_k^1$ from the two recursion relations relating $\tilde{P}_{k-1}^{11}/\tilde{P}_k^1$ to $\tilde{P}_k^{11}/\tilde{P}_k^1$ and $\tilde{P}_k^1/\tilde{P}_k^{11}$ to $\tilde{P}_{k+1}^1/\tilde{P}_k^{11}$. The fix point of iteration (70) can again be calculated, resulting in

$$c(1-c)\frac{\tilde{P}_2^1}{\tilde{P}_1^{11}}=\frac{b}{2}\left[1-\left(1-\frac{4a}{b^2}\right)^{1/2}\right] \tag{71}$$

with

$$a=\frac{c(1-c)^3(s+1-c+c^2)}{s+c} \tag{72}$$

and

$$b=s+1-c+c^2+\frac{c(1-c)^3-c(s+c)^2}{s+c} \tag{73}$$

The expansion of $\tilde{\phi}(s)$ for small s yields the mean relaxation time as

$$\bar{\tau}=\frac{1-2c+5c^3-5c^4-3c^5+5c^6-c^7+c^9-c^{10}}{c^4(1-c)^3} \tag{74}$$

This formula is quite involved, but it is seen directly that

$$\bar{\tau}\sim c^{-4} \qquad \text{for} \quad c\ll 1 \tag{75}$$

The exponent increases by one when the length of the clusters is increased from $m=1$ to $m=2$. But still the exponent is too small to account for the true asymptotic behavior (which from Monte Carlo simulations is seen to be at least $\sim c^5$), indicating that the cluster approximation with $m=2$ also falls short for very small concentrations. It is interesting to note that the corresponding asymptotic behavior in the case of the normal factorization is given by $\bar{\tau}\sim 1/(2c^4)$, which is smaller than (75) by a factor 1/2. It indicates that the compensating factorization method may yield results which are somewhat better than the results obtained from the normal factorization, at least for small concentrations.

Also in this case, the behavior of $\phi(t\to\infty)$ can be calculated. Again the rightmost zero of the root in Eq. (71) yields the asymptotic behavior.

This time the polynomial under the root is of order 4 in s and we have four zeros. For small concentrations the rightmost singularity can be written as

$$s_1 = -\frac{c^4}{4} + O(c^5) \tag{76}$$

From this, the asymptotic behavior can be calculated to be

$$\phi(t \to \infty) \propto t^{-3/2} e^{-c^4/4t} \qquad \text{for small } c \tag{77}$$

which has the form of the result (46) of the defect-diffusion model for the case $m = 1$, but with a diffusion constant $D = c^2$ instead of c. This "renormalization" of the diffusion constant can be derived from Eq. (68) for $k \geqslant 2$. Elimination of $\tilde{P}_k^{11}$ for $|s| \ll c$ leads to the equation

$$[s + c^2(2-c)]\tilde{P}_k^1 = c^2(1-c)\tilde{P}_{k-1}^1 + c^2\tilde{P}_{k+1}^1 \tag{78}$$

which represents a discretized diffusion equation with drift term, where $D = c^2(1 - c/2) \sim c^2$ and $BF = -c^3$. The origin of the extra factor of c in D lies in the fact that the up-spin front propagates only via the "excited" state of probability $\tilde{P}_k^{11}$, which has a second up-spin immediately behind the front.

In Fig. 3 we present a plot of $\phi(t)$ for different concentrations, comparing the $(m = 2)$-cluster approximations with the exact relaxation functions.

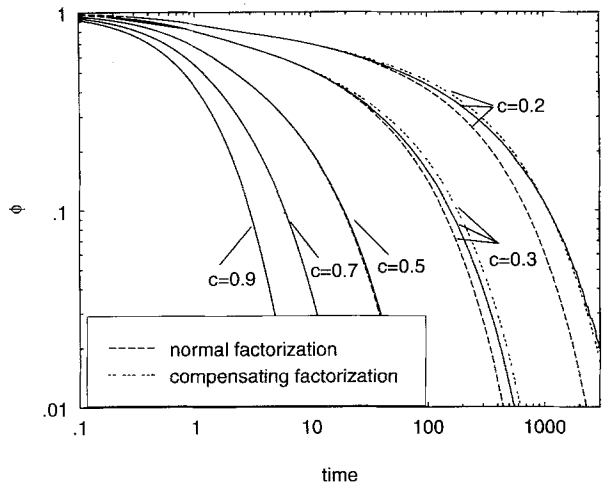

Fig. 3. Double-log plot of $\phi(t)$ for various concentrations c. The dashed lines are obtained from the cluster approximations with $m = 2$. Full lines represent the exact results (obtained from numerical results for finite chains[1] which are indistinguishable from exact results for the given concentrations and time domain; in the case of $c = 0.3$ and $c = 0.2$ the Monte Carlo results are taken).

For $c=0.2$ and $c=0.3$, the curves for the two factorization methods are somewhat apart from each other and for both concentrations the compensating factorization yields better results than normal factorization. It is also seen that the curves from the compensating factorization have a mixed convergence behavior—for short times they are above the exact curve and for long times they are below it. It seems that the error from normal factorization is overcompensated for short times and undercompensated for long times.

3.5. Clusters of Arbitrary Length

We now turn to the general case where the relaxation function $\phi(t)$ is approximated by clusters of length m. The equations of motion for the probabilities $P_k^{(m)}$ of clusters of fixed length m can be directly deduced from the master equation:

$$\begin{aligned}
\partial_t P_k^{1,j_1,\ldots,j_{m-1}} &= -cP_k^{1,j_1,\ldots,j_{m-1}} + (1-c)\underline{P_{k-1}^{1,1,j_1,\ldots,j_{m-1}}} \\
&\quad + j_1\{-(1-c)P_k^{1,1,j_2,\ldots,j_{m-1}} + cP_{k+1}^{1,j_2,\ldots,j_{m-1},0} + cP_{k+1}^{1,j_2,\ldots,j_{m-1},1}\} \\
&\quad + \sum_{i=1}^{m-2} j_{i+1}\{-[c+(1-2c)j_i]P_k^{1,j_1,\ldots,j_{m-1}} \\
&\quad + [1-c-(1-2c)j_i]P_k^{1,j_1,\ldots,(1-j_i),j_{i+1},\ldots,j_{m-1}}\} \\
&\quad - [c+(1-2c)j_{m-1}]\underline{P_k^{1,j_1,\ldots,j_{m-1},1}} \\
&\quad + [1-c-(1-2c)j_{m-1}]\underline{P_k^{1,j_1,\ldots,(1-j_{m-1}),1}} \qquad (79)
\end{aligned}$$

The pairs of loss and gain terms on the r.h.s. of (79) result from the flipping of spins number $k-1$ to $k+m-1$. Because of the kinetic constraint, there is no contribution from the spins number $i<k-1$. For $k=1$, in the first pair of loss and gain terms

$$-cP_1^{1,j_1,\ldots,j_{m-1}} + (1-c)P_0^{1,1,j_1,\ldots,j_{m-1}}$$

which is the contribution of flips of spin 0; the probability $P_0^{1,1,j_1,\ldots,j_{m-1}}$ needs to be expressed by the probability $P_1^{1,j_1,\ldots,j_{m-1}}$, as discussed above. Using the identity $n_0 = -(1-n_0)+1$, we can write the above contribution as

$$-P_1^{1,j_1,\ldots,j_{m-1}} + c(1-c)\prod_{i=1}^{m-1}[1-c-(1-2c)j_i] \qquad (80)$$

Also the flip of spin k needs a special comment. We have the contribution

$$j_1[-(1-c)P_k^{1,1,j_2,\ldots,j_{m-1}} + cP_k^{0,1,j_2,\ldots,j_{m-1}}$$

$$P_{k+1}^{1,j_2,\ldots,j_{m-1},0} + P_{k+1}^{1,j_2,\ldots,j_{m-1},1}$$

The last case requiring a special comment is the flip of spin $k+m-1$—the right end of the cluster. This spin can only flip if its right neighbor is up, which is taken into account by prolonging the cluster with a 1.

Note that the underlined terms in Eqs. (79) are connected to clusters of length $m+1$ which are to be approximated. The structure of Eq. (79) is quite simple. There are 2^{m-1} internal cluster states $(j_1,\ldots,j_{m-1})$. We number these states by binary numbers as discussed in ref. 1, except that we reverse the order of $(j_1,\ldots,j_{m-1})$. The corresponding variables $P_k^{(m)}$ are collected in the vector $\mathbf{x}_k^{(m)}$. To form the total vector $\mathbf{x}$, we collect all vectors $\mathbf{x}_k^{(m)}$ into

$$\mathbf{x} = (x_1^{(m)}, \mathbf{x}_2^{(m)},\ldots)$$

Let $A_1^{(m)}$ and $A^{(m)}$ denote the matrices containing all internal couplings between elements of $\mathbf{x}_1^{(m)}$ and $\mathbf{x}_{k>1}^{(m)}$, respectively. The sign of these matrices

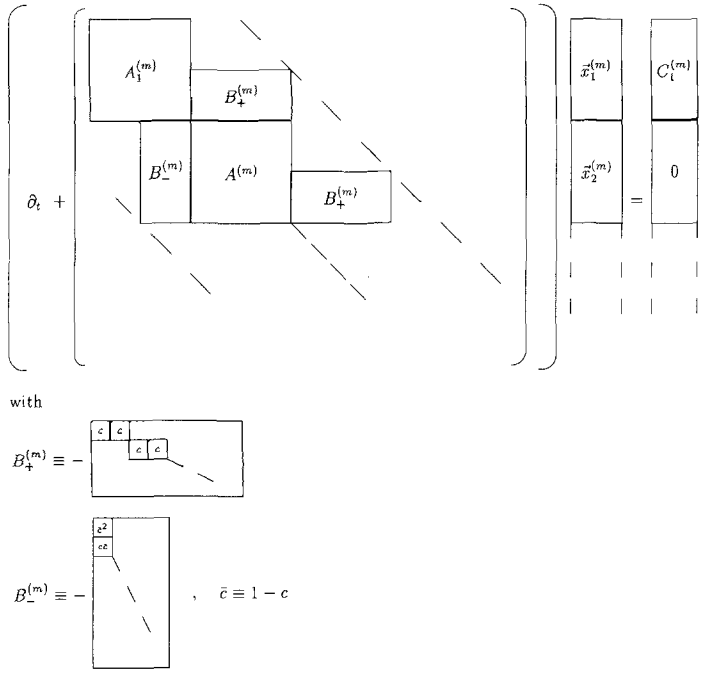

Fig. 4. Visualization of the total system of equations (79).

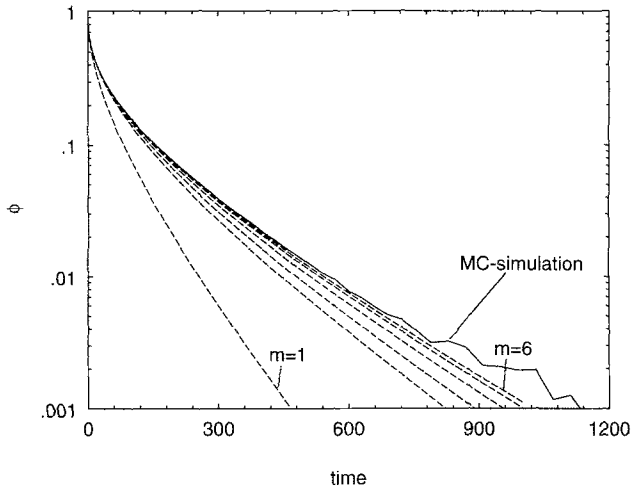

Fig. 5. Semilog plot of $\phi(t)$ for $c = 0.3$. The Monte Carlo result is compared with cluster approximation of different orders m. Normal factorization is used.

is chosen such that the loss terms are positive and the gain terms negative. Collecting all constants for $k = 1$ into the vector $C_1^{(m)}$, we can visualize the total system of equations as in Fig. 4. For a more detailed discussion of this visualization we refer to ref. 6. Clearly, the total matrix is a band matrix with a bandwidth of $3 \cdot 2^{m-1}$. It enables us to use an adequate numerical algorithm with a moderate amount of required storage space. The total system of equations can also be transformed into a matrix continued fraction,[13,14] with the effect that the desired storage space is even smaller and that it is easier to find the stable fix point.

In Fig. 5 we present an example of a relaxation function $\phi(t)$ calculated from the cluster approximation of order $m \leqslant 6$ and concentration $c = 0.3$. The curves obtained with normal factorization are given for $m = 1,..., 6$. For comparison, the corresponding Monte Carlo curve is plotted, too. The figure shows that the curves from normal factorization convergence for increasing m to the exact $\phi(t)$ curve from below. This indicates that normal factorization of cluster functions yields lower bounds to the exact relaxation function.

3.6. Validity of the Approximation

As seen in Section 3.5, the curves obtained with normal factorization converge with increasing m to $\phi(t)$ from below. This property makes the mean relaxation time $\bar{\tau} \equiv \int_0^\infty \phi(t)\, dt$ a well-suited parameter to discuss the

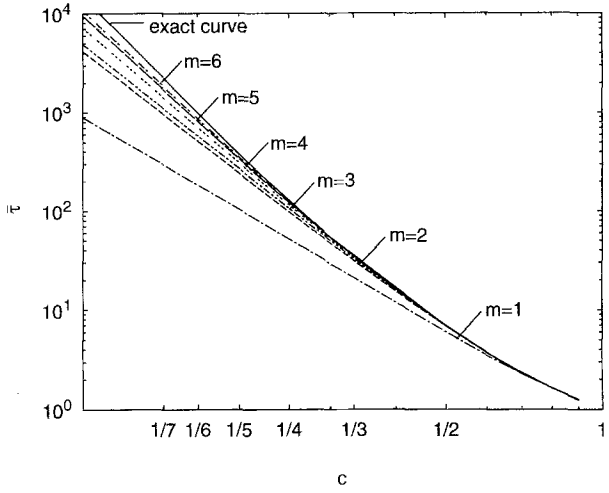

Fig. 6. Mean relaxation time of the infinite chain as a function of c for different cluster lengths m compared with the exact curve.

validity of the approximation. In Fig. 6 we present the functions $\bar{\tau}(c)$ for $m = 1,..., 6$ together with the corresponding exact curve. Starting from $c = 1$, the curves from the cluster approximation follow the exact curve for decreasing c until they fall off below the exact curve (as expected). It is important to note that the points where the approximated $\bar{\tau}$ are 90% of the exact curve are at $c \simeq 1/(m+1)$. Thus we can say that clusters of length m yield good approximations to $\phi(t)$ as long as

$$c \gtrsim \frac{1}{m+1} \tag{81}$$

The length $m+1$ may be interpreted as the site of the factorized spin counted from the first up spin and $1/c$ is the characteristic length of a fraction of the chain in which exactly one up spin is found. It is the only static length scale inherent to our model. Therefore, if the clusterlength is chosen such that it is very probable to find an up spin inside the clusters, the factorization yields useful results. On the other hand, if it is improbable to find an up spin inside the clusters, the factorization works on an essential spin and the results are poor approximations. Note that we found not only a criterion for the validity of the cluster approximation, but also a characteristic length scale on which clusters are important. On bigger length scales, we may look upon the clusters as objects moving on the chain.

3.7. The Asymptotic Long-Time Behavior of $\phi(t)$ for $c \to 0$

As shown above, for the cluster approximations $m=1$ and $m=2$ the long-time form of $\phi(t)$ for $c \to 0$, which is given by

$$\phi(t) \sim e^{s_1 t}/t^{3/2} \tag{82}$$

corresponds to a defect-diffusion model with diffusion in a constant force field. The characteristic rate $(-s_1)$ is determined by a defect-diffusion constant $D^{(m)}(c)$, which depends on the approximation m as

$$-s_1 = D^{(m)}(c)c^2/4 \tag{83}$$

For $m=1$ and $m=2$ the values $D^{(1)}=c$ and $D^{(2)}=c^2$ were derived, respectively $(c \to 0)$. We conjecture that the exact asymptotic time dependence of ϕ, which corresponds to the limit $m \to \infty$, is of the same form (82), (83) with a renormalized defect diffusion constant $D^{(\infty)}(c)$. Figure 7, in which the long-time portion of the Monte Carlo data for $\phi(t)$ at different concentrations is fitted by Eq. (82), supports this conjecture. An estimate of $D^{(\infty)}(c)$ for $c \to 0$ which has a nonanalytic concentration dependence is derived from the following considerations.

In ref. 6 it has been shown by a renormalization procedure in which every other spin is eliminated that for long times and for $c \to 0$ the spin

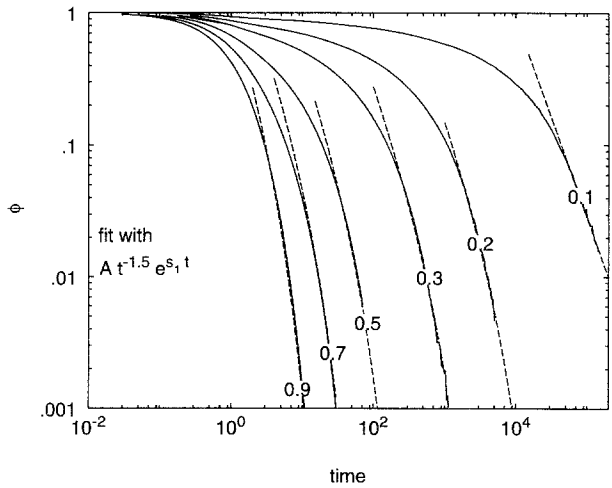

Fig. 7. Double-log plot of $\phi(t)$ for various concentrations c. The dashed lines represent asymptotic fits of the form (82).

autocorrelation function for a chain with free end of length $2L-1$ equals that for a chain of length $L-1$ with the time t rescaled as

$$t \to t' = \frac{c}{2} t \tag{84}$$

In this renormalization step the set of equations of the cluster approximation for clusters of length $m = 2^k + 1$ is transformed into that for clusters of length $m' = 2^{k-1} + 1$ with the same rescaling (84) of the time. (The reason for this particular choice of cluster sizes is this: Since in the renormalization step the front up spin at the left edge of a cluster and its left neighbor spin are replaced by a "block spin," m must be odd. For the cluster size number to be odd after all renormalization steps but the last, the original m must be given by $2^k + 1$, with integer k.) Repeating this procedure k times, we end up with the $(m=2)$-cluster approximation with rescaled time $t' = (c/2)^k t$. Therefore the diffusion constant $D^{(m)}$ is given by

$$D^{(m)} = D^{(2)} \left(\frac{c}{2}\right)^k = c^2 \left(\frac{c}{2}\right)^{\mathrm{lb}(m-1)} \tag{85}$$

We assume that $D^{(m)} \approx D^{(\infty)}$ when the cluster length m equals the average distance $1/c$ between neighboring up spins. Evidence supporting this assumption is given in the preceding section. This yields our estimate

$$D^{(\infty)} = c^2 \left(\frac{c}{2}\right)^{\mathrm{lb}(1/c-1)} \approx 4 \left(\frac{c}{2}\right)^{\mathrm{lb}(1/c)+2} \tag{86}$$

It is important to note that the renormalization procedure only works for $c \to 0$. In ref. 6 it has been shown that the renormalization procedure gives increasingly unreliable results when the number of renormalization steps becomes larger than $\mathrm{lb}(1/c)$. This is the reason for (85) not converging to (86) when $m \to \infty$.

The leading factor $c^{\mathrm{lb}(1/c)}$ in expression (86) can be explained by the following argument. The propagation of the up-spin front to the left over a distance l requires the "excitation" of a minimum number $z(l)$ of additional up spins. For $l = 2^k$ $(k = 1, 2, 3, \ldots)$ this number is given by[6]

$$z(2^k) = k + 1 \tag{87}$$

This result follows from the recurrence relation

$$z(2^{k+1}) = z(2^k) + 1 \tag{88}$$

in combination with the particular value $z(2) = 2$. Since $z-1$ of the additional up spins are auxiliary, we conclude that the rate of propagation to

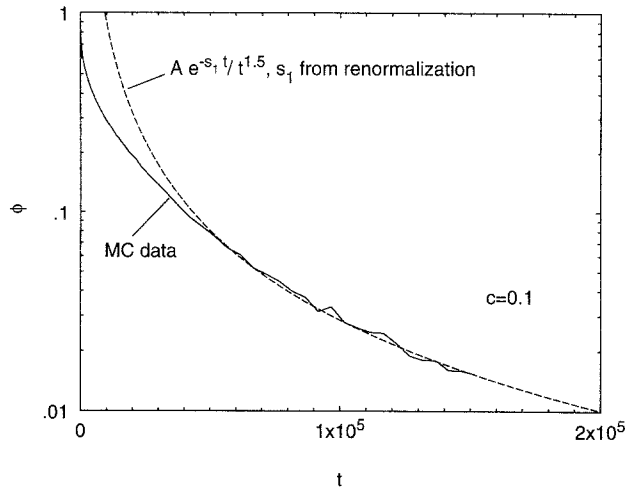

Fig. 8. Comparison of the Monte Carlo data for $\phi(t)$ at $c=0.1$ with the prediction of Eqs. (82) and (86).

the left over a distance $l=2^k$ is controlled by an extra factor c^k for low c values. Similarly, the withdrawal of the up-spin front to the right over a distance $l=2^k$ requires a minimum of k additional up spins between the front up spin and the up spin at the right end of the interval. Therefore, for either direction, the motion of the up-spin front over an up-spin-free interval of length $l=2^k$ slows down the proportional to an extra factor c^k for $c \to 0$. Since the average length of up-spin-free intervals is $1/c$, we conclude that the renormalized diffusion constant of the up-spin front (the "defect diffusion constant") contains the extra factor $c^{\mathrm{lb}(1/c)}$, where $\mathrm{lb}\, l = \log 2$ denotes the binary logarithm.

In Fig. 8 we show a comparison of the Monte Carlo data for $\phi(t)$ at $c=0.1$ with the prediction of Eqs. (82) and (86). Fitting the factor of proportionality in Eq. (82), we obtain good agreement for the longest times $0.5 \cdot 10^5 < t \leqslant 1.5 \cdot 10^5$. Unfortunately, this is not a test of our estimate, Eq. (86), since in this time region the exponent $|s_1|\, t$ in expression (82) is negligible, because our estimate yields $|s_1| = 10^{-9}$.

4. SUMMARY AND CONCLUSIONS

In this paper, the hierarchically constrained kinetic Ising chain first presented in ref. 1 is reviewed and three approximation methods for the calculation of the single-spin autocorrelation function are presented. The results can be summarized as follows:

1. The standard approximation schemes, the effective-medium approximation (EMA) (Section 2.1) and the mode-coupling approximation (MCA) (Section 2.2), are not suited for our model. Results are not only quantitatively inaccurate, but reveal qualitatively erroneous features. Namely, the EMA exhibits a blocking transition for $c < 0.5$ [see property Eq. (8)] and the relaxation function from the MCA diverges when $c \lesssim 0.5$ (see B in Section 2.2 and Fig. 1). For these approximation schemes similar results have also been found for other kinetic Ising models with kinetic constraints.[8,9]

2. The cluster approximation (Section 3) was designed in close relation to our model and is clearly more successful in yielding good results than the other two (see Fig. 2 and 3 for the first two orders of the approximation). The order of the approximation can be increased in a straightforward manner. This yields results converging to the exact solution for all concentrations (see Fig. 5). Equation (81) gives an estimate of the required order m of the approximation as a function of concentration. It should be worthwhile trying to construct a similar approximation method for related models.

3. The cluster approximation has also been useful for clarifying some general aspects of the hierarchical spin model. These concern the connection with defect-diffusion models. In Sections 3.3 and 3.7 we found that in the long-time limit, the clusters can be viewed as defects diffusing on the chain. From that the asymptotic long-time form of the spin-autocorrelation function can be infered to be $\phi(t) \sim e^{s_1 t}/t^{3/2}$ [see Eqs. (64), (77), and (82) and Fig. 7]. The renormalized diffusion constant (86) occurring in the asymptotic formula was estimated using the result of a renormalization procedure described in ref. 6.

With these results, the time dependence of the spin-autocorrelation function $\phi(t)$ of the semi-infinite hierarchical spin chain can be characterized as follows. There are three time regimes, in each of which $\phi(t)$ can be approximated by a Kohlrausch–Williams–Watts function

$$\phi_{\mathrm{KWW}}(t) = \exp(-[t/\tau]^{\beta})$$

with exponents $0 < \beta \leqslant 1$ and relaxation times τ (Fig. 9).

From the master equation we infer that $\phi(t)$ decays exponentially ($\beta = 1$) like $\exp(-ct)$ at short times. For $c = 0.1$, for example, this expression is a good approximation to $\phi(t)$ for the first 5% of its decay from the initial value of one. A short-time behavior of this sort is common to many kinetic Ising models. According to our asymptotic formulas (82), (86), the long-time behavior of $\phi(t)$ is also dominated by an exponential. The

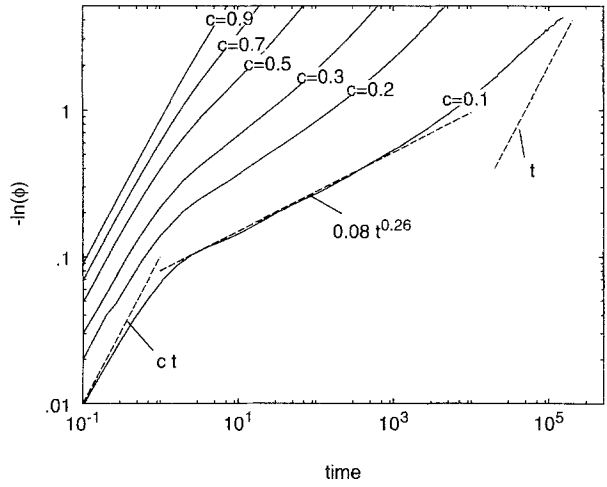

Fig. 9. KWW plot of $\phi(t)$ for various concentrations c. For $c = 0.1$ the three time regimes are sketched with dashed lines and the respective KWW-exponents are written down.

algebraic factor $t^{-3/2}$ can be considered as a logarithmic correction to the exponent. Between the short-time and the long-time domains there is a crossover regime, where $\phi(t)$ can again be fitted to the KWW formula over an extended time interval. However, in this regime the effective exponent β decreases markedly with decreasing up-spin concentration c. Possibly β goes to zero for $c \to 0$ as $[\ln(1/c)]^{-1}$. For $c = 0.1$, the KWW formula with $\beta = 0.26$ gives a good fit of the decay of $\phi(t)$ from about 95 to 50% of its initial value (see Fig. 9). The transition from this intermediate to the asymptotic long-time regime is very slow, for low concentrations in particular. Therefore the long-time regime is difficult to reach by Monte Carlo simulation. This is related to the difficulty of measuring the asymptotic decay of the relaxation function for real systems with slow cooperative dynamics.

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NOTE ADDED IN PROOF

In the meantime it could be proved (J. Jäckle, *J. Non-Cryst. Solids*, to be published) that the solution of the MCA-equation of motion (19, 21) not only no longer decays monotonically, but even diverges exponentially for $t \to \infty$ at up spin concentrations $c < 1/3$.

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