Phase-ordering simulation of one-dimensional conserved kink system

Hiroyasu Toyoki*
Department of Ecosocial System Engineering, University of Yamanashi, Kofu 400-8511, Japan

Tomoyuki Nagaya†
Department of Electrical and Electronic Engineering, Okayama University, Okayama 700-8530, Japan
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The kink-antikink kinetics of one-dimensional phase ordering under conserved order parameter dynamics is studied numerically. The average domain size is found to grow logarithmically, and the distribution of domain size and order parameter correlation function are shown to satisfy a scaling relation. The two-time autocorrelation function follows a power law of $A_{t_0}(t) \sim t^{-\lambda}$, where λ depends on the start time of the calculation t_0. If t_0 is in the scaling regime, λ takes a constant value of 3.0. Thus the scaling functions are sensitive to the initial configuration of domains. When the initial kink positions are given by uniform random numbers, the scaling functions agree with those obtained by cell dynamical system simulation.

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The growth of an ordered phase following quenching from a disordered phase satisfies a form of dynamical scaling in most cases [1]. For the vector order parameter $\boldsymbol{\psi}(\mathbf{r},t)$, the correlation function $C(r,t)=\langle \boldsymbol{\psi}(\mathbf{r}_0,t)\cdot\boldsymbol{\psi}(\mathbf{r}_0+\mathbf{r},t)\rangle$ is known to be cast into a scaling form $C(r,t)=f(r/\ell)$ and the characteristic length grows algebraically in time, $\ell(t)\sim t^{1/z}$. The form of the scaling function and the exponent, z are determined by the symmetry of the ordered state and conservation laws. The spatial structure of the order parameter is governed by topological defects, such as vortices and hedgehogs, the long-range interaction of which leads to algebraic growth. The one-dimensional (1D) scalar order parameter, on the other hand, exhibits logarithmic growth due to the exponential interaction of kinks.

For the case of nonconserved order parameter (NCOP) dynamics, the kink equation has been derived from the time-dependent Ginzburg-Landau (TDGL) equation [2], and the domain distribution and logarithmic growth have been obtained by kinetic study of the kink equation in the mid-1980s [3]. Around the same time, the logarithmic growth was observed experimentally in neutron scattering studies of a layered antiferromagnet [4]. The kink equation for the conserved order parameter (COP) case was also derived from the TDGL equation by Kawakatsu and Munakata (KM), who also identified logarithmic growth [5]. In their work, however, the spatial characteristics of the ordering process were not investigated due to a lack of available computing power. As no experimental system for 1D COP was known until the recent work by Nagaya and Gilli (NG) [6], little attention has been paid to such systems over long periods. Nagaya and Gilli studied the coarsening process of the undulated domain wall in a layered nematic system, and found that the application of a magnetic field to a nematic layer yields a straight domain wall in the layer. They also found that low-frequency electric fields induce zigzag undulation of the wall, with the undulation coarsening over time. This is equivalent to a 1D kink-antikink system with conserved order parameter. It has been shown that the average domain size grows logarithmically, and scaling laws for the distribution function of domain length, structure factor, and autocorrelation function have been derived. The domain length only grew up to two times the initial length in the NG experiments. Thus longer-term observation is desirable in order to check the scaling behavior.

This report presents numerical results for a wide time range, in which the domain length grows to over one hundred times the initial length. In the 1D case, thermal random forces may be dominant over deterministic forces due to the high thermodynamic energy of the system. At the thin limit of the wall, the system is well simulated by the kinetic Ising model, which exhibits power-law growths of $t^{1/2}$ for NCOP and $t^{1/3}$ for COP [7]. In contrast, when the interaction between kinks is dominant, logarithmic growth occurs. The NG experiments correspond to the latter case, which will also be the focus of this paper. An interactive kink model based on a modification of the Ising model has been proposed by Majumdar and Huse [8]. Noting that the interaction between kinks is a short-range phenomena, they used an update scheme by which the shortest domain is collapsed at each time step without moving other kinks, and is assigned to domains on both sides belonging to the same phase. Although they have shown that the correlation functions can be scaled by the average domain length, the time dependence cannot be known in that system. Furthermore, the equivalence to the equation of motion for kinks has yet to be adequately verified.

In the present work, the cell dynamical system (CDS) model was employed as a discrete-time version of the TDGL equation and the KM equation for kinks. CDS is frequently used for analysis of growth dynamics, and the results are known to agree with the analytical results for high-dimensional cases [1]. For the 1D case, however, CDS incurs extremely long calculation times due to the short-range interaction of kinks. Accordingly, CDS is used only to check

*Electronic adddress: toyoki@yamanashi.ac.jp
†Electronic addresss: nagaya@elec.okayama-u.ac.jp

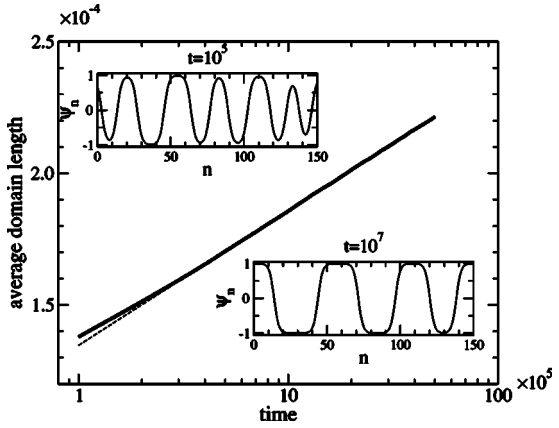

FIG. 1. Average domain length against time obtained by CDS simulation. The dotted line is the best fit. Insets show the profiles of the order parameter ψ_n. The time represents the number of updates.

the early stage of growth, and the KM equation is employed to study long-time behavior.

The CDS model for the scalar order parameter $\psi(n,t)$ is given by

$$\psi(n,t+1) = \mathcal{F}[\psi(n,t)] - \langle\langle \mathcal{F}[\psi(n,t)] - \psi(n,t)\rangle\rangle, \qquad (1)$$

$$\mathcal{F}(\psi) = \Delta[f(\psi) + D(\langle\langle\psi\rangle\rangle - \psi)], \qquad (2)$$

where $\langle\langle A(n)\rangle\rangle - A(n)$ is the discrete Laplacian, which is simply given by $[(A(n+1)+A(n-1)-2A(n)]/2$ for the 1D case. The local map $f(\psi)=(1-|\psi|^2)\psi$ is used, corresponding to a double-well potential. Figure 1 shows the growth of the average domain length for $\Delta=0.01$, $D=10.0$, and $N=2^{16}$ sites. The initial distribution of ψ_n is given by uniform random numbers of $|\psi_n|<0.4$. The domain length is well fitted by a logarithmic line above $t=3\times10^5$, where t denotes the number of updates. This lower bound of the logarithmic growth corresponds to the stage in which most kinks exhibit a stationary profile, as shown in the insets. The increment of the domain length in this simulation is less than twice the lower edge, and is considered to be too small to confirm the scaling behavior of the structure factor or correlation function. It takes several months of computation to obtain domain length growth of several times.

The stationary profile of a kink derived from the TDGL equation is given by $\psi_{x_0}(x)=\tanh(x-x_0)$, where x_0 is the kink core position. Inserting an N-kink state $\psi(x)=-1+\Sigma_{n=0}^{N-1}(-1)^n[\psi_{x_n}(x)+1]$ into the TDGL equation, it is possible to derive the equation for $\{x_n\}$. As the driving force for kinks is yielded by excess energy related to the superposition of exponential tails of the kink, the dominant term should be extracted as a function of the separation of adjacent kink pairs $\{x_{n+1}-x_n\}$. For the conserved case, Kawakatsu and Munakata showed that the relation can be written in a simpler form in terms of $\ell_n=x_{n+1}-x_n$ instead of x_n, as follows:

$$\dot{\ell}_n = I_n^{(+)} + I_n^{(-)}, \qquad (3)$$

where

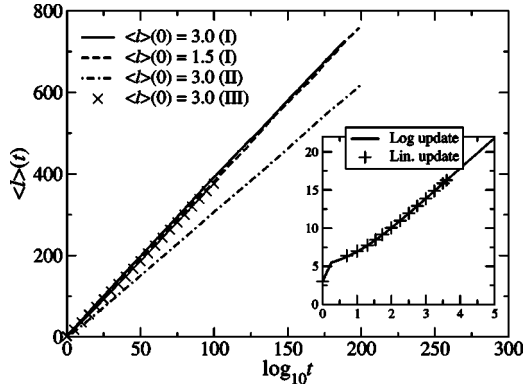

FIG. 2. Average domain length against time for three types of initial distribution. The inset shows a comparison between the results obtained using a constant logarithmic time step of $\Delta\tau=\Delta\log_{10}t=0.005$, and those obtained using a linear time step of $\Delta t=0.1$.

$$I_n^{(+)} = -I_{n+2}^{(-)} = \frac{1}{\ell_{n+1}}\left(e^{-\ell_{n+2}} - e^{-\ell_n}\right). \qquad (4)$$

One can interpret that $I_n^{(-)}$ and $I_n^{(+)}$ represent the *flow* transferring from ℓ_{n-2} and ℓ_{n+2}, respectively, due to the kink interaction. The condition $I_n^{(+)}=I_{n+2}^{(-)}$ satisfies the conservation law.

As expected from the exponential interaction between kinks, the numerical results show logarithmic growth. To calculate the long-term behavior, simulations were performed by using a logarithmic time of $\tau=\ln t$, where the growth equation (3) is written as $d\ell_n/d\tau=\exp(\tau)[I_n^{(+)}+I_n^{(-)}]$. For a given number of kinks N, equal to the number of antikinks, the total length of the system is given by $\Sigma_{n=0}^{2N-1}\ell_n$, which is conserved in each run. A periodic boundary condition was used, with $d\tau=0.005$. The system was updated using a fourth-order Runge-Kutta scheme. When a kink-antikink pair approach to within a unit length (i.e., $\ell_n<1$), the pair is considered to be annihilated. As it is not obvious what initial distribution corresponds to that just after the early transient stage that kinks are formed in a system quenched from a disordered state, three initial distributions of kink positions were tested and compared with the results of CDS. Case I has initial kink positions given by uniform random numbers, where the initial domain size distribution is an exponential function. The other cases have domain lengths, rather than kink positions, given by Gaussian (case II) and uniform (case III) random numbers. Figure 2 shows the growth of domain size averaged over 50 runs for these three initial configurations. The initial numbers of kinks and antikinks are $N=5\times10^4$. The growth of the average domain size $\langle\ell\rangle(t)$ fits the logarithmic curve well above $\langle\ell\rangle(t)\approx10$. The upper bound of this calculation was $\langle\ell\rangle(t)=750$, corresponding to $N(t)=300$, which is sufficiently large to avoid finite-size effects. As shown in the inset, the calculation using a logarithmic time step was consistent with the linear-update model in the early stage.

Figure 3 shows the domain size distribution function scaled by the average domain size $\langle\ell\rangle(t)$ for the three initial conditions. The size distribution function grows toward a single scaling function of $g(\ell/\langle\ell\rangle)$ in all cases. Cases I and

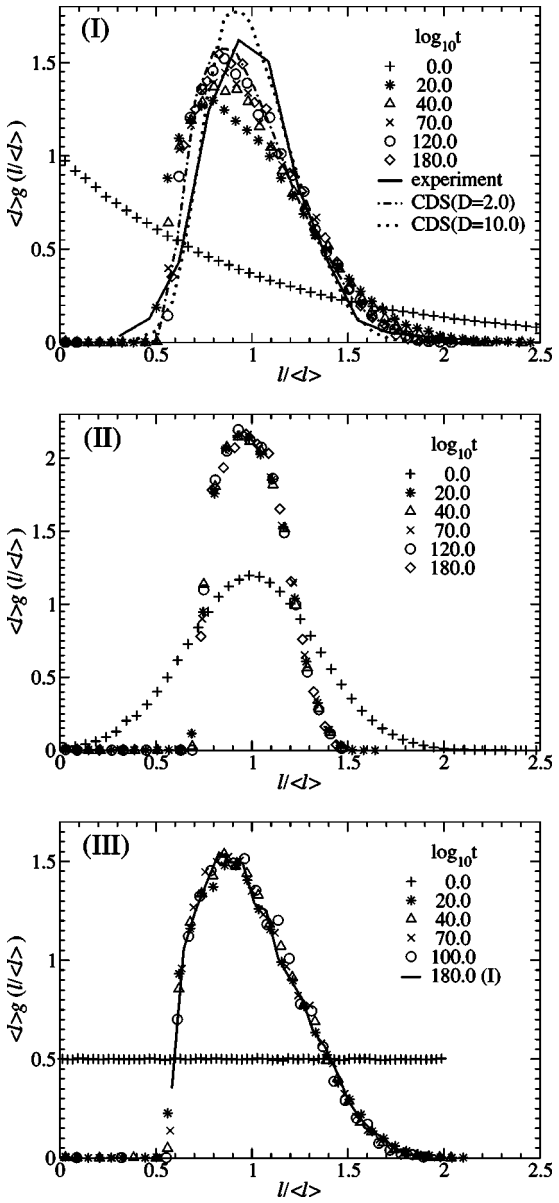

FIG. 3. Scaled distribution function of domain size. (I)–(III) correspond to cases I–III in the text. CDS results for two values of D are also plotted in (I). The solid line in (I) indicates experimental results presented previously [6]. The data for $\tau=180.0$ in (I) is shown in (III) as a solid line for comparison.

III collapse to a similar scaling function, whereas case II reaches a steeper scaling function.

The distribution function for case I has a long transient regime and seems to be progressing to a scaling regime within the time range of the present calculations, as suggested by the longer tail of the initial distribution compared to the other two cases. Thus the ordering dynamics for the present kink system depends remarkably on the initial condition.

As shown by the lines in Fig. 3 (I), the experimental and CDS data are in reasonable agreement with the results of cases I and III. The CDS results for the case of a thin domain wall ($D=2.0$) is fitted best, while the other distributions are slightly more symmetrical than the kink kinetics results.

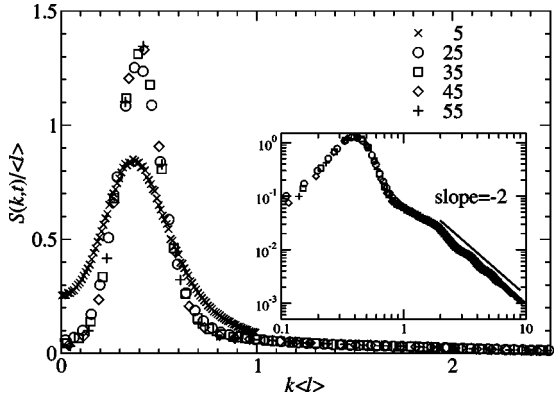

FIG. 4. Scaled structure factor. The inset shows the same data on a logarithmic scale.

These results indicate that the kink kinetic results follow an asymptotic curve in large systems.

The spatial configuration of the Ising-like order parameter $\psi(x)$ defined by $\psi(x)=(-1)^n$ was also examined for $\Sigma_{i=0}^{n-1}\ell_i < x < \Sigma_{i=0}^{n}\ell_i$. The structure factor in this case is given by $S(k,t)=|\Sigma_{n=0}^{M-1}\psi(x_n)\exp(i2\pi k x_n/M)|^2$, where $\{x_n\}$ represent M points equally dividing the system length. Figure 4 shows the structure factor scaled by $\langle\ell\rangle(t)$, obtained by averaging 200 runs with $M=2^{15}$ and 3×10^4 initial kinks for case I. The correlation function of the order parameter $C(r,t)$ is shown in Fig. 5, as obtained by Fourier transformation of $S(k,t)$. The power-law tail k^{-2} and the linear decay in the short-distance region of $C(r,t)$ are evidence of a kink structure. The scaling holds reasonably well, but still continues to shift slightly as the periodicity becomes stronger over time. Case I (Fig. 4) is the most remarkable case, where the first minimum located at $r/\langle\ell\rangle=0.70$ grows from -0.46 to -0.52 as τ changes from 25 to 55. The first minimum in case III is located at $r/\langle\ell\rangle=0.62$ and changes slightly from -0.578 to -0.591 during the same period, while case II changes by less than 1%: -0.323 at $\tau=15$ and -0.326 at $\tau=45$. This indicates, considering the behavior of $g(\ell/\langle\ell\rangle)$, that cases II and III almost reach the scaling regime within this period.

The two-time autocorrelation function is known to be characterized by an independent exponent λ via

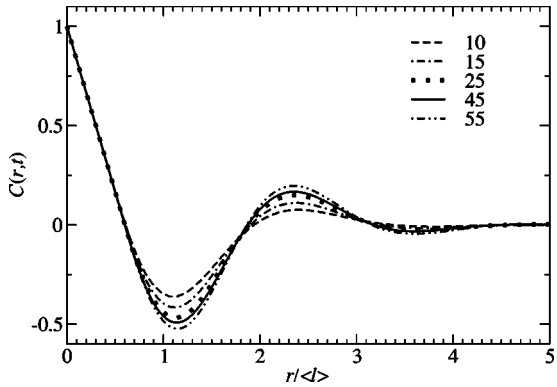

FIG. 5. The scaled equal-time two-point correlation function.

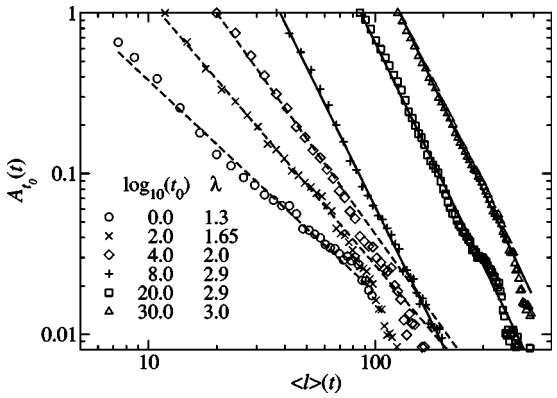

FIG. 6. Two-time autocorrelation function for some base times t_0. The best-fit values of the exponent λ are indicated by dashed and solid lines, corresponding to $\langle \ell \rangle(t) < 70.0$ and $A_{t_0}(t) > 0.02$, respectively.

$$A_{t_0}(t) = \langle \psi(x,t_0)\psi(x,t_0+t)\rangle \sim \langle \ell \rangle(t)^{-\lambda}. \quad (5)$$

The autocorrelation function was determined at 300 points for a run starting with 3×10^4 kinks and antikinks, and the function was averaged over all points and 200 runs. Figure 6 shows $A_{t_0}(t)$ for case I, plotted against the average domain size. The autocorrelation function exhibits power-law decay except for a certain region at longer times, where a finite-size effect would occur. The values of λ indicated in Fig. 6 were calculated in the power-law regions of $\langle \ell \rangle(t) < 70$ for $\log_{10}t_0 = 0.0$, 2.0, and 4.0, and $A_{t_0}(t) > 0.02$ for other t_0. The behavior of $A_{t_0}(t)$ can be divided into two regimes; an early transient regime at small t_0, and the scaling regime at all calculation times. In the former case, λ increases with t_0, whereas in the latter case, λ takes a universal value of 3.0. The data of $t_0 = 2.0$ and 4.0 are considered to crossover to the regime with $\lambda = 3.0$ at around $\langle \ell \rangle(t) = 80$. It was found that $A_{t_0}(t)$ decreases slowest in case II ($\lambda = 2.1$) and fastest in case III ($\lambda = 3.2$). Thus the exponent λ is also dependent on the initial configuration.

This report presented numerical results for the ordering dynamics of a conserved scalar order parameter system. It is shown that the average domain size can be fitted to a single logarithmic curve over a wide range of time including the pre-scaling regime. The scaling regime for the distribution functions of domain length and structure factor was identified. The CDS results were most accurately reproduced by cases I and III of the kink kinetics system. Thus the ordering after quenching from the thermal disordered state is considered to correspond to cases I and III. The scaling function of case II differs from those of the other cases. As the scaled function of case I moves slightly in the opposite direction to that of case II, they do not seem to collapse to a single function. Consequently, the present results are considered to progress out of the pre-scaling regime, and to indicate the existence of more than one stable scaling structure.

The power-law decay of the autocorrelation function was also investigated, and it was found that the exponent λ also depends on the initial configuration. The exponent λ is, however, robust with respect to the initial time t_0, as long as t_0 is within the scaling region. This robustness was also recognized by Yeung *et al.* [9] for 2D systems. The value of λ also satisfies the lower bound suggested by Yeung *et al.*

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[1] For reviews, see A. J. Bray, Adv. Phys. **43**, 357 (1994); A. Onuki, *Phase Transition Dynamics*, Part III (Cambridge University Press, Cambridge, England, 2002).
[2] K. Kawasaki and T. Ohta, Physica A **116A**, 573 (1982).
[3] T. Nagai and K. Kawasaki, Physica A **120A**, 587 (1983); K. Kawasaki and T. Nagai, *ibid.* **121A**, 175 (1983).
[4] H. Ikeda, J. Phys. Soc. Jpn. **52**, 33 (1983)
[5] T. Kawakatsu and T. Munakata, Prog. Theor. Phys. **74**, 11 (1985).
[6] T. Nagaya and J-M Gilli, Phys. Rev. E **65**, 051708 (2002); Phys. Rev. Lett. **92**, 145504 (2004).
[7] S. J. Cornell, K. Kaski, and R. B. Stinchcombe, Phys. Rev. B **44**, 12 263 (1991); see also, for example, F. Corberi, C. Castellano, E. Lippiello and M. Zannetti, Phys. Rev. E **65**, 066114 (2002); S. N. Majumdar and D. S. Dean, *ibid.* **66**, 056114 (2002).
[8] S. N. Majumdar and D. A. Huse, Phys. Rev. E **52**, 270 (1995).
[9] C. Yeung, M. Rao, and R. C. Desai, Phys. Rev. E **53**, 3073 (1996).