Ordering Kinetics in the Two-Dimensional Classical Coulomb Gas of Half-Integer Charges on a Square Lattice: Temperature Dependent Growth and Roughening Transition

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The ordering kinetics in the Coulomb gas (CG) of half-integer charges is investigated via Monte Carlo simulations. Because of the long range Coulomb interaction, the phase ordering of this system is governed by an activation energy barrier with a logarithmic dependence on the domain size. This results in a genuine temperature-dependent growth and a roughening transition of the domain-wall morphology above $T_R \simeq 0.09 \pm 0.01$. An analytical argument with numerical verification indicates that the classical CG of half-integer charges belongs to a new universality class from the viewpoint of Lai *et al.*'s classification of ordering kinetics [Phys. Rev. B **37**, 9481 (1988)]. [S0031-9007(97)03761-7]

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The subject of phase ordering kinetics of statistical systems, which deals with the approach to equilibrium under a rapid thermal quench from a disordered phase to a low temperature ordered phase, has attracted research interest for several decades [1–3].

One of the important questions in the ordering kinetics of statistical systems is the effect of thermal fluctuations and identification of a universality class of the ordering kinetics, which was first addressed by Lai, Mazenko, and Valls (LMV) [4]. According to LMV, an important criterion is the domain size dependence of the activation barrier. The class I system is characterized by no activation barrier and therefore systems in this class show no freezing at zero temperature, i.e., thermal fluctuation is irrelevant in the ordering dynamics. In class II systems, a local energy barrier exists for growth of a domain, where the magnitude of the energy barrier is independent of the size of the domain. These systems exhibit freezing in the limit of zero temperature, and at finite temperature the average domain size $L(t)$ behaves as $L(t) = L_0 + A[t/\tau(T)]^{\phi}$ with the activated time scale $\tau(T) = \tau_0 \exp(E_0/T)$, where L_0, A, and τ_0 are weakly temperature dependent, and E_0 is an activation energy determined by the local barriers. Here L_0 is related to the average size of frozen domains at $T = 0$. Lastly, class III and IV systems are characterized by energy barriers depending on the domain size as a positive power law, resulting in growth laws (at finite temperature) of logarithmic power form $L(t) \sim (\ln t)^m$. Each of these systems exhibits a *temperature-independent* growth law (growth exponent).

This LMV scheme is of course not exhaustive, but it turns out that this scheme is quite general, making it difficult to find a new universality class which is not included in the LMV classification. In connection with this issue, a recent simulation study [5] on the phase ordering kinetics of the two-dimensional (2D) fully frustrated *XY* model (FFXYM) [6] revealed interesting features of growth kinetics such as a temperature-dependent growth exponent and finite temperature roughening transition of the domain-wall morphology, thus raising a possibility of finding a new class of ordering kinetics. But this simulation could not provide a definitive answer to the question as to whether the temperature dependence of the growth exponent is truly genuine or is merely apparent due to the limitation of simulation time scale. Another related open question is the role of long range interaction between point defects present in FFXYM and its competition with the thermal fluctuations.

In the present Letter, in order to answer these questions, we have performed a direct Monte Carlo simulation of the 2D Coulomb gas (CG) of half-integer charges, which explicitly contains logarithmic long range interaction [7]. We have found the phase ordering kinetics of the CG retains basically the same features as that of FFXYM. We also find through a numerical calculation that the CG of half-integer charges is characterized by an activation energy barrier that has *logarithmic* dependence on the domain size. An analytic argument shows that this type of activation barrier leads to a *temperature dependent* growth exponent. Furthermore, it also explains the finite temperature roughening transition in the domain-wall morphology via a Kosterlitz and Thouless (KT)-like argument on the one-dimensional domain wall. All these results are nicely confirmed by our simulation results. Therefore, we can view the CG of half integer charges (and FFXYM) as belonging to a new universality class of ordering dynamics with continuously varying (temperature dependent) growth exponents.

General 2D CG on a square lattice is described by the following Hamiltonian that can be mapped from the uniformly frustrated *XY* model via Villain transformation [8],

$$\mathcal{H}_{\mathrm{CG}} = \frac{1}{2}\sum_{ij}(n_i - f)G(r_{ij})(n_j - f), \qquad (1)$$

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where $n_i = 0, \pm 1, \pm 2, \ldots$ corresponds to the integer vorticity of the phase angle at site i dual to the XY lattice. The charge at site i is defined as $q_i \equiv n_i - f$ where f is called the frustration parameter and $-f$ can be considered as a negative uniform background charge distribution. The CG of half-integer charge corresponds to the case of $f = 1/2$. The lattice Green function $G(r_{ij})$ solves the equation

$$\Delta^2 G(r_{ij}) = -2\pi\delta_{r_{ij},0}\,, \tag{2}$$

where Δ^2 is the discrete lattice Laplacian. By Fourier transforming (2) for a square lattice of linear size N with periodic boundary condition, one obtains

$$G(\vec{r}) = \frac{\pi}{N^2}\sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{2 - \cos(\vec{k}\cdot\hat{x}) - \cos(\vec{k}\cdot\hat{y})}\,, \tag{3}$$

where the summation is over all wave vectors $\{\vec{k}\} = \{(\frac{m_1}{N})\vec{b}_1 + (\frac{m_2}{N})\vec{b}_2\}$ with $m_1, m_2 = 0, 1, 2, \ldots, N-1$ consistent with periodic boundary conditions, and $\{\vec{b}_1, \vec{b}_2\} = \{2\pi\hat{x}, 2\pi\hat{y}\}$ the basis vectors of the reciprocal lattice. Equation (3) diverges for $\vec{k} = 0$, which reflects the infinite self-energy of a point charge. To remove this self-energy term and keep the CG energy finite, we impose the neutrality condition $\sum_i q_i = \sum_i (n_i - f) = 0$, i.e., $\sum_i n_i = Nf$. Since the self-energy term exactly cancels in the neutral system, we can use the nonsingular potential $G'(\vec{r}) \equiv G(\vec{r}) - G(\vec{r} = 0)$ in (1), which is evaluated numerically by using (3) for a given lattice size N. For large separation r, $G'(\vec{r}) \simeq -\ln|\vec{r}|$.

For the case of $f = 1/2$, charges with lowest magnitude are $1/2$ and $-1/2$. The ground state is a configuration of charges $1/2$ and $-1/2$ forming a checkerboard pattern with the same symmetry as an Ising antiferromagnet [9]. Since the continuous spin degree of freedom has been left out in the duality mapping, the ground state of the model now possesses only twofold discrete Z_2 symmetry. This model system can have two types of excitations. One is a charge pair excitation involving the interchange of a given $+1/2$, $-1/2$ pair separated by a distance r. The other is an Ising-like domain excitation, originating in the formation of oppositely ordered Ising domains.

To investigate the ordering kinetics of the model, we carry out Monte Carlo simulations on a square lattice of linear size $N = 64$ with periodic boundary conditions. We have also done some simulations with a bigger system size of $N = 80$, but found no essential difference in the results. Restricting the charges to have the lowest magnitude $+1/2$ or $-1/2$ only, we update the initial disordered random configuration by exchanging the charges at randomly selected nearest neighbor pairs according to the standard Metropolis algorithm. The presented results are averages over 20 to 40 different random initial configurations. We stress here that we are dealing with a nonconserved order parameter, namely the staggered charge variable defined as $\sigma_i = 2(-1)^{i_x + i_y} q_i$, (i_x, i_y) being the integer coordinate of a lattice site i, although the net charge is conserved. The main quantity of interest is the two-point equal-time correlation function of the Ising order parameter $C(r,t) = \frac{1}{N^2}\sum_i \langle \sigma_i(t)\sigma_{i+r}(t)\rangle$, where $\langle\cdots\rangle$ represents the average over different random initial configurations. We also measure the total length of Ising domain walls, and the total number of the corners of the Ising domain walls to examine a morphological change.

For the case of zero-temperature quench, we find that the system is driven into a metastable state [10], preventing further ordering. Similar freezing behavior has also been observed in the FFXYM on a square lattice [5]. This can be contrasted with the case of exchange dynamics of the nearest neighbor antiferromagnetic Ising model in a square lattice, which is known to show no freezing at zero temperature [11]. This freezing behavior is simply due to the additional long range interaction which gives rise to activation barriers.

For finite temperature quenches, we try to collapse the Ising order parameter correlation functions $C(r,t)$ with a length scale $L(t)$, which is extracted from $C(r,t)$, for example, as $C[r = L(t), t] = 1/2$ for a given time t. A good data collapse for a given quenching temperature, as demonstrated in the inset of Fig. 1, indicates that a simple dynamic scaling of the form $C(\vec{r}, t) = F[r/L(t)]$ is satisfied for the equal time Ising correlation functions. The length scale $L(t)$ shows a power law growth in time $L(t) \sim t^{\phi}$ but the growth exponent ϕ shows a temperature dependence, as seen in Fig. 1. Note that it has a linear temperature dependence at low temperatures $\phi(T) = \alpha T$ with the slope $\alpha \simeq 8.57$.

Figure 2 shows the snapshots of the configurations of the Ising order parameter (staggered charge variable) for quenches to the temperatures $T = 0.04$ and 0.1,

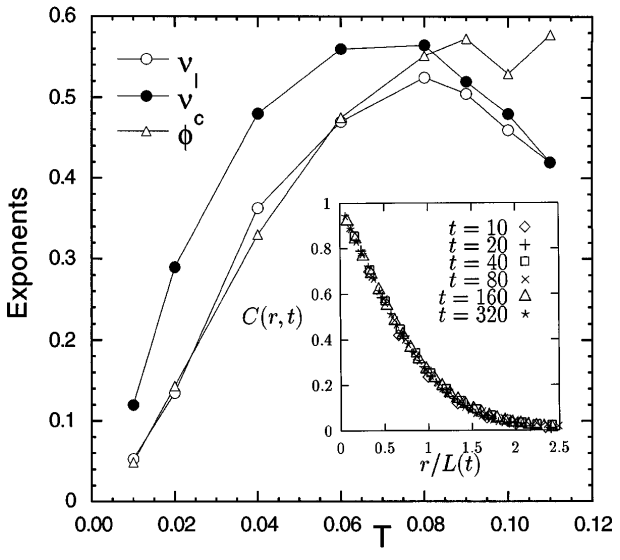

FIG. 1. The temperature dependence of various exponents ν_l, ν_c, and ϕ. Error bars are at most twice the size of symbols. Solid lines are guides to the eye. Inset: Scaling collapse of the equal-time correlation functions for the Ising spin at $T = 0.06$ with $L(t) \sim t^{\phi}$ where $\phi \simeq 0.48$.

respectively, where we can see a morphological transition from low temperature *faceted* domain walls to rough domain walls at high temperatures.

In order to locate the temperature at which the morphological transition takes place, we calculate the time dependence of the total number of domain-wall corners (N_c) and the total length (N_l) of the Ising domain walls. These quantities are expected to decay in time toward their equilibrium values with power law, i.e., $N_c(t) - N_c(\infty) \sim t^{-\nu_c}$ and $N_l(t) - N_l(\infty) \sim t^{-\nu_l}$. Figure 1 shows these exponents. We observe that ν_c is greater than ν_l for $T \leq T_R \simeq 0.09 \pm 0.01$, while $\nu_c \simeq \nu_l$ for $T > T_R$. As can be shown by a simple argument [5], the low temperature regime ($T < T_R$) corresponds to faceted domain-wall morphology and high temperature regime to rough domain walls (see Fig. 2). The decrease of the exponents ν_c and ν_l with increasing temperature at higher temperatures (for $T > 0.08$) can be attributed to the effect of thermal fluctuations that are competing with the ordering process. These thermal fluctuations can create more corners and domain walls and thus slow down the decay rate of these defects, resulting in smaller values of ν_c and ν_l as the temperature increases.

As for the temperature dependence of the growth exponent ϕ at low temperatures, we may argue as follows. At zero temperature, there exists freezing in the ordering process. At low but nonzero temperature, we expect the ordering proceeds via activated processes, where the domain walls tunnel across energy barriers. Since we observe faceted domain walls at low temperatures, we begin with a square-shaped domain of (-1) staggered charge variable with dimension $L \times L$ within an infinite background sea of opposite $(+1)$ staggered charge variable [see inset (a) of Fig. 3]. Suppose that our domain with (-1) staggered charge variable is represented by charge configuration beginning with $- + - + - + \ldots$ at the top left-end corner of the domain. It is easy to see that the first step in reducing the size of a domain with minimal energy cost is to exchange the $-1/2$ and $+1/2$ charges in the leftmost corner of the top row of the domain. Correspondingly, the domain will be reduced as shown in inset (b) of Fig. 3. This may be viewed as creating a pair of corners (we will call this a *step excitation*) in the domain wall, which will cost some positive energy. The next step will be to exchange again the leftmost charge pairs in the top row. Repeating these processes again and again, we reduce the total length of the domain wall by 2 lattice units. At this point, the energy of the system will now be lower than the initial energy. A question is, what is the maximum height of the energy barrier during these series of domain-wall motions delineated above?

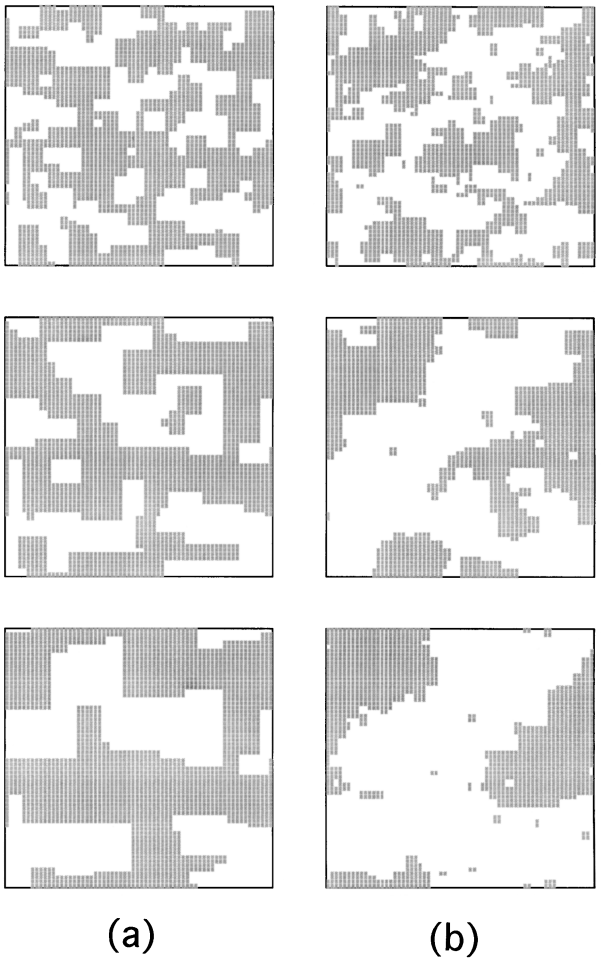

FIG. 2. The snapshots of configurations for Ising domains at (a) $T = 0.04$ and (b) $T = 0.1$. In each set, figures represent the snapshots taken at $t = 20$, 80, and 320, respectively, from top to bottom.

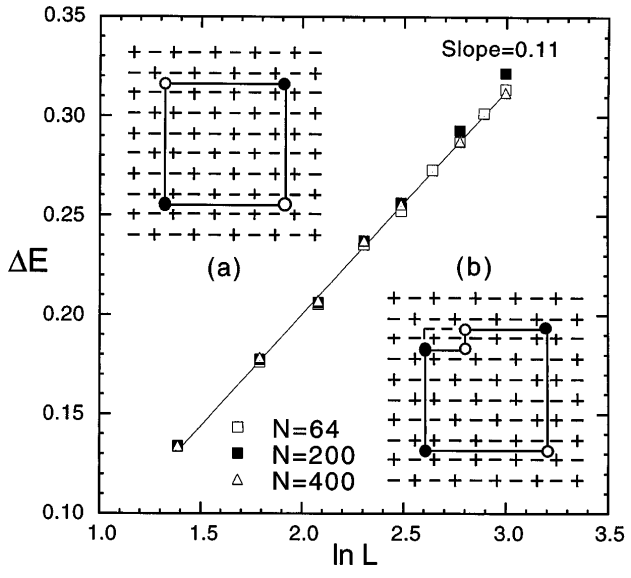

FIG. 3. The energy barrier ΔE versus the linear size L of a square shaped domain. Insets (a) and (b): The configuration of Ising domains. Open and filled circles represent negative and positive fractional charges, respectively.

Since each of the created corners can also be considered as a charge excitation of magnitude $1/4$ [12] interacting logarithmically with other charges separated by a length scale of order L (the domain size), we expect the energy barrier to behave as $\Delta E = E_0 \ln(L/L_0)$ where E_0 is a constant and L_0 is a length scale of the order of the lattice unit corresponding to the average size of the frozen domains at $T = 0$. In order to confirm this argument, we numerically calculated the domain-size dependence of the energy barrier using the Hamiltonian (1) and the domain size ranging from $\sim L = 4-20$ on a square lattice of size as large as $N = \sim 64-400$. We found that the maximum barrier appears when the step excitation reaches near the center $(L/2)$ of the domain wall or slightly beyond the center. Figure 3 shows a semi-log plot of the calculated energy barrier versus the linear domain size which gives a very nice fit to a logarithmic behavior with $E_0 = 0.11 \pm 0.01$ and $L_0 = 1.25 \pm 0.05$.

If we suppose that the ordering proceeds via an activated process with the barrier having logarithmic dependence on the domain size as above, then the time t taken for annihilation of a square domain of size $L \times L$ would be $t = t_0 \exp(\Delta E/T) = t_0 \exp[E_0 \ln(L/L_0)/T] = t_0 (L/L_0)^{E_0/T}$. That is, we get for the domain size $L(t) = L_0 (t/t_0)^{T/E_0}$, where t_0 is the time scale for reaching the average domain size L_0. Thus, we see that the growth exponent ϕ is proportional to the temperature T. Indeed, we can compare $1/E_0 = 9.09 \pm 0.90$ with the linear coefficient $\alpha = 8.57 \pm 0.38$ that is extracted from the linear temperature dependence of the growth exponents for $T = 0.01 \sim 0.06$ (see Fig. 1), which shows a reasonable agreement.

At higher temperatures, we no longer can assume that the ordering proceeds via activated dynamics alone, but proliferation of step excitations due to thermal fluctuations will make the domain walls become rough at $T > T_R$. This roughening transition will occur at the temperature for which an isolated step excitation on an infinitely long domain wall will cost no extra free energy. We can estimate this temperature roughly by matching the barrier energy for a step excitation $\Delta E = E_0 \ln(L/L_0)$ as the energy contribution of an isolated step excitation (or roughening excitation) with $T \ln(L/L_0)$ as the entropic contribution to the free energy. At the transition, we should have $E_0 \ln(L/L_0) \simeq T_R \ln(L/L_0)$, i.e., $T_R \simeq E_0 \simeq 0.11$. Taking the crudeness of our estimation into consideration, this gives a reasonable agreement with the value of $T_R \simeq 0.09 \pm 0.01$ obtained from direct calculation of morphological quantities. More rigorous treatment should include the effect of screening of other charges, which will lower the transition temperature that will probably give closer agreement.

In summary, we presented simulation results on the ordering dynamics of the 2D classical CG of half-integer charges on a square lattice. The phase ordering in this system is governed by the activation energy barrier with logarithmic dependence on the domain size, resulting in the temperature dependent growth exponent and a roughening transition of the domain walls at a finite temperature. This kind of low temperature ordering was not considered in the LMV classification. The present study strongly indicates that the CG with $f = 1/2$ and the FFXYM offer a new universality class of phase ordering dynamics.

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