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Phase-ordering dynamics in the continuum q-state clock model

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The order-parameter correlation function of the nonconserved, continuum q-state clock model is evaluated in the asymptotic scaling limit, during the phase-ordering process after a temperature quench. The short-distance behavior of the order-parameter scaling function exhibits explicit crossover from that characteristic of the Ising universality class to that of the O(2) model.

The phase-ordering process of a system quenched from a high-temperature disordered state into the ordered phase exhibit *universal* scaling behavior in the asymptotic late stages.¹ The characteristic scaling length for pure systems grows algebraically in time, $L(t) \sim t^n$, where *n* is called the growth exponent. In addition, the orderparameter correlation function satisfies similarity scaling

$$C(\mathbf{r},t) = \psi_0^2 \mathcal{F}(\mathbf{r}/L(t)) , \qquad (1)$$

where ψ_0 is the ordered magnitude of the order parameter. The set of factors that characterize a universality class, and, in particular, the functional form of \mathcal{F} , is known to include at least the dimensionality of space, whether the order parameter is conserved, and the degeneracy of the ground states.

We shall be concerned here with this last factor for a system with a nonconserved order parameter. The importance of the degeneracy of ground states lies in the fact that the symmetry property of the ground state uniquely determines the types of topological defect structures that control the late stage ordering in unstable systems. Recent studies of systems with continuous symmetries²⁻⁶ (with infinitely degenerate ground states) shows a variation in the behavior of the scattering structure factor $\Phi(k)$, the Fourier transform of $C(\mathbf{r}, t)$, from the usual scalar Ising-type systems. Namely, for large wave numbers, Porod's law, $\Phi(k) \sim k^{-(d+n)}$ for the general O(n) model.

In this paper we investigate the phase-ordering process for the continuum version of the q-state clock model⁷ (also referred to as the planar Potts model or the vector Potts model). This model provides an interesting *intermediate* case between the scalar Ising-type dynamics (where q = 2) and the model A dynamics with a complex order parameter (where $q = \infty$). Unlike the latter two limits, where the topological defects are interfaces and vortices respectively, the defects in the q-state clock model involve both interfaces and vortices reflecting the qfold degeneracy of the ground states.⁸ This model clearly is relevant to understanding the disorder-order transition in some alloys⁹ as well as in the evolution of cellular structures ubiquitous in nature.¹⁰

Many numerical studies have been devoted to the investigation of phase ordering of clock models¹¹ and the standard Potts models.¹² While it is by now well established that $L(t) \sim t^{1/2}$ in both models, there is considerable uncertainty in our understanding of the correlation functions. Numerical work generally shows independence of the correlation functions on the degeneracy q of ground states. On the theoretical front, Kawasaki⁸ extended the Ohta-Jasnow-Kawasaki¹³ method to the clock model but did not determine the explicit form of the correlation function. In this paper, we shall derive explicitly the short-distance behavior of the orderparameter correlation function in the asymptotic scaling regime. The auxiliary field method we adopt here has been proven useful in previous growth kinetics studies.14,15

The dimensionless free energy for the continuum qstate clock model¹⁶ ($q \ge 2$) can be written as

$$F = \int d\mathbf{r} \left[|\nabla \psi|^2 - |\psi|^2 + \frac{1}{2} |\psi|^4 + \frac{v}{q} (\psi^q + \psi^{*q} - 2|\psi|^q) \right], \qquad (2)$$

where $\psi(\mathbf{r},t) = |\psi(\mathbf{r},t)| e^{i\phi(\mathbf{r},t)}$ is the complex order parameter and v > 0 is a constant. By assuming the standard relaxation Langevin dynamics for the evolution of the order parameter we obtain the equation of motion

$$\frac{\partial \psi}{\partial t} = \nabla^2 \psi + \psi (1 - |\psi|^2) - v (\psi^{*q} - |\psi|^q) / \psi^* , \qquad (3)$$

where the noise term has been neglected for a zerotemperature quench. The q degenerate ground states are then given simply by $|\psi|=1$, $\phi_j=(2\pi/q)(j-\frac{1}{2})$ with

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j = 1, 2, ..., q, corresponding to q equivalent directions of a clock.

The phase ordering process of the clock model involves the motion and annihilation of both interfaces and vortices. Interfaces separate distinct ground states, while vortices are places where more than two interfaces meet. At the late stage of the ordering, it is reasonable to assume that only the topologically stable defect configurations with the lowest energy will be dominant. Such a defect configuration is simply a vortex where all q-distinct interfaces meet, so that the phase of the order parameter changes by 2π going around the vortex. The order parameter field around an isolated defect can be described by the inhomogeneous solution of the equation of motion (3). The *far-field* solution for a vortex centered at $\mathbf{r}=\mathbf{0}$ can easily be found to be of the form

$$\psi_{\rm far}(\mathbf{r}) \sim \exp \frac{2\pi i}{q} \left| \frac{\theta(\mathbf{r})}{2\pi/q} \right| , \qquad (4)$$

r

where θ is the polar angle of **r** and we introduce the notation that [a] is the largest integer not exceeding a. To examine the solution near an interface but far away from the vortex core, we extract from (3) the effective equation of motion for the variation of phase degrees of freedom only and obtain

$$\phi''(z) + v \sin[q\phi(z)] = 0 , \qquad (5)$$

where z is the effective coordinate perpendicular to the domain wall. Equation (5) is of the sine-Gordon form and has the soliton-type solution

$$\phi(z) = \frac{4}{q} \tan^{-1} \exp(\sqrt{qv} z) + \frac{2\pi j}{q}$$
(6)

near the *j*th domain wall.

In the context of growth kinetics the key question is the structure of the scaling behavior at long time and large distances. As usual we assume that, in this asymptotic scaling regime, the order parameter structures can be associated with an auxiliary Gaussian field.⁴ In our present case, a complex scalar (or equivalently twovector) auxiliary field $m(\mathbf{r}, t)$ is appropriate. The magnitude |m| has the interpretation of the *distance* to the nearest vortex and the phase of *m* specifies the relative positions of interfaces. The nonlinear transformation relating the order parameter field to this auxiliary field $\psi(\mathbf{r},t)=\psi(m(\mathbf{r},t))$ is chosen as the stationary inhomogeneous solution of (3) near an isolated vortex, however, with *m* the coordinate.

We now proceed to evaluate the correlation function by writing

$$C(\mathbf{r},t) = \langle \psi(m_1)\psi^*(m_2) \rangle$$

= $\langle \psi_{\text{far}}(m_1)\psi^*_{\text{far}}(m_2) \rangle + O(L^{-1}(t))$ (7)

where $m_1 \equiv m(\mathbf{r}, t)$, $m_2 \equiv m(0, t)$. The average is now over probability distributions of the auxiliary field m. It is essential to note that by extracting out the far-field term in (7) we have absorbed any nonuniversal, potential-dependent contributions into a term of order $O(L^{-1})$.⁴ Hence, in the scaling limit $L(t) \rightarrow \infty$ the asymptotic correlation function is independent of the detailed structure of the potential. Anticipating scaling in this case we write

$$\mathcal{F}_{q} = \langle \psi_{\text{far}}(m_{1})\psi_{\text{far}}^{*}(m_{2}) \rangle .$$
(8)

It is easy to show from (4) that

$$g(\theta_1,\theta_2) \equiv \psi_{\text{far}}(m_1)\psi_{\text{far}}^*(m_2) = e^{2\pi i (k-l)/q}$$
(9)

for $\theta_1 \in [2\pi(k-1)/q, 2\pi k/q]$, $\theta_2 \in [2\pi(l-1)/q, 2\pi l/q]$ and $k, l=1,2,\ldots,q$. Here θ_1, θ_2 are the polar angles of m_1 and m_2 , respectively. Now the average over the auxiliary field is of the form

$$\mathcal{F}_q = \int d^2 m_1 d^2 m_2 g\left(\theta_1, \theta_2\right) \Phi(m_1, m_2) \tag{10}$$

with the probability density function

$$\Phi(m_1, m_2) = \left[\frac{\gamma}{2\pi \langle m^2 \rangle}\right]^2 \\ \times \exp\left[\frac{-\gamma^2(m_1^2 + m_2^2 - 2fm_1m_2^*)}{2\langle m^2 \rangle}\right], \quad (11)$$

where $\gamma = (1 - f^2)^{-1/2}$ and $f(\mathbf{r}, t) = \langle m(\mathbf{r}, t)m^*(0, t) \rangle / \langle m^2 \rangle$. By suitably rescaling the arguments, (10) can be cast into the form

$$\mathcal{F}_{q}(f) = \int \frac{d^{2}x_{1}d^{2}x_{2}}{4\pi^{2}\gamma^{2}} g(\theta_{1},\theta_{2}) \exp[-x_{1}^{2}/2 - x_{2}^{2}/2 + x_{1}x_{2}f\cos(\theta_{1} - \theta_{2})] .$$
(12)

Note that the dependence of \mathcal{F} on \mathbf{r}, t is implicitly contained in the correlator $f(\mathbf{r}, t)$. In principle,¹⁴ this function should be determined self-consistently from the equation of motion. Here we shall only need the property that f scales and has the short-distance expansion: $f = f(\mathbf{r}/L(t)) = 1 - \text{const} \times (r/L)^2 + \cdots$.

The radial part of (12) can be easily evaluated first to give

$$\mathcal{F}_{q} = \int_{0}^{2\pi} \int_{0}^{2\pi} \frac{d\theta_{1}d\theta_{2}}{4\pi^{2}\gamma^{2}} g\left(\theta_{1},\theta_{2}\right) Q\left(f\cos(\theta_{1}-\theta_{2})\right) , \qquad (13)$$

where

$$Q(\alpha) = \frac{1}{1 - \alpha^2} + \frac{\alpha}{(1 - \alpha^2)^{3/2}} \left[\frac{\pi}{2} + \arcsin\alpha \right].$$
 (14)

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It is advantageous to exhaust the symmetry properties of g and further restrict the limits of integration to obtain more explicitly that

$$\mathcal{F}_{q} = \int_{0}^{2\pi/q} \int_{0}^{2\pi/q} \frac{d\theta_{1} d\theta_{2}}{4\pi^{2} \gamma^{2}} \left[q \mathcal{Q}(f \cos(\theta_{1} - \theta_{2})) + 2 \sum_{j=1}^{q-1} (q-j) \cos\left[\frac{2\pi j}{q}\right] \mathcal{Q}(f \cos(\theta_{1} - \theta_{2} - 2\pi j/q)) \right].$$
(15)

Finally we complete the θ integrations in (15) and obtain the main result of our paper

$$\mathcal{F}_{q}[f] = \frac{q}{2\pi^{2}} \sin^{2} \left[\frac{\pi}{q} \right] \sum_{j=0}^{q-1} \cos \left[\frac{2\pi j}{q} \right] (\pi \lambda_{j} + \lambda_{j}^{2}) , \quad (16)$$

where $\lambda_j = \arcsin[f \cos(2\pi j/q)]$.

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Equation (16) shows explicit dependence of the scaling function upon the degree of degeneracy of the ground states q. Several limits can be scrutinized at once. In the Ising case of q=2 one recovers the well-known result¹³⁻¹⁵ for the scaling function

$$\mathcal{F}_2 = (2/\pi) \arcsin f \quad . \tag{17}$$

The case q = 3 is interesting because the three-state clock model is identical to the standard three-state Potts model. In this case (16) gives

$$\mathcal{F}_{3} = \frac{9}{8\pi^{2}} \left[\pi \arcsin f + \pi \arcsin \frac{f}{2} + (\arcsin f)^{2} - \left[\arcsin \frac{f}{2} \right]^{2} \right].$$
(18)

The scaling function for q = 4 gives the interesting result $\mathcal{F}_4 = (2/\pi) \operatorname{arcsin} f$, which is identical to \mathcal{F}_2 . This result, surprising at first sight, is, upon reflection, not unexpected, since it is known that the four-state clock model is isomorphic to a pair of noninteracting Ising models.¹⁷ Note that this behavior occurs because of the accidental symmetry property of the model; therefore we do not expect this to recur for larger q. While we could similarly

regard the eight-state clock model as isomorphic to four Ising models, these Ising models are now coupled, and there is no simple relation to the uncoupled Ising-type dynamics. It can be shown that (16) can be further simplified if even and odd q are treated separately. We shall, however, not dwell on this any further. Let us finally examine the limit $q \rightarrow \infty$ when we expect the ∞ state clock model to approach the planar rotator or O(2) model. To see this explicitly, we may simply replace the sum in (16) by an integral as $q \rightarrow \infty$. Straightforward algebra leads to

$$\mathcal{F}_{\infty} = f \int_{0}^{1} \left[\frac{1 - z^2}{1 - f^2 z^2} \right]^{1/2} dz = \frac{\pi f}{4} F(\frac{1}{2}, \frac{1}{2}; 2; f^2) , \qquad (19)$$

where F is the hypergeometric function. Equation (19) is of the same form as is obtained for the O(2) model.^{3,4}

We next proceed to analyze the short-distance behavior of the scaling function, since it gives rise to the anomalous power-law decay of the scattering form factor $\Phi(k)$ at large wave numbers. The limit of short distances, i.e., $x = r/L(t) \rightarrow 0$, is associated with the limit $f \rightarrow 1$. Keeping the leading terms for f near 1, (16) can be rewritten in the form

$$\mathcal{F}_q(f) = 1 - a(q)(1 - f^2)^{1/2} - b(q)(1 - f) + \cdots$$
, (20)

where

$$a(q) = \frac{q}{\pi} \sin^2 \left(\frac{\pi}{q}\right)$$
(21)

and

$$(q) = \frac{q}{\pi} \sin^2 \left[\frac{\pi}{q} \right] \sum_{j=1}^{q-1} \frac{1 - 2j/q}{\sin(2\pi j/q)} + \frac{1}{\pi} \sin \left[\frac{\pi}{q} \right] \left[(q-1)\sin\frac{\pi}{q} + \cos\frac{\pi}{q} \right].$$
(22)

Recalling that $1-f \sim x^2$ at small x, the second term on the right-hand side of (20) gives a linear dependence on x, for any finite value of q. This can be understood as the consequence of the presence of interfaces in the system. Alternatively speaking, this term is responsible for the power-law decay $\Phi(k) \sim k^{-(d+1)}$ at large k. Thus Porod's law remains valid for all q-state clock models. However, the Porod's tail gets weaker as the degeneracy q increases. Evidently, as the limit $q \to \infty$ is approached, we have $a(q) \sim q^{-1} \to 0$. More importantly, notice that the expansion (20) is no longer valid in the limit $q \to \infty$, due to the noninterchangeable order of the two limits $\lim_{f \to 1} \operatorname{and} \lim_{q \to \infty}$. And the coefficient b(q) diverges,

$$b(q) \sim 2\pi \ln q + O(1)$$
 (23)

The logarithmic divergence hints some novel behavior. In fact, in the limit $q \rightarrow \infty$, we have using (19) instead of (22), the result

$$\mathcal{F}_{\infty} = 1 + \frac{1}{4} (1 - f^2) \ln(1 - f^2) + \cdots,$$
 (24)

which gives a $x^{2}\ln x$ singularity at small x. In Fourier space, this corresponds to $\Phi(k) \sim k^{-(d+2)}$, the recently discovered result for the O(2) model.^{2-6,18}

The methodology we adopted here for the clock model could, in principle, be applied to the Potts model as well. And it is conceivable that our general conclusion about the q dependence of the scaling function is correct in the latter case too. This raises the need for more accurate

numerical simulations or experiments to further establish this dependence. Finally, the dynamics for the conserved clock model is certainly worthy of investigation. Knowing that $L(t) \sim t^{1/3}$ for q=2, while $L(t) \sim t^{1/4}$ for $q = \infty^2$, there must be crossover behavior as q is varied.

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(1988).

- ¹¹K. Kaski and J. D. Gunton, Phys. Rev. B 28, 5371 (1983).
- ¹²See M. P. Anderson, G. S. Grest, and D. J. Srolovitz, Philos. Mag. B 59, 293 (1989); S. Kumar, J. D. Gunton, and K. K. Kaski, Phys. Rev. B 35, 8517 (1987), and references therein.
- ¹³T. Ohta, D. Jasnow, and K. Kawasaki, Phys. Rev. Lett. 49, 1223 (1982).
- ¹⁴G. F. Mazenko, Phys. Rev. Lett. 63, 1605 (1989); Phys. Rev. B 42, 4487 (1990).
- ¹⁵Fong Liu and G. F. Mazenko, Phys. Rev. B 44, 9185 (1991); 45, 4656 (1992).
- ¹⁶Y. Enomoto, T. Aokage, and K. Isibasi, J. Phys. Condens. Matter 4, L133 (1992).
- ¹⁷D. D. Betts, Can. J. Phys. 42, 1564 (1964); M. Suzuki, Prog. Theor. Phys. 37, 770 (1967).
- ¹⁸A. P. Y. Wong, P. Wiltzius, and B. Yurke, Phys. Rev. Lett. 68, 3583 (1992).

- ¹For reveiws see, J. D. Gunton, M. San Miguel, and P. S. Sahni, in Phase Transitions and Critical Phenomena, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8; H. Furukawa, Adv. Phys. 34, 703 (1985); K. Binder, Rep. Prog. Phys. 50, 783 (1987).
- ²M. Mondello and N. Goldenfeld, Phys. Rev. A 42, 5865 (1990); 45, 657 (1992).
- ³A. J. Bray and S. Puri, Phys. Rev. Lett. 67, 2670 (1991).
- ⁴Fong Liu and G. F. Mazenko, Phys. Rev. B 45, 6989 (1992); 46, 5963 (1992).
- ⁵H. Tovoki, Phys. Rev. B 45, 1965 (1992).
- ⁶A. J. Bray and K. Humayun, J. Phys. A 25, 2191 (1992).
- ⁷R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).
- ⁸K. Kawasaki, Phys. Rev. A **31**, 3880 (1985).
- ⁹S. E. Nagler et al., Phys. Rev. Lett. 61, 718 (1988); S. Katano et al., Phys. Rev. B 38, 2659 (1988).
- ¹⁰For a recent review, see H. V. Atkinson, Acta. Metall. 36, 469