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Phase ordering dynamics of a vector order parameter

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Abstract. Mazenko's theory of phase ordering dynamics is generalized to an n -component non-conserved vector order parameter. The scaling functions for the equal-time and two-time correlation functions are calculated, as well as the exponent characterizing the decay of autocorrelations. The equal-time correlation function is numerically quite close to that recently calculated by Bray and Puri, and by Toyoki, and exhibits the same power-law tail in its Fourier transform, the time-dependent structure factor.

1. Introduction

The calculation of two-point correlation functions, for systems undergoing phase ordering following a quench into the ordered phase from high temperatures, is a long-standing challenge [1]. For a non-conserved scalar order parameter field $\phi(\mathbf{r}, t)$ it is well established that, in the late stages of growth, the equal-time correlation function is described by the scaling form

$$C(\mathbf{r}, t) \equiv [\phi(\mathbf{x}, t)\phi(\mathbf{x} + \mathbf{r}, t)] = f(r/L(t)) \quad (1)$$

where the domain scale $L(t) \sim t^{1/2}$. Square brackets in (1) indicate an average over the ensemble of possible initial conditions. Although the origin of the $t^{1/2}$ growth has been understood for a long time [2], being due to the motion of domain walls driven by their curvature, the scaling function $f(x)$ has eluded exact calculation from first principles. Exact results are available in a few special cases, namely the one-dimensional Glauber model [3], the one-dimensional $O(n)$ -model with $n = 2$ [4], and the $O(n)$ model for $n = \infty$ for any d [5, 6], but not for the most physically interesting cases of small finite n and $d = 2$ and 3.

A promising recent approach is due to Mazenko [7], building on the earlier work of Ohta, Jasnow and Kawasaki (OJK) [8]. The key idea in both theories is to introduce a nonlinear mapping between the order parameter field $\phi(\mathbf{r}, t)$, which has 'sharp' (on the scale of $L(t)$) discontinuities at domain walls, and an auxiliary field $m(\mathbf{r}, t)$ that varies smoothly near walls. In the OJK theory $m(\mathbf{r}, t)$ obeys a simple diffusion equation and is normally distributed. In the Mazenko approach, only the assumption that $m(\mathbf{r}, t)$ is normally distributed is required. The Mazenko approach has the virtues that (i) the scaling function $f(x)$ depends, unlike that of OJK, explicitly on spatial dimension d ; (ii) the known exact result for $d = 1$ is recovered [9] in the limit $d \rightarrow 1$; and (iii) the exponent describing the decay of autocorrelations [6, 10] emerges naturally, and a non-trivial value for this exponent is obtained [11].

There has been much recent interest in phase ordering in systems with more complicated symmetries such as n -component vector models [4–6, 12] and the nematic phase of liquid crystals [13]. In this paper we extend Mazenko's approach to a general n -component non-conserved vector order parameter with $O(n)$ symmetry. A key ingredient of the calculation is the analogue for general n of the OJK scaling function. This function has been derived very recently by Bray and Puri [14] (Note that the scaling variable is taken to be $r/2\sqrt{t}$ in this paper, rather than r/\sqrt{t} as in [14].), and independently by Tbyoki [15]. It has the interesting feature that the Fourier transform $g(k)$ of the scaling function $f(x)$ has the power-law tail $g(k) \sim k^{-(d+n)}$, a simple generalization of the familiar 'Porod's law' [16] for $n = 1$. We shall find that this feature is preserved by the Mazenko scaling function.

The outline of the paper is as follows. In the following section we review Mazenko's theory for a non-conserved scalar order parameter ($n = 1$). This serves as a useful background to the case of general n discussed in section 3. There are many simplifications for $n = 1$, the most important being that the 'smooth' field m can ultimately be eliminated to derive an equation for the scaling function $f(x)$ itself. For general n this is not possible, and the mathematics is consequently more involved, although the treatment is as conceptually simple as before. Section 4 contains a discussion of the correlation function between the fields at different times. The results are presented in section 5, while section 6 considers the relation of the present theory to earlier approaches. Section 7 concludes with a discussion and summary.

2. The Mazenko theory for $n = 1$

We start from the time-dependent Ginzburg–Landau equation in the form

$$\partial\phi/\partial t = \nabla^2\phi - V'(\phi) \quad (2)$$

where $V'(\phi) \equiv dV/d\phi$ and the potential function $V(\phi)$ has the usual 'double well' shape, with stable minima at $\phi = \pm 1$ and a local maximum at $\phi = 0$. It may help to keep in mind the familiar quartic potential, $V(\phi) = -\phi^2/2 + \phi^4/4$, but the precise form of $V(\phi)$ is not important in what follows.

It is useful to consider the general two-time correlation function

$$C(12) = [\phi(1)\phi(2)] \quad (3)$$

where we have introduced the compact notation in which '1' stands for the spacetime point (\mathbf{x}_1, t_1) , etc. Multiplying (2), evaluated at the point '1', by $\phi(2)$ and averaging over initial conditions, gives

$$\partial C(12)/\partial t_1 = \nabla_1^2 C(12) - [\phi(2)V'(\phi(1))] \quad (4)$$

where ∇_1^2 indicates the Laplacian with respect to coordinate \mathbf{x}_1 . Since, by translational invariance, $C(12)$ depends on \mathbf{x}_1 only through the relative coordinate $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$, we can drop the subscript on ∇^2 in (4) and regard it as the Laplacian with respect to \mathbf{r} .

The key step in simplifying (4) is to introduce the nonlinear transformation

$$\phi(\mathbf{r}, t) = \sigma(m(\mathbf{r}, t)) \quad (5)$$

where the function $\sigma(m)$ is a 'sigmoid' function, i.e. $\sigma(m)$ increases monotonically from -1 at $m = -\infty$ to $+1$ at $m = +\infty$. A very convenient choice for this function is defined by the equation

$$\frac{1}{2} \frac{d^2 \sigma}{dm^2} = V'(\sigma). \quad (6)$$

The factor $\frac{1}{2}$ in (6) is conventional. Comparison with (2) shows that, with the choice (6), $\sigma(m)$ gives essentially the equilibrium order parameter profile across a domain wall, with m interpreted as a coordinate normal to the wall. In particular, the positions of the walls are obtained from the zeros of the field $m(r, t)$. As a concrete example, $V(\phi) = -\phi^2/2 + \phi^4/4$ gives $\sigma(m) = \tanh(m)$. Using (6) in (4) gives

$$\frac{\partial C(12)}{\partial t_1} = \nabla^2 C(12) - \frac{1}{2} \left[\frac{d^2 \sigma(m(1))}{dm(1)^2} \sigma(m(2)) \right]. \quad (7)$$

So far there are no approximations. Mazenko now makes the key assumption [7] that the field $m(x, t)$ has a Gaussian distribution (with zero mean) at all times. Then the final term in (7) can be expressed in terms of $C(12)$ itself, as follows. For a Gaussian distribution (with zero mean), the joint probability distribution $\Phi(m(1), m(2))$ can be expressed in terms of the second moments, i.e. in terms of

$$S_0(1) = [m(1)^2] \quad S_0(2) = [m(2)^2] \quad C_0(12) = [m(1)m(2)]. \quad (8)$$

In fact

$$\begin{aligned} \Phi(x_1, x_2) &= [\delta(x_1 - m(1)) \delta(x_2 - m(2))] \\ &= N \exp \left\{ -\frac{1}{2(1-\gamma^2)} \left(\frac{x_1^2}{S_0(1)} + \frac{x_2^2}{S_0(2)} - \frac{2\gamma x_1 x_2}{\sqrt{S_0(1)S_0(2)}} \right) \right\} \end{aligned} \quad (9)$$

where

$$N = \frac{1}{2\pi \sqrt{(1-\gamma^2)S_0(1)S_0(2)}} \quad \gamma \equiv \gamma(12) = \frac{C_0(12)}{\sqrt{S_0(1)S_0(2)}}. \quad (10)$$

To exploit this distribution we write $C(12)$ in terms of the Fourier components of $\sigma(m)$:

$$\begin{aligned} C(12) &= [\sigma(m(1))\sigma(m(2))] \\ &= \sum_{k_1, k_2} \sigma_{k_1} \sigma_{k_2} [\exp\{ik_1 m(1) + ik_2 m(2)\}] \\ &= \sum_{k_1, k_2} \sigma_{k_1} \sigma_{k_2} \exp\{-\frac{1}{2}(S_0(1)k_1^2 + 2C_0(12)k_1 k_2 + S_0(2)k_2^2)\} \end{aligned} \quad (11)$$

where the final line follows from (8) and (9). Similarly, it follows immediately that

$$\begin{aligned} \left[\frac{d^2 \sigma(m(1))}{dm(1)^2} \sigma(m(2)) \right] &= \sum_{k_1, k_2} \sigma_{k_1} \sigma_{k_2} (ik_1)^2 [\exp\{ik_1 m(1) + ik_2 m(2)\}] \\ &= 2 \frac{\partial C(12)}{\partial S_0(1)}. \end{aligned} \quad (12)$$

With this useful result (7) can be simplified to

$$\frac{\partial C(12)}{\partial t_1} = \nabla^2 C(12) - \frac{\partial C(12)}{\partial S_0(1)}. \quad (13)$$

Finally we need an expression for $C(12)$ in terms of $S_0(1)$, $S_0(2)$ and $C_0(12)$. The essential simplification here is that, in the late stages of growth, where the domain scale $L(t)$ is much larger than the intrinsic thickness of the domain walls, the walls may be treated as sharp, i.e. for the evaluation of $C(12)$ equation (5) may be replaced by

$$\sigma(\mathbf{r}, t) = \text{sgn}(m(\mathbf{r}, t)) \quad (14)$$

in the scaling regime, to give

$$\begin{aligned} C(12) &= [\text{sgn}(m(1)) \text{sgn}(m(2))] \\ &= \frac{2}{\pi} \sin^{-1}(\gamma) \end{aligned} \quad (15)$$

the last line following from the Gaussian average over $m(1)$ and $m(2)$ with the weight given by (9).

The derivative in (13) can now be evaluated:

$$\begin{aligned} \frac{\partial C(12)}{\partial S_0(1)} &= \frac{dC(12)}{d\gamma} \frac{\partial \gamma}{\partial S_0(1)} = -\frac{2}{\pi} \frac{1}{\sqrt{1-\gamma^2}} \frac{\gamma}{2S_0(1)} \\ &= -\frac{1}{\pi S_0(1)} \tan\left(\frac{\pi}{2} C(12)\right). \end{aligned} \quad (16)$$

Putting this in (13) gives Mazenko's nonlinear differential equation for $C(12)$:

$$\frac{\partial C(12)}{\partial t_1} = \nabla^2 C(12) + \frac{1}{\pi S_0(1)} \tan\left(\frac{\pi}{2} C(12)\right). \quad (17)$$

This equation describes the space and time dependence of the two-time correlation function $C(12) = [\phi(\mathbf{x}_1, t_1)\phi(\mathbf{x}_2, t_2)]$. As a consequence of the translational invariance of the ensemble of initial conditions, we have observed that $C(12)$ depends on $\mathbf{x}_1, \mathbf{x}_2$ only through $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$. However, it does depend separately on t_1 and t_2 . It is possible to solve (17) for the full dependence on t_1 and t_2 , but as a first step one needs to consider the equal-time correlation function, with $t_1 = t_2 = t$. This is the function whose Fourier transform, the equal-time structure factor, is directly measurable via small-angle scattering experiments. We will return to the case of general t_1, t_2 in the following section where the theory is extended to arbitrary n .

For $t_1 = t_2 = t$, the differential operator $\partial/\partial t$ hits both fields in $C(12)$, so instead of (17) the equation for the equal-time correlation function is

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = \nabla^2 C(12) + \frac{1}{\pi S_0(1)} \tan\left(\frac{\pi}{2} C(12)\right). \quad (18)$$

In the late stages of growth, one expects a scaling solution of the form (1). Looking at the dimensions of the three terms in (18), one sees that this implies $L(t) \sim t^{1/2}$,

and that for consistency one must have $S_0(1) \sim t$. The latter is consistent with the definition $S_0(1) = [m(1)^2]$, the interpretation of m as a length, and the scaling of lengths as $t^{1/2}$. Therefore we write

$$S_0(1) = t/\lambda = L(t)^2/\lambda \quad (19)$$

$$C(12) = f\left(\frac{r}{\sqrt{t}}\right) \quad (20)$$

where the dependence on $r = |\mathbf{r}|$ follows from isotropy. Then one obtains the following differential equation for the scaling function $f(x)$:

$$0 = f'' + \left(\frac{d-1}{x} + \frac{x}{4}\right) f' + \frac{\lambda}{\pi} \tan\left(\frac{\pi}{2} f\right) \quad (21)$$

where primes indicate derivatives with respect to x . Note that our notation in (19) differs from that of Mazenko.

To solve (21) for the scaling function $f(x)$ we need to supply initial conditions and also to determine the value of λ . We first discuss the initial conditions. Clearly $f(0) = 1$ follows immediately from (1) when we remember that $\phi = \pm 1$ are the equilibrium values of the order parameter. For $x \rightarrow 0$, the divergence of the final term in (21) (as $f \rightarrow 1$) must be cancelled by a corresponding divergence of the term $(d-1)f'/x$. This implies that $1 - f(x) \sim x$, for $x \rightarrow 0$. Substituting this into (21) gives

$$f(x) = 1 - \frac{1}{\pi} \sqrt{\frac{2\lambda}{d-1}} x + \dots \quad x \rightarrow 0. \quad (22)$$

The required initial conditions are thus $f(0) = 1$, $f'(0) = -(1/\pi)\{2\lambda/(d-1)\}^{1/2}$. For any given λ , (21) can now be integrated forward (numerically) to obtain the solution for all x . So what determines λ ?

As discussed by Mazenko [7], λ is fixed by requiring the correct behaviour at large x . For $x \gg 1$, $f(x)$ will be small and $\tan(\pi f/2)$ in (21) can be replaced by its argument, giving a linear equation for f valid at large x . This equation has two linearly independent solutions, f_1 and f_2 , whose large x behaviour is easily determined:

$$f_1(x) \sim x^{-(d-2\lambda)} \exp(-x^2/8) \quad (23)$$

$$f_2(x) \sim x^{-2\lambda}. \quad (24)$$

For general λ , the solution obtained by integrating (21) forward from (22) will be, for large x , a linear combination of f_1 and f_2 , i.e. $f(x) = A(\lambda)f_1(x) + B(\lambda)f_2(x)$ for $x \rightarrow \infty$. However, for a typical initial field configuration (with only short-range spatial correlations), as would be obtained by quenching from the high temperature phase, only f_1 is physically sensible. This determines λ from the condition $B(\lambda) = 0$, i.e. the coefficient of the unphysical power-law term f_2 should vanish. We have noted elsewhere [17], however, that the solution $f_2(x)$ can have physical meaning, if the system is quenched from an initial state where *long-range correlations are already present*, e.g. the equilibrium state at the critical point. In this case a family of solutions

exists, with continuously varying λ (such that $B(\lambda) > 0$), the value of λ being related to the exponent of the power-law decay of spatial correlations in the initial state. This phenomenon has been discussed quite generally using renormalization group arguments [18].

We have discussed the Mazenko theory for a scalar order parameter in some detail, as the extension to general n requires little extra work and involves no new points of principle. However, the results are mathematically neater for $n = 1$: no simple equation like (21) can be derived for $n > 1$.

3. Phase ordering for general n

The general approach is the same as for $n = 1$, the main difference being that the important topological structures are no longer domain walls but vortices (or vortex lines) for $n = 2$ and monopoles (or 'hedgehogs') for $n = 3$. The field $m(\mathbf{r}, t)$ will become, for general n , a vector field $\vec{m}(\mathbf{r}, t)$ which, in the vicinity of a topological singularity in the field $\vec{\phi}$, plays the role of a position vector from the singularity to the point \mathbf{r} .

For a vector field with $O(n)$ symmetry, the analogues of equations (2)–(4) are

$$\partial \vec{\phi} / \partial t = \nabla^2 \vec{\phi} - \partial V / \partial \vec{\phi} \quad (25)$$

$$C(12) = [\vec{\phi}(1) \cdot \vec{\phi}(2)] \quad (26)$$

$$\partial C(12) / \partial t_1 = \nabla_1^2 C(12) - [\vec{\phi}(2) \cdot \partial V / \partial \vec{\phi}(1)]. \quad (27)$$

By analogy with (5) we introduce the nonlinear transformation

$$\vec{\phi}(\mathbf{r}, t) = \vec{\sigma}(\vec{m}(\mathbf{r}, t)) \quad (28)$$

where $\vec{m}(\mathbf{r}, t)$ is a vector field with the same internal dimension as $\vec{\phi}$, i.e. n . We define the function $\vec{\sigma}(\vec{m})$ by analogy with (6):

$$\frac{1}{2} \nabla_m^2 \vec{\sigma} = \frac{\partial V}{\partial \vec{\sigma}} \quad (29)$$

where ∇_m^2 is the Laplacian operator with respect to the vector \vec{m} . Comparison with (25) shows that $\vec{\sigma}(\vec{m})$ represents the equilibrium field due to a single vortex (vortex line, hedgehog, etc) with \vec{m} interpreted as (apart from a factor of $1/\sqrt{2}$) a position vector from the vortex core. Clearly there is a family of such solutions, related by rotations, just as the relevant solution of (6), representing a domain wall, is determined only up to an overall sign. For the scalar case we chose the solution for which σ and m have the same sign. For the vector case we will choose the solution where $\vec{\sigma}$ and \vec{m} are everywhere parallel (such a solution clearly exists, by symmetry).

At this juncture we should note that the physical picture of \vec{m} as a position vector in the real d -dimensional space of necessity requires $n \leq d$. We will return to this point later, but for the moment will continue to regard n as arbitrary.

Following the treatment of $n = 1$, we take \vec{m} to have a Gaussian distribution with zero mean. This means, in particular, that each Cartesian component of $\vec{m}(\mathbf{r}, t)$ is independently distributed. Thus the joint probability distribution of $\vec{m}(1)$ and

$\vec{m}(2)$ is simply a product of the separate distributions for each component. The joint distribution for a single component is described by equations (8)–(10), where $m(1)$, $m(2)$ are the (same) specified component of $\vec{m}(1)$, $\vec{m}(2)$.

Using the distribution (9), obvious generalizations of (7), (11) and (12) lead once more to (13). As before, the final step is to express $C(12)$ in terms of $S_0(1)$, $S_0(2)$ and $C_0(12)$ so that the derivative in the final term of (13) can be taken, i.e. we need an analogue of (14) for vector fields. Just as, in the scalar case, the magnitude of the field is saturated ($\phi^2 = 1$) at late times except near a domain wall, so in the vector case the field will be saturated ($\vec{\phi}^2 = 1$) except near topological singularities such as vortex lines. The effect on $C(12)$ of the depletion of $\vec{\phi}^2$ near, e.g. a vortex core, will be negligible at late times (the change in the *direction* of $\vec{\phi}$ due to a vortex is, however, important), since the ‘core size’ is independent of time and therefore negligible compared to $L(t)$ at late times. By analogy with (14) we therefore write

$$\vec{\sigma}(\mathbf{r}, t) = \vec{m}(\mathbf{r}, t) / |\vec{m}(\mathbf{r}, t)| \quad (30)$$

instead of (28), recognizing that $\vec{\sigma}$ is a unit vector nearly everywhere at late times. In the scaling regime, therefore, one obtains,

$$C(12) = \left[\frac{\vec{m}(1)}{|\vec{m}(1)|}, \frac{\vec{m}(2)}{|\vec{m}(2)|} \right]. \quad (31)$$

It remains to evaluate the average, using a product of n distributions of the form (9), one for each component of the field. This calculation was done in [14]. The result is

$$C(12) = \frac{n\gamma}{2\pi} \left[B\left(\frac{n+1}{2}, \frac{1}{2}\right) \right]^2 F\left(\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; \gamma^2\right) \quad (32)$$

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function, $F(a, b; c; z)$ is the hypergeometric function, and γ is given by (10). One can verify that (15) is recovered for $n = 1$.

Following (16) precisely, we can evaluate the derivative appearing in the final term of (13) as

$$\frac{\partial C(12)}{\partial S_0(1)} = -\frac{\gamma}{2S_0(1)} \frac{\partial C(12)}{\partial \gamma}. \quad (33)$$

Substituting this into (13) gives a generalized version of (17),

$$\frac{\partial C(12)}{\partial t_1} = \nabla^2 C(12) + \frac{\gamma}{2S_0(1)} \frac{\partial C(12)}{\partial \gamma} \quad (34)$$

and, for $t_1 = t_2 = t$, a generalized version of (18),

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = \nabla^2 C(12) + \frac{\gamma}{2S_0(1)} \frac{\partial C(12)}{\partial \gamma} \quad (35)$$

For the special case $n = 1$, for which (32) reduces to (15), it is easy to eliminate γ in favour of $C(12)$, and one can verify that (17) and (18) are recovered. For general n , however, it is not possible to eliminate γ . We are therefore forced to

work with γ as our independent variable, rather than C . Defining a parameter λ through (19), and imposing the scaling form (20) once more, yields the following differential equation for equal times:

$$0 = \gamma'' + \frac{C_{\gamma\gamma}}{C_\gamma}(\gamma')^2 + \left(\frac{d-1}{x} + \frac{x}{4}\right)\gamma' + \frac{\lambda}{2}\gamma. \quad (36)$$

Here primes indicate derivatives with respect to the scaling variable $x = r/\sqrt{t}$, C_γ means $dC/d\gamma$ etc, and $C(\gamma)$ is the function given by (32).

This procedure is a little complicated, so we will pause to summarize the main points. Equation (36) is our main result for general n , equivalent to (21) for $n = 1$. Equation (36) is an equation for the function $\gamma(x)$, where x is the scaling variable r/\sqrt{t} . The equal-time correlation scaling function $f(x)$, the quantity of physical interest, is obtained by substituting the solution $\gamma(x)$ of (36) into the right-hand side of (32). This procedure is straightforward to implement numerically. First, however, we must discuss once more the initial conditions and the value of λ .

The initial condition $\gamma(0) = 1$ follows immediately from the definition (10) of γ and the definitions (8). Similarly, one can show from (35) and (36) that $\gamma'(0) = 0$ for any n . We shall discuss the precise small- x form of $\gamma(x)$, and the corresponding form of $f(x)$, in more detail in section 6, when we show that $f(x)$ has a leading singularity of order $(x^2)^{n/2}$ (plus a $\ln x$ factor for even n), implying a power-law tail, $g(k) \sim k^{-(d+n)}$, in the structure factor (the Fourier transform of $f(x)$), in accordance with the predictions of Bray and Puri [14] and Toyoki [15]. For the moment, we simply note that, for any n , $\gamma(0) = 1$, $\gamma'(0) = 0$ are the appropriate initial conditions for (36).

The value of λ is determined exactly as for $n = 1$, by demanding that the solution obtained by integrating forward from the initial conditions match on to the correct physical solution at large x . For $x \rightarrow \infty$ we have $\gamma \rightarrow 0$, and (36) can be linearized in γ , by dropping the second term. This linear equation then has exactly the same form as the linearized version of (21) (in fact from (32) it is clear that $C(12)$, i.e. $f(x)$, and $\gamma(x)$ differ only by an overall factor for $\gamma \rightarrow 0$), so the large- x solutions have the form (23) and (24) for any n (although λ will depend on n). So we determine λ once more by demanding that the amplitude of the power-law solution $f_2(x)$ vanish.

Before presenting the numerical results for the equal-time scaling function we complete, in the following section, the presentation of analytical results by considering general two-time correlations. In particular, we will see that the parameter λ determines [11] the exponent that characterizes non-equilibrium autocorrelations in the phase ordering process [6, 10].

4. Two-time correlation functions

Our treatment here follows that presented by Liu and Mazenko [11] for $n = 1$. The correlation $C(12)$ between fields at general spacetime points (\mathbf{x}_1, t_1) , (\mathbf{x}_2, t_2) satisfies (34). For simplicity, we will specialize to the case $t_1 \gg t_2$, although the general case can also be handled using the methods of [11]. For $t_1 \gg t_2$, the correlation $C(12)$ will be small and the final, nonlinear, term in (34) can be linearized. Since, for $\gamma \rightarrow 0$, $C(12) \rightarrow \text{constant } \gamma$, we have $\gamma(\partial C/\partial \gamma) = C$ to linear order.

For general t_1, t_2 we also need $S_0(1) = t_1/\lambda$ instead of (19). Then (34) becomes

$$\frac{\partial C(12)}{\partial t_1} = \nabla^2 C(12) + \frac{\lambda}{2t_1} C(12). \quad (37)$$

To solve this equation we Fourier transform in space, and then integrate forward from an initial condition at $t_1 = \alpha t_2$, with $\alpha \gg 1$, so that the linear equation (37) is valid for all $t_1 \geq \alpha t_2$. Calling $S_k(t_1, t_2)$ the Fourier transform of $C(12)$, we obtain

$$S_k(t_1, t_2) = \left(\frac{t_1}{\alpha t_2}\right)^{\lambda/2} \exp\{-k^2(t_1 - \alpha t_2)\} S_k(\alpha t_2, t_2). \quad (38)$$

Imposing the scaling form $S_k(\alpha t_2, t_2) = (8\pi t_2)^{d/2} g_\alpha(k^2 t_2)$, with $g_\alpha(0) = \text{constant}$, and Fourier transforming back to real space gives, for $t_1 \gg \alpha t_2$,

$$C(12) = \frac{g_\alpha(0)}{\alpha^{\lambda/2}} \left(\frac{t_2}{t_1}\right)^{(d-\lambda)/2} \exp\left(-\frac{r^2}{4t_1}\right). \quad (39)$$

By construction, $g_\alpha(0)/\alpha^{\lambda/2}$ must be independent of α for large α , so our final result for the two-time correlation function is

$$C(12) = \text{constant} \left(\frac{t_2}{t_1}\right)^{(d-\lambda)/2} \exp\left(-\frac{r^2}{4t_1}\right) \quad t_1 \gg t_2. \quad (40)$$

To determine the constant prefactor would require integrating the full nonlinear equation (34), which can be done numerically.

The pre-exponential factor in (40) has the form $\{L(t_2)/L(t_1)\}^{\bar{\lambda}}$, with

$$\bar{\lambda} = d - \lambda. \quad (41)$$

In particular, putting $r = 0$ in (40) shows that $\bar{\lambda}$ describes the decay of autocorrelations as a function of t_1 at fixed t_2 . This exponent has been measured in simulations of vector spin systems [4, 19], and also calculated in a $1/n$ expansion [6], and in the following section we will compare the predictions of the current theory with both simulation results and $1/n$ results.

5. Results

Table 1 contains the values of λ , for various n and d , determined as described earlier. Also listed are the corresponding values λ_{sim} obtained, via (41), from simulation results [4, 19] for $\bar{\lambda}$. Equivalent results for $n = 1$ have already been given in [7], so we specialize here to $n \geq 2$.

The blank entries in the table indicate either that no simulation results for $\bar{\lambda}$ are available ($d = 2, n = 2$), or that the behaviour of the system is in some way anomalous. For example, the $d = 1, n = 2$ system has a domain scale growing as $t^{1/4}$, rather than $t^{1/2}$, a Gaussian scaling function $f(x)$, and an autocorrelation function of 'stretched exponential' form [4]. None of these features is recovered by

the Mazenko scheme, naively applied. However, one can argue that the way in which the calculation is set up restricts its applicability to systems with $n \leq d$.

Table 1. Values of the exponent λ , obtained using the Mazenko theory. Equivalent simulation results, λ_{sim} , are shown where available.

d		$n = 2$	$n = 3$	$n = 4$
1	λ	0.301	0.378	0.414
	λ_{sim}	—	0.352(5) ^a	0.420(8) ^a
2	λ	0.829	0.883	0.912
	λ_{sim}	—	—	0.89(1) ^b
3	λ	1.382	1.413	1.432

^a [4]

^b [19]

This is because the n -component vector field $\vec{m}(r, t)$ has a physical interpretation as a position vector from a topologically stable singularity (e.g. a vortex) in the field $\vec{\phi}(x, t)$ to the point r , when r is close to the singularity. Clearly this interpretation only makes sense if the dimension n of the vector \vec{m} is less than or equal to the dimension d of space. The equations derived using this interpretation, however, show no peculiarities for $n > d$, and indeed the values of λ obtained for $d = 1$, $n = 3, 4$ and for $d = 2$, $n = 4$ are in quite reasonable agreement with the simulation results. The case $d = 2$, $n = 3$ is another apparently anomalous system and does not seem to exhibit simple scaling [19]. We shall return to the general question of the validity of our approach for $n > d$ in section 7.

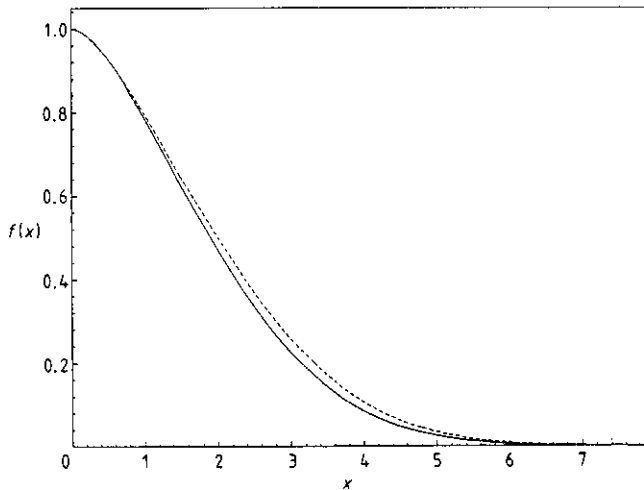


Figure 1. Scaling function $f(x)$ for the equal-time correlation function plotted against scaling variable $x = r/\sqrt{t}$, for $n = d = 2$: full curve, Mazenko theory; broken curve, Bray-Puri function [14].

Figures 1 and 2 display the scaling functions $f(x)$ for $d = 2$, $n = 2$ and $d = 3$, $n = 3$. Recall that these are obtained by solving (36) numerically, with initial conditions $\gamma(0) = 1$, $\gamma'(0) = 0$ and λ given in table 1, and substituting the result

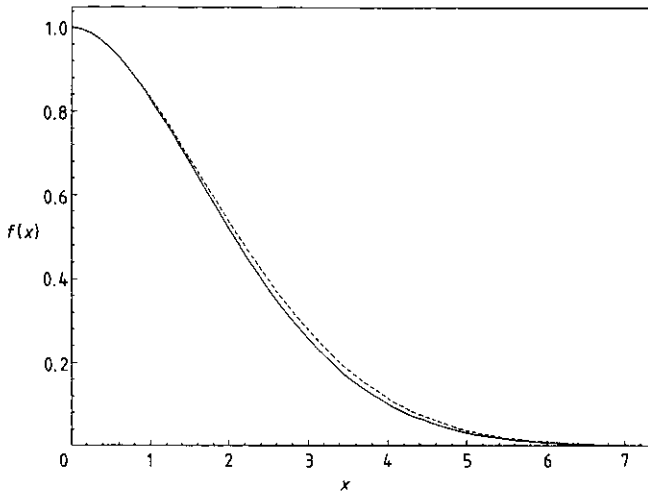


Figure 2. Same as figure 1, but for $n = d = 3$.

into (32). These are fairly smooth functions with, on the surface, no interesting features. The large- x behaviour has the form (23). A close inspection of the small- x limit, however, reveals that $f(x)$ is singular at $x = 0$, and this in turn leads to a power-law decay of the form $k^{-(d+n)}$ in the Fourier transform of $f(x)$, the scaling function for the equal-time structure factor $S_k(t, t)$. The case $n = 1$ is the familiar Porod's law [16], whose form follows from (22). The general n result was suggested by Bray and Puri [14], and by Toyoki [15], from a somewhat simpler treatment of the scaling function. The Bray-Puri (BP) scaling functions are included in figures 1 and 2 for comparison, and are not too different from the ones calculated earlier. A detailed comparison of the present theory to that of BP is given in the following section where, in particular, we explicitly consider the small- x form of the scaling function in both theories.

6. Comparison with other theories

The BP scaling functions [14] were derived using a generalization to arbitrary n of earlier approaches to the scalar theory by Kawasaki *et al* (KYG) [20], and by Ohta *et al* (OJK) [8]. These two approaches, while conceptually different, lead to the same scaling function $f(x)$.

The KYG theory starts from (2), with $V'(\phi) = -\phi + \phi^3$. Ignoring the ϕ^3 term yields a linear equation with the solution $\phi_0(\mathbf{x}, t) = \exp\{t(1 + \nabla^2)\}\phi(\mathbf{x}, 0)$. Reinstating the ϕ^3 term perturbatively leads to a divergent perturbation series which can, however, be summed approximately for late times by retaining only the dominant (as $t \rightarrow \infty$) divergence in each diagram and neglecting the momentum dependence in certain factors (the perturbation theory is done in momentum space). The result is

$$\phi_{\text{KYG}}(\mathbf{x}, t) = \frac{\phi_0(\mathbf{x}, t)}{\{1 + (\phi_0(\mathbf{x}, t))^2\}^{1/2}}. \quad (42)$$

Since ϕ_0 blows up exponentially with time, at late times (42) can be simplified to

$$\phi_{\text{KYG}}(\mathbf{x}, t) = \text{sgn}(\phi_0(\mathbf{x}, t)). \quad (43)$$

The exponential factor in ϕ_0 is now irrelevant, since it drops out when the sign is taken. The final result can therefore be written more simply in terms of a function $m(\mathbf{x}, t)$ that obeys the diffusion equation:

$$\phi_{\text{KYG}}(\mathbf{x}, t) = \text{sgn}(m(\mathbf{x}, t)) \quad (44)$$

$$\partial m / \partial t = \nabla^2 m. \quad (45)$$

This result is now in the form (14), i.e. the original field ϕ , with its discontinuities at domain walls, has been written in terms of a 'smooth' field m . If the initial condition on m has a Gaussian distribution, then the m distribution is Gaussian for all times since m obeys the linear equation (45). Therefore (15) can be taken over, with γ given by (10) and (8), i.e.

$$\gamma = \frac{[m(1)m(2)]}{[m(1)^2]^{1/2}[m(2)^2]^{1/2}}. \quad (46)$$

In the Mazenko theory, γ is determined self-consistently using only the assumption that m has a Gaussian distribution: the result is that γ obeys (36). In KYG, m obeys the diffusion equation (45), giving γ explicitly (for equal times) as $\gamma = \exp(-r^2/8t)$, and

$$C_{\text{KYG}}(12) = (2/\pi) \sin^{-1}(\exp\{-r^2/8t\}). \quad (47)$$

OJK again use a mapping of the form (44), but deal directly with the motion of interfaces, i.e. the surfaces on which $m = 0$. A sort of mean-field treatment of the resulting equation again leads to (45), but with a diffusion constant of $(d-1)/d$ instead of unity. Thus the form (47) is again obtained, but with $8 \rightarrow 8(d-1)/d$. The factor $(d-1)/d$ reflects the absence, for $d = 1$, of driving forces due to wall curvature.

The KYG arguments have been used for general n by Bray and Puri [14], and essentially equivalent results obtained by Toyoki [15]. The special case $n = 2$ had previously been treated by Puri and Roland [21] and by Puri [22]. The only change from the scalar theory is that ϕ and ϕ_0 become n -component vectors giving, instead of (44) and (45),

$$\tilde{\phi}_{\text{BP}}(\mathbf{x}, t) = \frac{\tilde{m}(\mathbf{x}, t)}{|\tilde{m}(\mathbf{x}, t)|} \quad (48)$$

$$\partial \tilde{m} / \partial t = \nabla^2 \tilde{m}. \quad (49)$$

With a Gaussian distribution for the field \tilde{m} at $t = 0$, the final result is simply (32), but with γ taking the specific form

$$\gamma_{\text{BP}} = \exp(-x^2/8) \quad x = r/\sqrt{t}. \quad (50)$$

Since $C(12) \sim \gamma$ for small γ , the large- x behaviour of $f_{\text{BP}}(x)$ is the same as (23), apart from the power-law prefactor. To investigate the small- x behaviour of both theories we need to look at the limit $\gamma \rightarrow 1$. To determine the small- x behaviour

of γ within the theory of section 3, we return to (36). From the properties of the hypergeometric functions [23] one can show that, for $\gamma \rightarrow 1$,

$$\begin{aligned} \frac{C_{\gamma\gamma}}{C_\gamma} &= \frac{2-n}{2}(1-\gamma)^{-1} + \dots & n < 2 \\ &\sim \{(1-\gamma)|\ln(1-\gamma)|\}^{-1} & n = 2 \\ &\sim (1-\gamma)^{(n-4)/2} & 2 < n < 4 \\ &\sim |\ln(1-\gamma)| & n = 4 \\ &\sim \text{constant} & n > 4. \end{aligned} \tag{51}$$

With these results one can see that (36) has a small- x solution of the form

$$\gamma = 1 - \alpha x^2 + \dots \tag{52}$$

Substituting this into (36), and using (51), we see that the nonlinear term in (36) only survives for $x \rightarrow 0$ for $n < 2$, and that

$$\begin{aligned} \alpha &= \frac{\lambda}{4} \frac{1}{d+n-2} & n \leq 2 \\ &= \frac{\lambda}{4d} & n \geq 2. \end{aligned} \tag{53}$$

These results, which should be compared with $\alpha_{\text{BP}} = \frac{1}{8}$, justify our use of initial conditions $\gamma(0) = 1$, $\gamma'(0) = 0$ in solving (36).

It should be noted that the BP scaling function is independent of the spatial dimension d , as is clear from (32) and (50). Liu and Mazenko [9] have noted that, for $n = 1$, the KYG scaling function (i.e. the $n = 1$ case of BP) is recovered from the full Mazenko theory in the limit $d \rightarrow \infty$. A similar result, in fact, holds for all n . Taking d large in (36), it is clear that λ must vary as d for large d so that the final term in (36) cancels the term $(d/x)\gamma'$. Retaining only these two terms gives $\gamma = \exp(-\lambda x^2/4d)$ for large d . Requiring that this match the form (23) at large x fixes $\lambda = d/2$ and $\gamma = \exp(-x^2/8)$ for $d \rightarrow \infty$, i.e. the BP result (50) is recovered in this limit.

From the small- x behaviour of γ one can extract the small- x behaviour of the scaling function $f(x)$. This is accomplished by using the transformation formulae for the hypergeometric function [23] to rewrite (32) in the form

$$\begin{aligned} C(12) &= \gamma F\left(\frac{1}{2}, \frac{1}{2}; \frac{2-n}{2}; 1-\gamma^2\right) \\ &+ \frac{n\gamma}{2\pi} \left[\Gamma^2\left(\frac{n+1}{2}\right) \Gamma\left(-\frac{n}{2}\right) \right] \left[\Gamma\left(\frac{n+2}{2}\right) \right]^{-1} (1-\gamma^2)^{n/2} \\ &\times F\left(\frac{n+1}{2}, \frac{n+1}{2}; \frac{n+2}{2}; 1-\gamma^2\right). \end{aligned} \tag{54}$$

As has been stressed by Bray and Puri, the second term is non-analytic in $(1-\gamma^2)$, i.e. in x^2 , for $x \rightarrow 0$, generating a term of order x^n (plus logarithmic corrections

when n is even). The result is that the equal-time structure factor $S_k(t, t)$ has a power-law tail of the form $L(t)^{-n} k^{-(d+n)}$ for $kL(t) \gg 1$ [14]. Hence this tail is common to both Mazenko-type and KYG-type theories, since they both have the same small- x form (52) for γ , differing only in the value of α . The tail has been observed in simulations [15, 24], and it would be interesting to seek experimental confirmation of it.

It is also interesting to look at the theory in the limit $n \gg 1$, where exact results are known [5, 6]. From (32) it is easy to show that

$$C(12) = \gamma - \frac{1}{2n} \gamma(1 - \gamma^2) + O(n^{-2}). \quad (55)$$

This forms the basis for a perturbative solution in powers of $1/n$. The calculation is straightforward, so we will omit the details. The most interesting result is that λ is given by

$$\lambda = \frac{d}{2} \left(1 - 3^{-d/2} \frac{1}{n} + O(n^{-2}) \right) \quad (56)$$

which can be compared with the exact $O(1/n)$ result [6]

$$\lambda = \frac{d}{2} \left(1 - \left(\frac{4}{3} \right)^{d/2} \frac{4}{9} (d+2) B \left(\frac{d}{2} + 1, \frac{d}{2} + 1 \right) \frac{1}{n} + O(n^{-2}) \right) \quad (57)$$

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function. The difference between these results, which is numerically small, implies that the Mazenko-type theories are not exact in general, though they capture most of the important physics. We recall that KYG-type theories, such as BP, give $\lambda = d/2$ for all n .

7. Discussion and summary

Mazenko's theory of phase ordering dynamics [7] has been generalized to systems described by an n -component vector order parameter with $O(n)$ symmetry. The key idea was to write the order parameter field $\vec{\phi}$ as a nonlinear function (defined by (29)) of a field \vec{m} such that \vec{m} varies smoothly in space at points where $\vec{\phi}$ has topological defects. The vector \vec{m} is everywhere parallel to $\vec{\phi}$, but its magnitude measures, close to a defect, the distance from the defect. The single assumption is that \vec{m} can be treated as a Gaussian random field.

The main result is contained in (32) and (36), which together determine the scaling function $f(x)$ for the equal-time correlation function $C(12)$. The parameter λ appearing in equation (36) has, as shown in section 4 and [11], physical significance as the exponent characterizing different time correlations [4, 6, 10]. It is determined by the condition that the equal-time correlation function have the correct large distance behaviour. The values of λ for $2 \leq n \leq 4$, and $1 \leq d \leq 3$, are given in table 1.

The scaling functions $f(x)$ for $n = d = 2$ and $n = d = 3$ are displayed in figures 1 and 2, where the equivalent functions obtained from the approach of Bray and Puri [14] are included for comparison. Note that these comparisons are *absolute*, i.e. the scaling variable is r/\sqrt{t} in all cases. In comparing the theory with experiment

or simulations, the absolute units of time, to be used in (2), will not in general be known (unless (2) is solved directly), and the characteristic scale $L(t)$ will have one overall free parameter to be fitted. If one allows such a free parameter in figures 1 and 2, by rescaling the abscissa for the Bray-Puri curves (which would correspond to changing the 'diffusion constant' from unity in (49)), the agreement is very good indeed. We recall that the Mazenko theory reduces exactly to Bray-Puri in the limit $d \rightarrow \infty$.

While the scaling functions in figures 1 and 2 are almost featureless, we have shown that they carry a (leading) short-distance singularity of the form x^n , with an extra $\ln x$ factor when n is even. This leads to a power-law tail, $S_k(t, t) \propto k^{-(d+n)}$ in the structure factor, i.e. the Fourier transform of the equal-time correlation function. This tail, which for $n = 1$ is the familiar 'Porod's law' [16], is common to both Mazenko and Bray-Puri theories. Tbyoki [15] has independently obtained the same result by assuming that topological defects in the system can be modelled by the zeros of a Gaussian random field. This raises the interesting question of whether such a tail is to be expected in systems where no topologically stable defects exist. For scalar fields, for example, it is quite clear that Porod's law is a simple consequence of sharp domain walls. The probability that two points a distance r apart are in different phases, for $r \ll L(t)$, is just the probability that a domain wall passes between the points, and is of order $r/L(t)$. This gives $C(12) = 1 - \text{constant}r/L + \dots$ for $r \ll L$, which leads directly to Porod's law. For $n \geq 2$, Bray and Puri's generalization of Porod's law can also be derived by a direct consideration of the role of topological defects. To illustrate the point we consider the case $n = d = 2$, for which the defects are vortices.

Consider the field $\vec{\phi}$ at points \mathbf{x} and $\mathbf{x} + \mathbf{r}$ in the presence of a vortex at the origin. We make the natural assumption that the vortex density is of order L^{-2} and take $|\mathbf{r}| \ll |\mathbf{x}| \ll L$, i.e. we are looking at two nearby points whose separation is much smaller than their distance from the vortex, but which are much nearer to the given vortex than to any other. Then the field $\vec{\phi}$ at the two points is saturated in length and, up to a global rotation, can be taken to be directed radially outward from the origin. Thus

$$\begin{aligned} \vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(\mathbf{x} + \mathbf{r}) &\simeq \frac{\mathbf{x} \cdot (\mathbf{x} + \mathbf{r})}{|\mathbf{x}| |\mathbf{x} + \mathbf{r}|} \\ &\simeq 1 - \frac{1}{2} \left(\frac{r^2}{x^2} - \frac{(\mathbf{x} \cdot \mathbf{r})^2}{x^4} \right) + O(r^4/x^4). \end{aligned}$$

With \mathbf{r} held fixed we now average the result over all possible relative positions of the vortex, i.e. over all values of \mathbf{x} within an area L^2 around the pair of points:

$$\begin{aligned} C(12) &= [\vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(\mathbf{x} + \mathbf{r})] \\ &\simeq 1 - \text{constant} \frac{r^2}{L^2} \int_r^L \frac{x \, dx}{x^2} + \dots \\ &\simeq 1 - \text{constant} \frac{r^2}{L^2} \ln \left(\frac{L}{r} \right) + \dots \end{aligned}$$

Fourier transforming this gives $S_k(t, t) \sim 1/k^4 L^2$ for $kL \gg 1$, which is the special case $d = n = 2$ of the general $k^{-(d+n)}$ tail. This argument can be extended to general $n \leq d$, where stable defects occur.

Given that the tail can be ascribed directly to the role of topological defects, is the tail still present in the absence of stable defects? This is an open question at present. The case $d = 1$, $n = 2$ presents a counter-example with no power-law tail [4]. The Bray–Puri and Mazenko approaches both give a tail for all n and d . However, the interpretation of the Mazenko theory is problematical for $n > d$, since the dimension of the vector \vec{m} , which is supposed to represent a spatial vector, would then be greater than that of the space in which it resides. It may be that there is a variant of the Mazenko theory which avoids this problem for $n > d$.

We began by mentioning some of the strengths of the Mazenko approach: the explicit d -dependence, the recovery of the exact result for $d = 1 = n$, and the emergence of the exponent λ in a natural way. We conclude by noting a residual deficiency, which we illustrate for $n = 1$, namely its inability to reproduce correctly the structure of the domain walls. Real walls have a well-defined profile, given by the stationary solution of (2) with ϕ varying only in, say, the x -direction, with boundary conditions $\phi(\pm\infty) = \pm 1$. For such a wall, $|\nabla\phi|$, evaluated in the interface (i.e. where $\phi = 0$), has a precise value. This implies that $|\nabla m|$ should have a precise value. In fact, comparing (2) and (6) implies $|\nabla m| = 1/\sqrt{2}$ in the interface for an 'exact' solution. In the Mazenko theory, however, m is a Gaussian random field, so each component $\partial m/\partial x_i$ of ∇m is an independent Gaussian field, and is independent of m itself. Therefore $|\nabla m|$ will have a distribution of values, rather than a unique value, at interfaces, i.e. there is a distribution of interfacial widths. It is interesting, however, that in the limit $d \rightarrow \infty$ the central limit theorem ensures that $|\nabla m|$ does have a precise value: $|\nabla m| \rightarrow (d[(m')^2])^{1/2}$, where $m' = \partial m/\partial x_i$ for some i , gives (using (8) and (10)) $|\nabla m| \rightarrow (d\{[(m')^2]/[m^2]\}[m^2])^{1/2} = (d\{-\gamma''(x)/t\}S_0(1))^{1/2}$. Using (19) for $S_0(1)$ and (52) for $\gamma(x)$ gives $|\nabla m| \rightarrow 1/\sqrt{2}$ for $d \rightarrow \infty$, which is the correct result. We conclude that the Mazenko theory is unlikely to be exact for general d , but may well become exact for large d . It will be interesting to see if one can use this approach to develop a systematic expansion around the large d limit.

After this manuscript was essentially complete, we learned of very similar work by Liu and Mazenko [25] (note that these authors use the symbol λ for what we call $\bar{\lambda} \equiv d - \lambda$). Where our results overlap we agree completely, except for some discrepancies in the values of the exponent λ . Liu and Mazenko only quote results for $n = 2$. Their results for λ , to be compared with the $n = 2$ column of table 1, read 0.315 ($d = 1$), 0.832 ($d = 2$) and 1.382 ($d = 3$). There is no discrepancy for $d = 3$, a small one (0.4%) for $d = 2$ and a somewhat larger one (4.7%) for $d = 1$. In the latter two cases, the differences are greater than the expected errors on our results (no greater than ± 1 in the last figure quoted). We have checked our results and believe them to be correct.

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