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Slow domain growth in a system with competing interactions

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We carry out a numerical study of the growth of domains following a quench in a three-dimensional scalar model with competing ferromagnetic J_1 and antiferromagnetic $J_2<J_1$ interactions. A "dynamical phase diagram" separates a region I of algebraic growth from a region II of logarithmic growth across an equilibrium "corner-rounding transition," confirming a previous claim. In region II, up to the late times we study, the correlation functions are *anisotropic* and *violate dynamical scaling*. This arises from the presence of two distinct length scales—the distance between interfaces R and the distance between corners L, both of which grow logarithmically slowly. In the scaling limit $(t\rightarrow\infty)$, $L/R\rightarrow 0$, restoring scaling and isotropy. Under the assumption of analyticity, the asymptotic scaling function is identical to the pure Ising model. The slow logarithmic growth arises from a renormalization of the kinetic coefficient at the smaller length scale L, and can be associated with the dangerously irrelevant operator J_2 at the zero-temperature fixed point (ZFP). This implies that at the ZFP, the two models, with and without J_2, belong to the same universality class.

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A zero-temperature fixed-point (ZFP) [1] governs the late-time evolution of domains following a quench from a disordered to an ordered phase. Generically, this fixed point is associated with a *single* dominant length scale, $R(t)$, which is the characteristic length over which spins order (distance between interfaces). A variety of studies [2] indicate that in the vicinity of the ZFP, the equal time correlation function $g(\vec{r},t)\equiv\langle\phi(0,t)\phi(\vec{r},t)\rangle$ exhibits a scale invariant (isotropic) form, $g(r/R(t))$, with $R(t)\sim t^{1/z}$ (z is the dynamical exponent). This diverging length implies that microscopic spatial and temporal details are irrelevant. This results in the emergence of universality classes (UC) characterized by the form of the scaling functions and the values of exponents such as z.

The presence of quenched randomness has a dramatic effect on dynamics, by pinning interfaces and retarding domain growth, $R(t)\sim(\ln t)^{\alpha}$. The energy barriers required to surmount interface pinning give rise to a scale-dependent renormalization of the bare kinetic coefficient [3], resulting in this slow logarithmic growth. In spite of this, however, the scaling functions and the exponents remain unaltered [3,4]. Randomness is associated with a dangerously irrelevant variable at the ZFP [3].

Recently, Shore and Sethna (SS) [5] and Shore, Holzer, and Sethna [6] studied domain growth dynamics in a *pure* three-dimensional (3D) (frustrated) Ising model (and an equivalent two-dimensional tiling model) with short range (isotropic) interactions. Quite surprisingly, they found that the dynamics of this model shares some features in common with the random field Ising model (RFIM). Their analysis, largely confined to the growth law, reveals that at temperatures below the "corner-rounding" temperature, the domains grow logarithmically slowly (reminiscent of growth in the RFIM) and are sharp and blocky (unlike pure Ising domains, which have rounded corners). From their limited Monte Carlo data on correlation functions, they arrive at the tentative conclusion that (a) the asymptotic correlation function obeys dynamical scaling (evidence for this is weak); (b) the scaling functions are *nonisotropic* (and thus different from the pure Ising case), *nonuniversal*, and *nonanalytic* in temperature T (below the critical temperature). These results would seem to indicate that short range (isotropic) interactions that produce frustration (and scale-dependent energy barriers to coarsening) are *relevant* at the conventional Ising ZFP [7] (this is quite distinct from the RFIM). These conclusions pose a serious challenge to conventional knowledge in domain growth kinetics.

In this Rapid Communication, we study the Langevin dynamics of a soft-spin version of the SS model, following a quench from the disordered to the ordered phase. We demonstrate a "dynamical phase diagram" separating a region I of algebraic growth from a region II of logarithmic growth across an equilibrium corner-rounding transition. We show that in region II, both growth behavior and asymptotic correlation functions are identical to those in generic quenched random models. This arises because of the presence of *two length scales* (just as in the RFIM [3]): $L\sim\ln t$, the distance between corners of cubic domains, and $R\sim(\ln t)^{3/2}$, the distance between interfaces. Since the numerical simulations of SS do not explore up to times when $R\gg L$, their conclusions (a) and (b) only reflect preasymptotic behavior. In the scaling limit, as $t\rightarrow\infty$, $L/R\rightarrow 0$, restoring scaling and isotropy of the asymptotic correlation functions. Under the assumption of analyticity, the scaling function is identical to the pure Ising model. The logarithmic growth arises from a scale-dependent renormalization of the kinetic coefficient at the smaller length scale L, and can be associated with the dangerously irrelevant operator J_2 (see below) at the ZFP. This implies that at the ZFP, the SS model, the pure Ising model, and the generic quenched random models, belong to the same UC.

The three-dimensional SS model [5] is an Ising model with nearest-neighbor (nn) ferromagnetic $J_1 \geqslant 0$ and weak next-nearest-neighbor (nnn) antiferromagnetic $J_2 \geqslant 0$ couplings. A coarse-grained free-energy functional $F[\phi]$ is obtained by a Hubbard-Stratonovich transformation [8], where the order parameter ϕ is a soft spin $(-\infty \leqslant \phi_i \leqslant \infty)$,

$$F[\phi_i]=\sum_{i=1}^{N}\left(-\frac{b}{2}\phi_i^2+\frac{u}{4}\phi_i^4\right)-J_1\sum_{\langle nn\rangle}\phi_i\phi_j+J_2\sum_{\langle nn\rangle}\phi_i\phi_j. \quad (1)$$

Although the competition promoted by J_2 leads to frustration, the ground state is ferromagnetic as long as $J_1/J_2 \geqslant 4$. The parameters b and u are temperature T dependent. The strict $T=0$ Ising limit is obtained by letting $b,u \rightarrow \infty$ such that $b/u=1$. However, in what follows, we shall treat b and u as independent parameters and restrict ourselves to the $T=0$ subspace (by setting the noise in the Langevin equation to zero). In this subspace, the up-down symmetry is spontaneously broken when $b>b_c=-6J_1+12J_2$.

A quench from $T=\infty$ to $T=0$ initiates the dynamics of $\phi_i(t)$ via the time-dependent Ginzburg Landau equation

$$\partial\phi_i/\partial t=b\phi_i-u\phi_i^3+J_1\sum_{\langle nn\rangle}\phi_j-J_2\sum_{\langle nnn\rangle}\phi_j, \quad (2)$$

into its ferromagnetic ground state. Time is measured in units of the bare kinetic coefficient Γ_0. We solve Eq. (2) using a first-order Euler scheme on a 128^3 and a 64^3 lattice with a time step $dt=0.1$. We average over 10 realizations of the initial configuration $\{\phi_i(0)\}$, which are uniformly distributed between -0.1 and 0.1 with zero mean. Without any loss of generality we fix $u=1$.

Our results on the growth of domains at various values of $b>b_c$ and J_2/J_1 are consistent with the results of SS. A region of I ($b_c<b<b_{CR}$) of algebraic growth separates a region II ($b>b_{CR}$) of logarithmic growth across a boundary $b_{CR}(J_2/J_1)$. A characteristic length scale, associated with the distance between interfaces, is extracted from the spherically averaged correlation function $(R(t),t)=g(0,t)/2$. In region I [Fig. 1(a)], $R(t)\sim t^{1/z}$, with $1/z=0.45\pm0.05$, consistent with the usual diffusive growth, $z=2$, for model-A systems. In region II [Fig. 1(b)], however, after an early algebraic growth (whose "range" increases with decreasing J_2/J_1), we obtain a reasonable fit to $R(t)\sim[\ln t]^m$, with $m\approx\frac{3}{2}$ at late times (our data is not extensive enough to specify m accurately). From a simulation at different values of b and J_2/J_1 in region II, we claim that $R(t)\sim[(J_2/J_1)^{-1}\ln t]^{3/2}$ (this is different from the SS claim, $R(t)\sim\ln t$; see [9], however).

A clue to understanding a logarithmic growth in this model is provided by the instantaneous snapshots of order parameter configurations at late times, Fig. 2. In region I [Fig. 2(a)], the domains are smooth with no sharp edges or corners and resemble the domains of the pure Ising model. Region II [Fig. 2(b)], however, exhibits blocky domains with sharp corners and facets along simple cubic directions. Close to the boundary, $(b-b_{CR})\rightarrow 0^+$, the domains have rounded corners and some sharp edges. Following Ref. [6], we identify b_{CR} with the corner-rounding transition of the associated equilibrium crystal shape problem defined as the point at which the step free energy across the [11] interface goes to

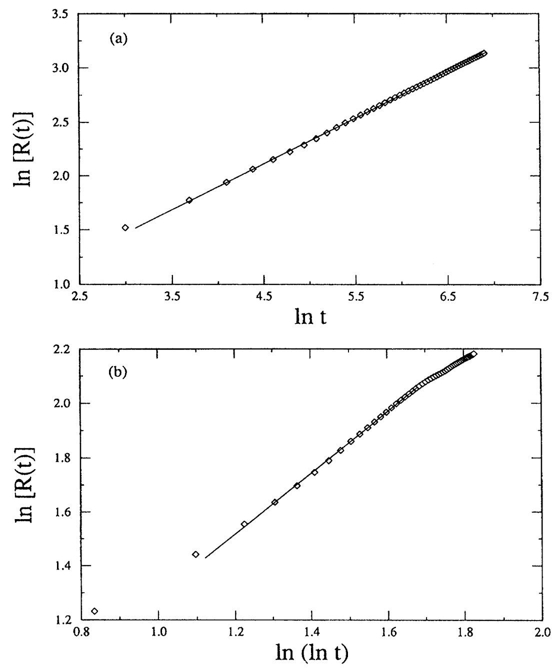

FIG. 1. (a) Growth of domain size $R(t)$ in region I ($b=-3$, $J_2/J_1=\frac{1}{6}$) plotted in a log-log plot. The slope of the straight line is 0.45 ±0.05. (b) Growth of domain size $R(t)$ in region II ($b=-0.1$, $J_2/J_1=0.01$). Here, $\ln[R(t)]$ is plotted against $\ln(\ln t)$. The slope of the straight line is 1.2 ± 0.2, consistent with $R(t)\sim[\ln t]^{3/2}$ (see text).

zero. We now repeat the argument [5] favoring logarithmic growth, which is compelling in its simplicity. After a quench with $b>b_{CR}>b_c$, the late-time morphology of the domains consists of sharp cubic blocks of, say, "down" spins, which shrink with time. The energy (in units of J_1) required to flip an entire edge of such a domain (for convenience, consider an isolated cube) of linear dimension L by single spin flips goes as $4J_2(L+1)/J_1$ (L is measured in units of lattice spacing a and is therefore dimensionless). Such scale-dependent energy barriers are reminiscent of energy barriers encountered in the RFIM [3] and lead to slow logarithmic growth, $L(t)\sim(J_2/J_1)^{-1}\ln t$ [10]. Note that this growth is different from that of $R(t)$, extracted from the bulk correlation function.

We investigate the nature of the correlation functions at late times. Region I follows standard dynamics at late times; the asymptotic correlation function is isotropic [the same along the lattice axes ($\times$) and the face ($\square$) and body ($+$) diagonals] and the spherically averaged $g(r,t)$ satisfies dynamical scaling. We find that the scaling function $g(r/R(t))$ is identical to that of the pure Ising model and thus independent of J_2. At large k, the scattering function [Fourier transform of $g(r/R(t))$] follows Porod's law $S(k/R(t))\sim k^{-4}$, consistent with the random interfaces being smooth and thin.

Region II contains several unusual features. It has been reported [6] that the correlation function is anisotropic with $g_\times \geqslant g_\square \geqslant g_+$ at fixed r/R. Further, $g_\times(r,t)$ exhibits dynamical scaling [6] at late times and the associated scaling function is independent of J_2/J_1 (and identical to that of the pure Ising model). There is a clear breakdown of scaling for $g_\square$, g_+, and the spherically averaged $g(r,t)$ (Fig. 3) even

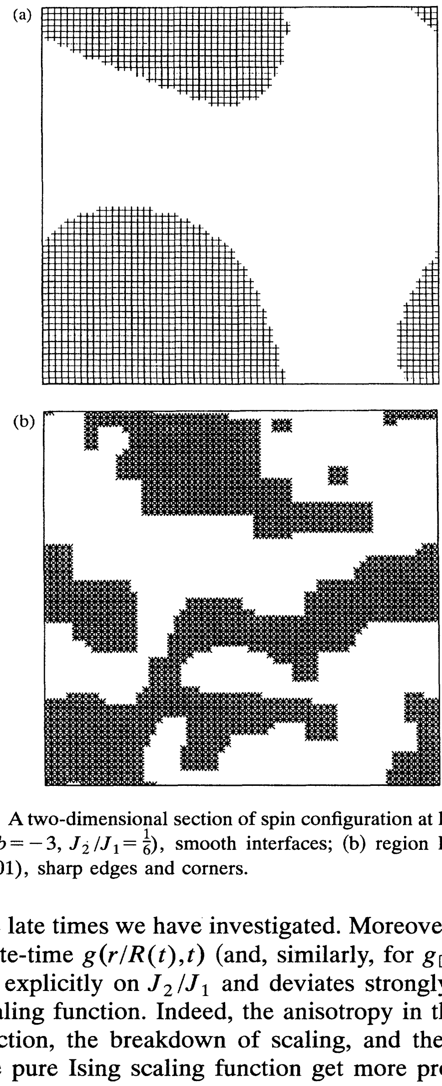

FIG. 2. A two-dimensional section of spin configuration at late times. (a) region I ($b=-3$, $J_2/J_1=\frac{1}{6}$), smooth interfaces; (b) region II ($b=-0.1$, $J_2/J_1=0.01$), sharp edges and corners.

up to the late times we have investigated. Moreover, the form of the late-time $g(r/R(t),t)$ (and, similarly, for $g_\square$ and g_+) depends explicitly on J_2/J_1 and deviates strongly from the Ising scaling function. Indeed, the anisotropy in the correlation function, the breakdown of scaling, and the deviation from the pure Ising scaling function get more prominent at larger J_2/J_1. The late-time $g(r,t)$ shows a linear dependence at small r, consistent with the presence of smooth interfaces. However the slope, which is proportional to the density of interfaces, depends on the value of J_2/J_1. These observations provoke the following set of questions. Why does dynamical scaling break down in region II at such late times? Why is the late-time $g(r/R(t))$ anisotropic and nonuniversal? Does dynamical scaling get restored at much later times? If restored, will the scaling function still be anisotropic (even though the free-energy functional is isotropic)? Will it still depend explicitly on J_2/J_1 in region II and thus be nonuniversal and different from the pure Ising scaling function? An affirmative answer would imply that the bulk dynamical scaling functions are *nonanalytic* at the corner-rounding transition b_{CR} (which is not associated with singularities of the bulk free energy). It would also mean that the scaling function explicitly depends on the short range interaction J_2 and the temperature T ($T<T_{\mathrm{CR}}<T_c$) and would hence be nonuniversal.

We will now provide a consistent explanation for all the questions just listed. A look at the configuration snapshots [such as Fig. 2(b)] in region II at various times immediately suggest that there are two independent length scales. One of

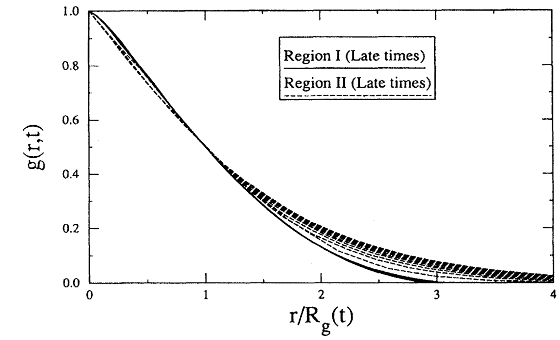

FIG. 3. Scaling function $g(r/R(t))$ vs $r/R(t)$ in region I ($b=-3$ and $J_2/J_1=\frac{1}{6}$) and in region II ($b=-1$, $J_2/J_1=\frac{1}{6}$) at various late times. Note the clear breakdown of scaling in region II. The corresponding plot in region I shows excellent scaling behavior.

these, $R(t)$, associated with bulk domain structure, is measured by the bulk correlation function $g(r,t)$ and corresponds to the typical distance over which spins change appreciably (distance between interfaces). The other length scale, $L(t)$, associated with the surface structure of domains (area of the face), corresponds to the typical distance over which "steps" are correlated (the distance between corners of the blocky domains). *In general, these two length scales grow at different rates.* In fact, in a generic pure spin model (e.g., the Ising model) above its roughening transition, $L=\xi_b$, the bulk correlation length, which is microscopic, while below the roughening transition, $R \gg L \geq \xi_b$. Thus the domains have rounded corners on a length scale R corresponding to the domain size. The bulk correlation function, which can be written as $g(r/R(t),L(t)/R(t))$, will assume its scaling form at late times, when $L(t)/R(t)\rightarrow 0$, which in generic pure systems happens quite soon. In the SS model, both $R(t)$ and $L(t)$ grow logarithmically slowly, perhaps with different powers, and so the scaling regime will be attained at very late times. In fact, as we have just seen, $R(t)$, measured from $g(r,t)$, grows as $[\ln t]^m$, where $m\approx\frac{3}{2}>1$, while $L(t)$ [obtained from competing the energy barrier to flip spins along the edge of a cube of size $L(t)$] grows as $\ln t$.

We provide a phenomenological "derivation" of the growth of these two length scales, in the spirit of Lai, Mazenko, and Valls (LMV) [11,6,12]. Since the dynamics of the spins does not conserve the total magnetization, the velocity $\dot{R}(t)$ should be curvature driven, albeit activated. The time scale of interface motion is dominated by the time required to flip the spins along its edge (recall the blocky domain pictures), and so the LMV equations read [13]

$$dR/dt=\Gamma_L/R, \tag{3}$$

where $\Gamma_L=\Gamma_0 e^{-f_B L}$ ($f_B \propto J_2$ is the free-energy barrier per unit length of the edge of a typical cubic domain of side L [14]) can be interpreted as the renormalized kinetic coefficient [3] due to the existence of scale-dependent energy barriers. To obtain the corresponding equations for $L(t)$, we consider the dynamics of spins restricted to the [111] interface [6]. This corresponds to the dynamics of rotating elementary hexagons (which consists of three tiles) in the associated two-dimensional tiling models [6]. It is easy to convince oneself that this dynamics is conservative [6] (and activated) and so, following LMV,

$$dL/dt=\Gamma_L/L^2. \qquad (4)$$

These coupled equations, valid at late times, admit the asymptotic solution, $L(t)\sim f_B^{-1}\ln t$ and $R(t)\sim[f_B^{-1}\ln t]^{3/2}$. The next leading-order corrections to $L\sim O(\ln(\ln t))$ and $R\sim O((\ln t)^{1/2}\ln(\ln t))$, and so the asymptotic ratio of the two-length scales is $L(t)/R(t)\sim[f_B^{-1}\ln t]^{-1/2}$. One has to simulate up to $t\sim e^{100}$ to see $R/L\sim 10$! It is clear, therefore, that even up to the late times we study, the correlations are characterized by these two slow growing length scales. This, as we had seen, results in a breakdown of dynamical scaling. At very late times, of course, a single length scale R would dominate and dynamical scaling would be restored. It is not surprising that the preasymptotic $g(r/R(t),t)$ is nonuniversal (J_2 dependent). It is reasonable to suggest that at late times, $g(r,t)$ can be written as $g(r,R(t),L(t))=g(r/R,L/R)\equiv g_0(r/R)+(L/R)g_1(r/R,L/R)$ [15]. The explicit J_2 dependence can be seen in the leading preasymptotic term. A similar expansion would hold for $g_\times$, $g_\Box$, and g_+ with the *same leading term* g_0. The scaling function $g_0(r/R)$ is clearly isotropic (since as $t\to\infty$, $L/R\to 0$, and the domains would look smooth on the length scale R and would lose their block morphology) and independent of J_2 and *hence identical with the Ising scaling function*. It is clear from geometry that $g_\times$ will not be affected by the formation of steps on the interface and so will be insensitive to the block morphology and hence to the length scale L. This explains why $g_\times$ attains its Ising universal form relatively quickly. $g_\Box$, g_+, and g are sensitive to the blockiness to varying degrees, giving rise to the anisotropic preasymptotic behavior. To conclude, the asymptotic dynamics of this model is indeed controlled by the Ising ZFP at which the competing interaction J_2 is irrelevant.

If J_2 is irrelevant at the ZFP, then why does it affect domain growth? From the singular dependence of the amplitude appearing in the logarithmic growth law as $J_2\to 0$, we conclude that J_2 is *dangerously irrelevant* at the ZFP [1,3]. Moreover, the presence of two length scales, $L(t)$ and $R(t)$, one of which grows sublinearly in the other, $L\sim R^{2/3}$ is characteristic of dangerously irrelevant variables. This is analogous to the situation in the RFIM [3], where the random field, responsible for generating scale-dependent energy barriers, is dangerously irrelevant at the ZFP. The logarithmic growth comes about because this dangerously irrelevant operator renormalizes the bare kinetic coefficient Γ_0 to a scale-dependent Γ_L. This renormalization occurs at the smaller length scale L at which scale-dependent energy barriers first appear. Since L is microscopic in the scaling regime (i.e., $L/R\to 0$ as $t\to\infty$), this renormalization does not affect the universal features of the Ising ZFP.

We conclude by asserting that the dynamics of the SS model following a quench to low temperatures is controlled by a ZFP. We have shown that the SS model, the pure Ising model, and generic models with quenched randomness belong to the same universality class at the ZFP.

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[1] A. J. Bray, Phys. Rev. B **41**, 6724 (1990).

[2] 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, London, 1983), Vol. 8.

[3] M. Rao and A. Chakrabarti, Phys. Rev. Lett. **71**, 3501 (1993).

[4] A. J. Bray, Adv. Phys. (to be published).

[5] J. D. Shore and J. P. Sethna, Phys. Rev. B **43**, 3782 (1991).

[6] J. D. Shore *et al.*, Phys. Rev. B **46**, 11 376 (1992).

[7] Because the scaling function depends explicitly on J_2, the $T-J_2/J_1$ parameter space would possess a whole "region" of fixed points.

[8] The Hubbard-Stratonovich transformation from the Ising variables S_i to the variables ϕ_i requires that the interaction matrix J_{ij} in the SS Hamiltonian written as $\mathcal{H}=-\frac{1}{2}\Sigma_{i,j}J_{ij}S_iS_j$ should be positive definite, which is ensured by defining nonzero diagonal elements $J_{ii}\geqslant 6$. The resulting local potential in ϕ_i, when expanded to lowest nontrivial order (universality at ZFP), gives the form in Eq. (1).

[9] A re-evaluation shows that $R(t)\sim[\ln t]^{3/2}$ is a better fit to SS data (J. D. Shore, private communication).

[10] This dynamical transition $b_{\rm CR}$ is determined by equating the free-energy barrier per unit length to flip all the spins along an edge of a cubic of size L (in the limit $L\to\infty$) to zero, which to leading order in J_2/J_1 is given by $b_{\rm CR}\approx(J_1^2/J_2)[1+O(J_2/J_1]$.

[11] Z. W. Lai *et al.*, Phys. Rev. B **37**, 9481 (1988).

[12] The LMV equations for generic models can be derived from the method of matched asymptotics.

[13] In region II, the domains are sharp and faceted (*as in the 3D Ising model for $T<T_c$*). The equilibrium interfacial energy (surface tension) is therefore anisotropic (*as in the 3D Ising model*). An anisotropic surface tension leads to an anisotropic kinetic coefficient in the coarse-grained equations of motion. *However, the asymptotic growth law remains unaffected*. See M. Siegert, Phys. Rev. A **42**, 6268 (1990) for the nonconserved model-*A* dynamics.

[14] The renormalized kinetic coefficient is given by $\Gamma_L=\Gamma_0\exp(-F_{\rm edge}/D)$, where $F_{\rm edge}$ is the *free-energy* barrier to moving the interface (face of the cube) by a unit length and D is the "diffusion coefficient" of the interface. The free-energy barrier $F_{\rm edge}$ is clearly dominated by the *energy* barrier to flip spins along an edge of the interface. This, for large L, is given by $4J_2L/J_1$. Thus, f_B to lowest order is proportional to J_2.

[15] The assumption is that the asymptotic correlation function is analytic in J_2. We believe, although we do not have proof, that if the bulk equilibrium correlation function $C(r;T,\{J_i\})$ is analytic in $(T,\{J_i\})$, then so is the asymptotic bulk dynamical correlation function $\lim_{t\to\infty}g(r,t;T,\{J_1\})$.