Two-point correlations near the phase transition in a compressible magnet

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Leading order in $\epsilon(=4-d)$ solutions of renormalization-group recursion relations are used to calculate the two-point correlation function in an n-component compressible magnet. The effect of finite compressibility on two-point correlations is studied and comparisons with the rigid system are made.

I. INTRODUCTION

One of the most useful tools in studying the critical-point behavior of magnetic systems is elastic neutron scattering. The coupling between the neutron and electron magnetic moments leads to a dependence of the differential scattering cross section on the Fourier transform of the spin-spin correlation function

$$G(\vec{q},t)=\sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}}\langle\vec{S}(\vec{R})\cdot\vec{S}(\vec{0})\rangle \quad . \tag{1.1}$$

Here $\vec{q}$ is the momentum transfer which is related to the scattering angle and $t=(T-T_c)/T_c$ is the reduced temperature. In rigid magnetic systems for wave vectors satisfying $qa \ll 1$ where a is the lattice constant G is expected to take on the asymptotic form (as $t\rightarrow 0$)

$$G(q,t)=Ct^{-\gamma}D(q^2\xi^2) \quad . \tag{1.2}$$

In the above, C is the amplitude of the susceptibility and ξ is the correlation length given by (as $t\rightarrow 0$)

$$\xi=fat^{-\nu} \quad , \tag{1.3}$$

where f is the amplitude of the second spatial moment of $G(\vec{R},t)=\langle\vec{S}(\vec{R})\cdot\vec{S}(\vec{0})\rangle$. The function $D(x^2)$ has been determined for both large and small values of its argument by Fisher and Aharony[1] correct to $O(\epsilon^2)$. For $x \ll 1$ (i.e., in the uncorrelated region) they obtain the Ornstein-Zernike form

$$D(x^2)=\frac{1}{1+x^2}+O(\epsilon^2) \quad , \tag{1.4}$$

while for $x \gg 1$ (i.e., in the strongly correlated region) $D(x^2)$ can be written

$$D(x^2)\approx\frac{D_0^\infty}{x^{2-\eta}}+\frac{D_1^\infty}{x^{2-\eta+(1-\alpha)/\nu}}+\frac{D_2^\infty}{x^{2-\eta+1/\nu}} \quad , \tag{1.5}$$

where $D_0^\infty=1+O(\epsilon^2)$,

$$D_1^\infty=\left(\frac{n+2}{4-n}\right)+\left(\frac{n+2}{n+8}\right)\frac{(7n+20)}{(4-n)^2}\epsilon+O(\epsilon^2)$$

and

$$D_2^\infty=-\frac{6}{(4-n)}-\left(\frac{n+2}{n+8}\right)\frac{(7n+20)}{(4-n)^2}\epsilon+O(\epsilon^2) \quad .$$

Their calculations were done for $T>T_c$ and in the absence of an external field. Combescot *et al.*[2] then extended these calculations to the case of nonzero external field. Although these and other[3] calculations gave detailed information about the small- and large-x behavior of $D(x^2)$, the properties of $D(x^2)$ for intermediate values of x remained unknown until Nelson[4] obtained results for $D(x^2)$ valid for all x which properly reproduced the large- and small-x behavior. Although these results only exponentiated singular behavior to $O(\epsilon)$, comparisons with high-temperature series expansions were encouraging.

The purpose of this paper is to present calculations of the two-point correlation function for an n-component magnetic system coupled to an isotropic elastic medium. The methods used are similar to those employed by Nelson[4] for the rigid system. A calculation including the effects of finite compressibility is worthwhile since a coupling between elastic and magnetic degrees of freedom can produce corrections to scaling behavior affecting two-point correlations and hence the analysis of scattering data. The paper is organized as follows. In Sec. II we review the model Hamiltonian and give solutions to renormalization-group[5] (RG) recursion relations obtained from it. Section III contains a calculation of the correlation function with a discussion of the RG matching conditions. The large and small $q\xi$ behavior of the function is obtained explicitly and compared to the rigid system results. We also present results of numerical calculations which display the dependence of G on both t and the strength of the magnetoelastic coupling. Section V contains a summary of results.

II. MODEL AND RECURSION RELATION SOLUTIONS

A model Hamiltonian useful for describing an n-component magnetic system coupled to an isotropic elastic medium is given in wave-vector space by[6,7]

$$H_{\rm eff}\left(=\frac{H}{T}\right)=\frac{L^{-d}}{2}\sum_{i,\vec{k}}(r+k^2)S_{i,\vec{k}}S_{i,-\vec{k}} + uL^{-3d}\sum_{i,j;\,\vec{k}_1,\vec{k}_2,\vec{k}_3} S_{i,\vec{k}_1}S_{i,\vec{k}_2}S_{j,\vec{k}_3} \times S_{j,-(\vec{k}_1+\vec{k}_2+\vec{k}_3)} + vL^{-3d}\left(\sum_{i,\vec{k}}S_{i,\vec{k}}S_{i,-\vec{k}}\right)^2 , \quad (2.1)$$

where the $S_{i,\vec{k}}$ constitute a set of nN collective coordinates, N being the number of spins in volume L^d and the wave-vector sums are restricted to the interior of a spherical Brillouin zone of unit radius. The first two terms in Eq. (2.1) are the usual terms found in the Ginzburg-Landau-Wilson (GLW) Hamiltonian[5] for a rigid magnetic system while the last term is a new mean-field-like interaction between the spins mediated by $\vec{k}=0$ phonons. The properties of Eq. (2.1) under RG transformation in $d=4-\epsilon$ have been studied previously, and the results of these works along with solutions to the differential RG recursion relations are summarized in our earlier paper[8] (hereafter referred to as I). The thermodynamic state of the system described by Eq. (2.1) is given by the fields r, u, and v and the set of differential RG recursion relations satisfied by these fields are given in I. The solutions[8] are

$$r(l)=t(l)-\tfrac{1}{2}\lambda(l)+\tfrac{1}{2}t(l)\lambda(l)\ln[1+t(l)]+O(\epsilon^2) , \quad (2.2a)$$

$$u(l)=ue^{\epsilon l}/Q(l)+O(\epsilon^2) , \quad (2.2b)$$

$$v(l)=\frac{ve^{\epsilon l}}{Q(l)^{A/C}f(l)}+O(\epsilon^2) , \quad (2.2c)$$

where $t(l)\equiv te^{2l}/f(l)$, $\lambda(l)\equiv Au(l)+Bv(l)$, $t\equiv r+\frac{1}{2}\lambda$, and the constants, A, B, and C are given by $A=(n+2)/2\pi^2$, $B=n/2\pi^2$, and $C=(n+8)/2\pi^2$. The functions $Q(l)$ and $f(l)$ are

$$f(l)=Q(l)^{A/C}[1+G(Q(l)^{1-2A/C}-1)] ,$$

$$Q(l)=1+(Cu/\epsilon)(e^{\epsilon l}-1) ,$$

where $G=Bv/Cu(1-2A/C)$; λ, r, u, and v are the $l=0$ values of these quantities and l is the logarithm of the spatial rescaling factor associated with the RG transformation. With these solutions at hand we now proceed to a calculation of the two-point correlation function.

III. CORRELATION FUNCTION AND RG MATCHING

The recursion relation method for calculating thermodynamic properties always involves making use of a scaling relation satisfied by the quantity of interest. In this case we use the relation[9]

$$G(q,\mu)=\exp\left(2l-\int_0^l\eta(l')dl'\right)G(e^lq,\mu(l)) , \quad (3.1)$$

where the set of fields $\mu=\{r,u,v\}$ defines the thermodynamic state of the near-critical system and $\mu(l)=\{r(l),u(l),v(l)\}$ corresponds to the thermodynamic state of a system onto which we map the near-critical system. With a suitable choice for l, one may be able to map onto a system whose two-point correlation function is easily calculated which means, in practice, that perturbation theory is applicable. One possible choice for l is a value, say l^*, which makes $r(l^*)=1$. This would make a calculation of $G(l^*)$ possible. The problem however with this choice is that, as pointed out by Nelson,[4] it leads to technical difficulties because as $T\to T_c$ (i.e., as $t\to 0$) l^* grows very large (it is approximately given by $e^{l^*}\approx t^{-\nu}$) and since e^lq must be bounded from above by unity this particular choice for l would only be useful for values of $q<e^{-l^*}\approx t^{\nu}$. This corresponds to values of $x=q\xi<1$. Another possible choice for l^* is given by $q^2e^{2l^*}=1$. The difficulty with this choice is that for wave vectors too small l^* will grow so large ($e^{l^*}\approx q^{-1}$) that for a given bare t, $t(l^*)$ will become larger than unity invalidating the solutions given in Eqs. (2.2). Thus this l^* is only useful for values of $x=q\xi>1$. In order to have results valid for any x we choose l^* by Nelson's compromise condition[4]

$$t(l^*)+e^{2l^*}q^2=1 . \quad (3.2)$$

With this l^* and ignoring η since it is of $O(\epsilon^2)$ Eq. (3.1) becomes

$$G(q,\mu)=e^{2l^*}G(e^{l^*}q,\mu(l^*)) . \quad (3.3)$$

We now need to calculate $G(e^{l^*}q,\mu(l^*))$ which may in fact be near critical depending on the values of μ and q. We write the Dyson equation[10] for $G(e^{l^*}q,\mu(l^*))$ which is shown graphically in Fig. 1.

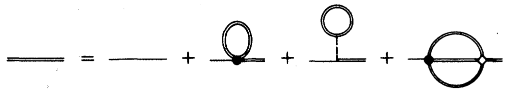

FIG. 1. Dyson equation for the two-point correlation function in terms of fully renormalized propagators and vertices. The broken line which carries no momentum is the bare v vertex while the solid dot and square are, respectively, the bare and fully renormalized four-point vertices u and u_R $(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4; l)$.

Analytically this reads

$$G^{-1}(e^{l^*}q, \mu(l^*)) = r(l^*) + e^{2l^*}q^2 + \frac{\lambda(l^*)}{K_4} \int \frac{d^dk}{(2\pi)^d} G(k, \mu(l^*)) \ , \quad (3.4)$$

where we have omitted the $O(\epsilon^2)$ terms in Eq. (3.4) since the condition (3.2) ensures that their contributions are less singular than those terms retained order by order in perturbation theory. The integral in Eq. (3.4) can be expressed in terms of the energy of a system in the thermodynamic state $\mu(l^*)$

$$E(\mu(l^*)) = -\tfrac{1}{2} n \int \frac{d^dk}{(2\pi)^d} G(k, \mu(l^*)) \ . \quad (3.5)$$

Since the energy of a compressible system was calculated in I we can carry over those results. We found that

$$E(r,u,v) = \tfrac{1}{8} n \frac{t}{u} \frac{1}{(4-n)} \left[\frac{F(t,u)^{1-2A/C} - 1}{1 + G(F(t,u)^{1-2A/C} - 1)} \right] , \quad (3.6)$$

where

$$F(t,u) \equiv 1 + (Cu/\epsilon)(t^{-\epsilon/2} - 1) \ . \quad (3.7)$$

Combining Eqs. (3.3)–(3.6) we find to leading order in ϵ

$$G(q,t,u^*,v) = e^{2l^*} \left[1 + \frac{\lambda(l^*) t(l^*)}{4K_4(4-n) u^*} [t(l^*)^{-(\epsilon/2)(4-n)/(n+8)} - 1] \right] , \quad (3.8)$$

where we have set $u = u^*$ for convenience (the fixed point we are referring to here is $F4$ of I — the rigid Heisenberg fixed point).

In order to remove the explicit l^* dependence from Eq. (3.8) we note that condition (3.2) with $u = u^*$ becomes

$$\frac{te^{\lambda_t l^*}}{(1-G)[1 + Ge^{\lambda_v l^*}/(1-G)]} + e^{2l^*}q^2 = 1 \ . \quad (3.9)$$

This expression is more conveniently given in terms of the nonlinear scaling fields appropriate to this problem. With the definitions $g_t(l) = g_t e^{\lambda_t l}$ and $g_v(l) = g_v e^{\lambda_v l}$ we find that [cf. Eqs. (5.17) of I]

$$g_t = t/(1-G), \quad g_v = \frac{v/\epsilon}{1-G} \ . \quad (3.10)$$

Making use of these results in Eq. (3.9) along with the substitution

$$e^{l^*} = g_t^{-\nu}\Phi(x,y) \ , \quad (3.11)$$

where $x \equiv q g_t^{-\nu}$ and

$$y \equiv n[(n+8)/2\pi^2(4-n)] g_v g_t^{-\phi_v} \quad (\phi_v = \nu\lambda_v = \alpha)$$

we obtain an equation satisfied by the function $\Phi(x,y)$

$$\frac{\Phi(x,y)^{\lambda_t}}{1 + y\Phi(x,y)^{\lambda_v}} + x^2\Phi(x,y)^2 = 1 \ . \quad (3.12)$$

Assuming that this equation can be solved for the function Φ we can now use Eq. (3.11) in the expression for G to obtain correct to $O(\epsilon)$

$$G(q,t,u^*,v) = g_t^{-2\nu}\Phi^2 \left\{ 1 + \left[\frac{n+2}{4-n} \right] \frac{\{1 + [6y/(n+2)]\Phi^{\lambda_v}\}}{(1 + y\Phi^{\lambda_v})^2} \Phi^{\lambda_t} \left[\left[\frac{\Phi^{\lambda_t}}{1 + y\Phi^{\lambda_v}} \right]^{-(\epsilon/2)(4-n)/(n+8)} - 1 \right] \right\} . \quad (3.13)$$

Writing G in the form

$$G(q,t,u^*,v) \equiv g_t^{-\gamma} D(x,y) \quad (3.14)$$

and realizing that $\gamma = 2\nu + O(\epsilon^2)$ we obtain for $D(x,y)$

$$D(x,y)=\Phi^2\left\{1+\left[\frac{n+2}{4-n}\right]\frac{\{1+[6/(n+2)]y\Phi^{\lambda_v}\}}{(1+y\Phi^{\lambda_v})}\Phi^{\lambda_t}\left[\left[\frac{\Phi^{\lambda_t}}{1+y\Phi^{\lambda_v}}\right]^{-(\epsilon/2)(4-n)/(n+8)}-1\right]\right\} . \tag{3.15}$$

We can now examine the small- and large-x behavior of $D(x,y)$. In doing this we will initially assume that $n>4$ to avoid complications associated with a first-order transition (see I). In this case y is positive since g_v is negative (the only physically admissible values of v are negative ones). Furthermore, since $\alpha<0$ for $n>4$, y will go to zero with g_t. Using Eq. (3.12) we obtain an expansion of the function Φ in x for $x<<1$ of the form

$$\Phi(x,y)=\Phi_0(x,y)\left[1+\frac{1}{2}\left[\frac{n+2}{n+8}\right]\epsilon\frac{\{1+[6/(n+2)]y\}}{(1+y)^2}\Phi_0(x,y)^2\ln\Phi_0(x,y)+O(\epsilon^2)\right] , \tag{3.16}$$

where

$$\Phi_0(x,y)=[x^2+1/(1+y)]^{-1/2} . \tag{3.17}$$

Substituting into Eq. (3.15) we obtain for $x<<1$

$$D(x,y)=\frac{1}{x^2+1/(1+y)}\left[1+\frac{1}{2}\left[\frac{n+2}{n+8}\right]\epsilon\frac{\{1+[6/(n+2)]y\}}{(1+y)^2}\frac{\ln(1+y)}{[x^2+1/(1+y)]}+O(\epsilon^2)\right] . \tag{3.18}$$

In the case when $v\rightarrow 0$ ($y\rightarrow 0$) this reduces to the rigid system result. Similarly when x is set to zero in this expression one obtains the scaling function for the susceptibility.[8] In the other extreme limit when $x>>1$ (deep within the critical region) the expansion of the function Φ is implemented by first writing

$$\Phi(x,y)=(1/x)\psi(w,z) , \tag{3.19}$$

where $w\equiv x^{-1/\nu}$ and $z\equiv yx^{-\alpha/\nu}$. The equation for ψ is

$$\psi(w,z)^2+\frac{\psi(w,z)^{\lambda_t}}{[1+z\psi(w,z)^{\lambda_v}]}=1 , \tag{3.20}$$

which can be expanded for small w (large x) to obtain

$$\psi(w,z)=\psi_0(w,z)\left[1+\frac{\epsilon}{2}\left[\frac{n+2}{n+8}\right]\frac{w\{1+[6/(n+2)]z\}}{(1+z)^2}\psi_0(w,z)^2\ln\psi_0(w,z)+O(\epsilon^2)\right] , \tag{3.21}$$

where

$$\psi_0(w,z)\equiv[1+w/(1+z)]^{-1/2} . \tag{3.22}$$

Substituting these results into Eq. (3.15) we obtain for $x>>1$

$$D(x,y)=\frac{1}{x^2}-\frac{1}{1+yx^{-\alpha/\nu}}\left[\frac{[6/(4-n)]y}{x^{2+(1+\alpha)/\nu}}+\frac{[6/(4-n)](1-y)}{x^{2+1/\nu}}-\frac{(n+2)/(4-n)}{x^{2+(1-\alpha)/\nu}}\right] . \tag{3.23}$$

This expression can be studied in two different regimes. The variable y can be written $y=[(v/v_3^*)/(1-v/v_3^*)]g_t^{-\alpha}$ where v_3^* is the value of v at fixed point $F3$ of I. In the limit of stiff lattice and/or weak spin-lattice coupling we have $v/v_3^*<<1$ and $y<<1$. In this case the system's critical behavior is controlled for all g_t by the rigid Heisenberg fixed point ($F4$ of I) and Eq. (3.23) becomes

$$D(x,y)=\frac{1}{x^2}-\frac{[6/(4-n)]y}{x^{2+(1+\alpha)/\nu}}-\frac{[6/(4-n)](1-y)}{x^{2+1/\nu}}+\frac{(n+2)/(4-n)}{x^{2+(1-\alpha)/\nu}} , \tag{3.24}$$

where we have ignored $yx^{-\alpha/\nu}$ compared to unity. The second term above is due entirely to the lattice coupling and since $\alpha<0$ it constitutes the leading correction to scaling. Note that when y is set to zero in Eq. (3.24) we recover the rigid system results of Fisher and Aharony[1] [neglecting the absence of η which is $O(\epsilon^2)$] with amplitudes correct to leading order in ϵ. The other regime is characterized by the inequality $[(v/v_3^*)/(1-v/v_3^*)]g_t^{-\alpha}>>1$. In this case the systems behavior is governed by fixed point $F3$ of I and Eq. (3.23) becomes

$$D(x,y)=\frac{1}{x^2}-\frac{6/(4-n)}{x^{2+1/\nu}}+\frac{6/(4-n)}{x^{2+(1-\alpha)/\nu}} , \tag{3.25}$$

where we have retained only terms which survive the $y \to \infty$ limit. This form for D will dominate for all $g_t > [(v/v_3^*)/(1-v/v_3^*)]^{1/\alpha}$. Since in the $y \to \infty$ limit the critical behavior is governed by fixed point $F3$ of I it is more appropriate to write the exponents in Eq. (3.25) (which are the exponents associated with the rigid Heisenberg fixed point) in terms of the exponents at fixed point $F3$. Making use of the relations[7] $\alpha = \alpha'/(\alpha'-1)$ and $\nu = \nu'/(1-\alpha')$ where the primed exponents are associated with fixed point $F3$ we obtain

$$D(x,y) = \frac{1}{x^2} + \frac{6/(4-n)}{x^{2+1/\nu'}} - \frac{6/(4-n)}{x^{2+(1-\alpha')/\nu'}} . \quad (3.26)$$

This has the same form as that given by Eq. (3.24) with y set to zero. This is to be expected since the short-distance expansion makes no reference to a specific fixed point.

Although Eqs. (3.18) and (3.24) correctly describe, respectively, the small and large x behavior of $D(x,y)$ for $y \ll 1$ it is more interesting to solve Eq. (3.12) numerically for intermediate values of x interpolating between the analytical results. In these calculations we have taken $\epsilon = 1$ and $n = 5$. Setting $n = 5$ we ensure that $\alpha < 0$: an assumption we have made throughout. The results are given in Fig. 2 where we plot $G(q,t(0),u^*,v)$ for different values of v/v_3^* as a function of $t(0)$. Here $t(0) = [T - T_c(0)]/T_c(0)$ is the temperature scale reduced with respect to T_c of the rigid system. Each curve is labeled by its respective value of v/v_3^* and since the lattice coupling raises T_c from $T_c(0)$ the curves corresponding to successively larger values of v/v_3^* begin at higher values of $t(0)$. It is interesting to compare the compressible system with the rigid system at fixed $t(0) > 0$. Two point correlations are enhanced in the compressible system relative to those in the rigid system. Furthermore the relative enhancement appears to increase as $q \to 0$. These results are plausible since the presence of the lattice coupling tends to favor long-range order. The insets of Figs. 2(a) and 2(b) give an expanded view of the maxima appearing at finite $t(0)$ in the function G. These maxima which occur due to a competition between the second and third terms in the short-distance expansion [which in the rigid system are proportional to $t(0)$ and $t(0)^{1-\alpha}$] are qualitatively similar to the maxima appearing in the high-temperature series expansion results of Ritchie and Fisher[11] for the Heisenberg model. Although the positions of the maxima at fixed angle will depend on v we have only given an expanded view of the rigid system maximum since all the maxima are qualitatively similar in appearance.

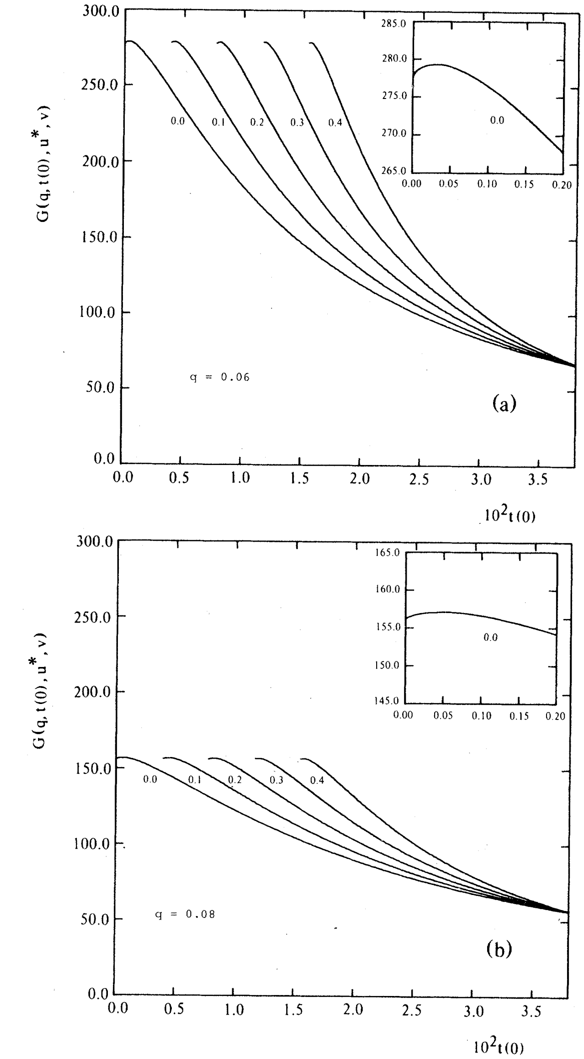

FIG. 2. Plot of $G(q,t(0),u^*,v)$ as a function of $t(0)$ for various values of v/v_3^* with (a) $q = 0.06$ and (b) $q = 0.08$. Here $t(0)$ is the temperature reduced with respect to T_c of the rigid system. Insets display expanded view of the maxima occurring in the rigid system curves for (a) $q = 0.06$ and (b) $q = 0.08$.

IV. SUMMARY

We have calculated the two-point correlation function with singularities exponentiated to $O(\epsilon)$ in an isotropic n-component compressible magnet for $T > T_c(v)$ and in the absence of an external field. We find that for $n > 4$ the lattice coupling produces a new correction to scaling in $G(q,t)$ which is more singular [it goes like $1/q^{(1+\alpha)/\nu}$] than the leading correction to scaling in the rigid system (which is proportional to $1/q^{1/\nu}$). The amplitude of this new correction to scaling is linear in $[T - T_c(v)]$ and the lattice coupling v. Although we have not explicitly given attention to the behavior of D when $n < 4$ and $\alpha > 0$, we believe that the analytical results given above can nevertheless be carried over. The only restriction on their use would be to exclude from consideration values of $t \lesssim t_c$ where t_c is the temperature at which a first-order transition occurs. In the Ising model, for example, we find $t_c = \frac{3}{2} K_4 u^* e^{-1} \times (4|v|/3u^*)^{1/\alpha}$ (see I). A simplification in our analysis involved setting $u = u^*$ which was not necessary. Letting u be arbitrarily small, for instance, would allow for a calculation of the Gaussian to Heisenberg crossover scaling function for two-point correlations.[12] We have also omitted a detailed study of the crossover behavior associated with the systems bare v being close to v_3^* (but still within the domain of attraction of the rigid Heisenberg fixed point).

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