Three-Point Correlations in Driven Diffusive Systems with Ising Symmetry

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For equilibrium systems with Ising symmetry, the three-point correlation function is always zero above criticality. When a lattice-gas version of this system is driven to a nonequilibrium steady state, this correlation becomes nontrivial. Its dominant large-scale behavior is found to be a consequence of both the manifest breaking of Ising symmetry by the driving force *and* the more subtle violation of the fluctuation-dissipation theorem.

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It is well known that symmetries play an important role in the understanding of physical systems and usually simplify our analyses drastically. A good example is the Ising model of a uniaxial magnet in the absence of an external magnetic field, where the Hamiltonian is symmetric under a global change of the signs of the spins —the Ising symmetry. Unless broken spontaneously, this symmetry ensures that all odd-point functions (static correlation functions with an odd number of spins) vanish. Such is the case when the system is in thermal equilibrium at temperature T above the critical T_c.

If a system is driven out of equilibrium into a steady state, however, then the symmetries associated with the driving forces must naturally be taken into account. Thus, when these forces do not respect the Ising symmetry, we expect odd-point functions to be nontrivial. This naive expectation is indeed borne out in a driven diffusive system, which recently received much attention [1-11]. However, by studying the three-point correlation function in the long-wavelength limit, we found that its dominant behavior depends *not only* on the explicit breaking of Ising symmetry by the driving force, but *also* on a less obvious effect, namely, the violation of the fluctuation-dissipation theorem (FDT). In the remainder of this Letter, we will briefly describe our models of the driven lattice gas, discuss the continuum version, derive the behavior of the three-point correlation within this context, and present Monte Carlo simulation data which confirm our conclusions.

The driven diffusive lattice gas, originally introduced as a model for superionic conductors [1], is one of the most useful proving grounds for studying phase transitions in nonequilibrium steady states. In this system, particles (i.e., the ions) occupy sites of a regular lattice. The dynamical evolution is governed by diffusion associated with the thermal bath, a nearest-neighbor attraction between the particles, and an external "driving" field E. This model may be cast into the Ising model, where + (−) spins are identified with particles (holes), so that Ising symmetry is just particle-hole symmetry. Particle conservation can be imposed by using Kawasaki's spin-exchange dynamics [12]. Thus, in systems with equal numbers of particles and holes, the magnetization (i.e., the one-point function) is identically zero at all times. As a result, up to a constant, the particle Hamiltonian, $\mathcal{H} = -4J\sum n_i n_j$, with $n_i = 0,1$ being the occupation number at site i, is identical to the Ising one: $-J\sum s_i s_j$, with $s_i = \pm 1$ being the spin at site i. To describe an attractive, short-ranged interaction, it is customary to let $J > 0$ and the sum be over nearest-neighbor sites.

Apart from the usual diffusion governed by $\mathcal{H}$ and T, there is an additional drive on the particles due to an external field $\mathbf{E}$, directed along one of the lattice axes. Jumps along (against) the field direction are enhanced (suppressed), with the rate depending on the (local) strength of E/T. Transverse jumps remain unaffected. Thus, a constant, uniform $\mathbf{E}$, in conjunction with periodic boundary conditions, sets up a positive average current in the steady state. Alternatively, one may consider an annealed random driving field whose *amplitude* fluctuates in space and time with zero mean, and, e.g., Gaussian correlations. In this case, the steady-state current vanishes due to the random average.

The uniformly and the randomly driven systems (referred to as UDS and RDS) clearly display different symmetries. In the former, the Ising symmetry of the system is obviously broken, and replaced by a symmetry [13] under the operation $(s_i, E) \to (-s_i, -E)$. Obviously, this system is also invariant under $(E, x_\parallel) \to (-E, -x_\parallel)$, where $x_\parallel$ denotes the spatial coordinate parallel to E. Combining these, we conclude that the UDS is symmetric under $(s_i, x_\parallel) \to (-s_i, -x_\parallel)$, an operation which we call CP. In contrast, for the RDS, the average over the randomness effectively restores the Ising symmetry.

These symmetries are clearly displayed in the continuum Langevin equations of motion, which result, in principle, from coarse graining the microscopic dynamics. Thus, we write equations for a mesoscopic magnetization density $\phi(x,t)$, keeping only the most relevant interactions. In the spirit of critical dynamics [14], these equations should provide an adequate description of the *long-wavelength* properties of our systems.

For the UDS [4], we have

$$\lambda^{-1}\partial_t\phi(x,t)=\tau_\parallel\partial^2\phi+\tau_\perp\nabla^2\phi-\nabla^4\phi+\mathcal{E}\partial\phi^2/2!-(\partial\cdot\zeta_\parallel+\nabla\cdot\zeta_\perp). \quad (1)$$

Here, ∂ and ∇ denote parallel (with respect to the driving field) and transverse gradients. The parameter $\mathcal{E}$ is an effective field, and, as all other coefficients, is a function of the microscopic T, J, and E. Of course, symmetry dictates that $\mathcal{E}$ is an odd function of E (while all others are even in E). This term is manifestly symmetric under CP, $(\phi,x_\parallel)\to(-\phi,-x_\parallel)$, while breaking the Ising symmetry, $\phi\to-\phi$. Its physical origin is an extra current, $j=c(\phi)\mathcal{E}$, where the conductivity c depends quadratically on ϕ, to leading order. The *thermal* noise terms $\zeta_\parallel$ and $\zeta_\perp$ are Gaussian distributed, according to $\exp[-\int dx\,dt\times(\zeta_\parallel^2/4\sigma_\parallel+\zeta_\perp^2/4\sigma_\perp)]$. Because of the strong anisotropy, the usual second-order phase transition is drastically modified. Here, it occurs when the transverse diffusion coefficient $\tau_\perp$ vanishes while the parallel $\tau_\parallel$ remains positive.

Similarly, the RDS is described by an effective equation [10],

$$\lambda^{-1}\partial_t\phi(x,t)=\rho_\parallel\partial^2\phi+\rho_\perp\nabla^2\phi-\nabla^4\phi+u\nabla^2\phi^3/3!-(\partial\cdot\xi_\parallel+\nabla\cdot\xi_\perp). \quad (2)$$

Because of the average over random E, a term like $c(\phi)\mathcal{E}$ must be absent, while the most relevant nonlinearity obeying the Ising symmetry is parametrized by u. Again, the theory is strongly anisotropic, so that criticality is characterized by $\rho_\perp=0$ and $\rho_\parallel>0$, with an anisotropic noise distribution according to $\exp[-\int dx\,dt(\xi_\parallel^2/4e a_\parallel+\xi_\perp^2/4\eta_\perp)]$.

Before proceeding to a discussion of the three-point function, we emphasize a major difference between the anisotropies appearing in our equations of motion and those suitable for describing systems near equilibrium with anisotropic couplings. For the latter, the FDT holds so that the ratios of the noise correlation widths to the diffusion coefficients are equal. In contrast, the violation of FDT in our nonequilibrium systems forces us to assume, generically, the inequalities $\sigma_\parallel/\tau_\parallel\neq\sigma_\perp/\tau_\perp$ and $\eta_\parallel/\rho_\parallel\neq\eta_\perp/\rho_\perp$ in UDS and RDS, respectively [4,10].

Returning to symmetries, we consider the consequences of having different nonlinear interactions in Eqs. (1) and (2). The most suitable quantity which can detect these differences is the three-point correlation function. In Fourier space, it is $G(k_1,k_2,k_3)\equiv\langle\phi(k_1)\phi(k_2)\phi(k_3)\rangle$, where $\langle\cdot\rangle$ stands for average over the steady state, with all ϕ's at equal times. Concentrating on $T>T_c$, we see that the Ising symmetry in a RDS forces G to be identically zero. On the other hand, CP symmetry in the UDS imposes $G(k_{i\parallel})=-G(-k_{i\parallel})$, so that it should be nontrivial generically. Using our continuum version and recasting the Langevin equation (1) in terms of the corresponding dynamic functional [15], we can calculate $G(k_i)$ perturbatively, provided T is not near T_c. Above criticality, this is straightforward since the disconnected parts vanish. To lowest order in $\mathcal{E}$, the result is

$$G(k_1,k_2,k_3)=\frac{-i\mathcal{E}\delta(k_1+k_2+k_3)}{\Gamma(k_1)+\Gamma(k_2)+\Gamma(k_3)}\left\{k_{1\parallel}\frac{\Sigma(k_2)\Sigma(k_3)}{\Gamma(k_2)\Gamma(k_3)}+\text{cyclic permutations}\right\}, \quad (3)$$

where $\Gamma(k)\equiv\tau_\perp k_\perp^2+\tau_\parallel k_\parallel^2+O(k^4)$ and $\Sigma(k)\equiv\sigma_\perp k_\perp^2+\sigma_\parallel k_\parallel^2$. Let us stress that (3) should capture the long-wavelength, or small-k, behavior of G.

Next, we turn our attention to the effects of FDT violation, which is characterized here by $\Gamma(k)$ *not* being proportional to $\Sigma(k)$, to lowest order in k. Instead, as $k\to0$, Σ/Γ is ~1, depending on the *direction* of k. (Indeed, this "discontinuity" singularity is responsible for long-range correlations [6,11] in the two-point function.) Thus, G diverges as $O(1/k)$, for generic, small momenta. As a result of particle conservation, G must be identically zero when any one of its momenta is zero. Thus, G exhibits an "infinitely" strong anisotropy as we approach $k=0$. In contrast, a recent study [11] provided a different expression for the three-point function. There the validity of the FDT was implicitly assumed in $\Gamma(k)=(k^2+\tau)\Sigma(k)$, so that $\Sigma/\Gamma(k\to0)$ is a nonsingular constant. The three permutations in Eq. (3) now add to zero trivially at this order and G *vanishes* as $O(k)$. While these naive powers are likely to become anomalous near T_c, we believe that our conclusion is valid for all T; namely, in the small-k limit, the leading behavior of G depends crucially on the breaking of the FDT.

The FDT also plays a decisive role at temperatures far above T_c where nearest-neighbor interactions are effectively zero [while the driving field is kept at $O(T)$]. In this region, the behavior of UDS is governed by an infinite-temperature, i.e., $J=0$, fixed point which *restores* detailed balance and the FDT [16]. Further, there would be no $O(k^4)$ terms in Γ so that Σ/Γ is a constant (for all k), leading to $G\equiv0$. Thus we expect G to be nontrivial for $T\sim J$ (e.g., near T_c) and to approach zero as the temperature is raised.

Below criticality, the situation is more complicated, since the expectation value of the order parameter, $\langle\phi(x)\rangle$, is inhomogeneous in the transverse $x_\perp$. Thus, the perturbation expansion inherent in the field-theoretic treatment must be set up around a nontrivial kink solution. Such expansions, though well known for equilibrium systems [17], are not fully established for driven nonequilibrium systems. Nevertheless, for the $T=0$ case, T should vanish again, since the bulk density is either 0 or 1 and the (extra) current is zero.

These predictions for the three-point function are tested in Monte Carlo simulations of both UDS and RDS, on an $L \times L$ periodic lattice, using saturation E fields. After reaching steady state, $\langle \phi(x_1)\phi(x_2)\phi(x_3)\rangle$ is measured. In this Letter, we present G for a particular choice of momenta, selected for simplicity and emphasis on the difference between UDS and RDS. Details and analyses of k dependence and finite-size effects will be published in a longer article [18]. To maximize the difference between the momenta, we choose k_1 to be purely longitudinal and k_2 to be purely transverse. Of course, $k_3 = -k_1 - k_2$ by translational invariance. The three terms in (3) reduce to two while G is proportional to $\Sigma(k_1)/\Gamma(k_1) - \Sigma(k_3)/\Gamma(k_3)$, which succinctly displays the role of FDT.

Since G is even in transverse momenta, we choose to "sum over $k_{2\perp}$" by setting $x_{2\perp} = x_{3\perp}$. For k_1, we use the smallest value allowed, namely, $2\pi/L$. The resultant, denoted by g, is plotted against T, as shown in Fig. 1, where T is measured in units of the Onsager T_c of the two-dimensional Ising model [19]. We see that, for RDS, both the real and imaginary parts of g are zero, up to fluctuations, for all T. For UDS, the real part vanishes, as expected implicitly from CP symmetry and shown explicitly in Eq. (3). The imaginary part of g, however, shows nontrivial behavior: It is negative [cf. Eq. (3)], with the minimum located around $T = 1.4$, the critical temperature of this system [1,3,20]. These comparisons confirm our first expectation, that the three-point function is a sensitive measure of CP versus Ising symmetries. Second, note that the predicted infinite-temperature behavior, i.e., $g \to 0$, already sets in at temperatures around $T = 3$. While the full understanding of the behavior of g below T_c requires further study, its decay toward zero agrees with $G(T=0) = 0$.

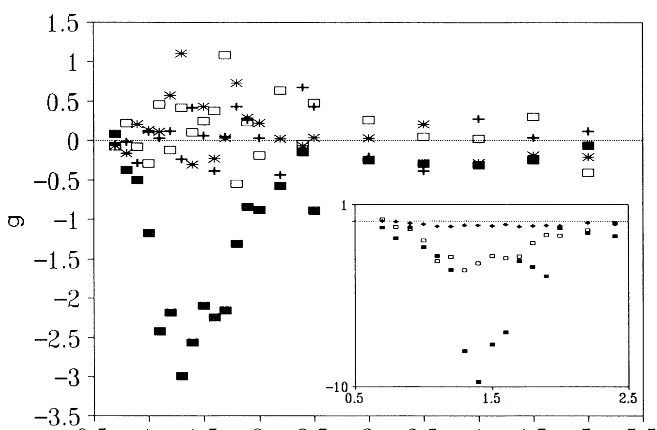

FIG. 1. Three-point correlation functions (g) in $L = 30$ systems vs T, which is in units of the Onsager temperature for the 2D Ising model. The symbols for the real and imaginary parts for the UDS are open and solid rectangles, respectively. Those for the RDS are plusses and asterisks, respectively. Inset: Im(g) vs T for the UDS with $L = 10$ (plusses), 30 (open rectangles), and 60 (solid rectangles).

Finally, in the inset, we see that $|g|$ increases with L. Since g is obtained from G by evaluating at the smallest momentum, $2\pi/L$, it would be difficult to explain this behavior with [11] $G \sim O(k)$. In contrast, it appears to be consistent with our $G \sim O(1/k)$. Further analysis is being performed [18], so that quantitative conclusions can be drawn. Similarly, considerable information about the critical properties of G is undoubtedly stored in the dramatic "dip" of g near $T = 1.4$. We believe that it reflects the "maximal" violation of the FDT at criticality, where the discontinuity of Σ/Γ at $k = 0$ goes to infinity. Work is in progress to extract the singular behavior of the three-point vertex function from a renormalized theory [10], so that a comparison with these data is possible.

To summarize, we have shown that the behavior of three-point correlation functions depends very sensitively on a subtle interplay between the breaking of Ising symmetry by a uniform drive and the violation of the FDT, due to nonequilibrium dynamics. Apart from their effects on the three-point function, the different symmetries typically lead to drastically different universality classes in the description of criticality. Thus, for instance, the upper critical dimension of the UDS [4] is $d_c = 5$ and the order parameter exponent $\beta = 0.5$ for all $d > 2$, whereas for the RDS [10] $d_c = 3$ and $\beta \approx 0.29$ in $d = 2$. Surprisingly, simulations with saturation fields [21] show *no detectable difference* in several key quantities (e.g., the order parameter, average number of nearest-neighbor pairs) in the entire temperature range. Therefore, it is significant that the three-point function sharply distinguishes the UDS from the RDS. Apart from the immediate issues concerning the k dependence of G at various temperatures, more extended ones come to mind. How do we understand the unexpected similarities in these two systems? Are the critical regions so minute that present data cannot yet resolve them, or is there another fixed point governing universal behavior of all systems driven with saturation fields? Finally, there is the most important question: Is it possible to observe a three-point correlation in physically realizable driven systems? In contrast to the two-point function (structure factor), there are very few articles [22] in the literature on measurements of higher correlations. It would be most interesting to develop experimental techniques and explore three-point functions in nature.

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[1] S. Katz, J. L. Lebowitz, and H. Spohn, Phys. Rev. B **28**,

1655 (1983); J. Stat. Phys. **34**, 497 (1984). For a recent review, see B. Schmittmann, Int. J. Mod. Phys. B **4**, 2269 (1990).

[2] H. van Beijeren and L. S. Schulman, Phys. Rev. Lett. **53**, 806 (1984); J. Krug, J. L. Lebowitz, H. Spohn, and M. Q. Zhang, J. Stat. Phys. **44**, 535 (1986); R. Dickman, Phys. Rev. A **38**, 2588 (1988).

[3] J. Marro, J. L. Lebowitz, H. Spohn, and M. H. Kalos, J. Stat. Phys. **38**, 725 (1985).

[4] K.-t. Leung and J. L. Cardy, J. Stat. Phys. **44**, 567 (1986); H. K. Janssen and B. Schmittmann, Z. Phys. B **64**, 503 (1986); K. Gawedzki and A. Kupiainen, Nucl. Phys. **B269**, 45 (1986).

[5] K.-t. Leung, J. Stat. Phys. **50**, 405 (1988); A. Hernandez-Machado and D. Jasnow, Phys. Rev. A **37**, 626 (1988); K.-t. Leung, K. K. Mon, J. L. Vallés, and R. K. P. Zia, Phys. Rev. Lett. **61**, 1744 (1988); J. L. Vallés, K.-t. Leung, and R. K. P. Zia, J. Stat. Phys. **56**, 43 (1989); and K.-t. Leung, J. Stat. Phys. **61**, 341 (1990).

[6] M. Q. Zhang, J.-S. Wang, J. L. Lebowitz, and J. L. Vallés, J. Stat. Phys. **52**, 1461 (1988).

[7] K.-t. Leung, B. Schmittmann, and R. K. P. Zia, Phys. Rev. Lett. **62**, 1722 (1989); R. Dickman, Phys. Rev. A **41**, 2192 (1990).

[8] F. J. Alexander and J. L. Lebowitz, J. Phys. A **23**, L375 (1990).

[9] G. E. Murch, Philos. Mag. A **41**, 157 (1980); H. Spohn, J. Phys. A **16**, 4275 (1983); J. V. Andersen and O. G. Mouritsen, Phys. Rev. Lett. **65**, 440 (1990); H. C. Fogedby and A. Svane, Phys. Rev. B **42**, 1056 (1990).

[10] B. Schmittmann and R. K. P. Zia, Phys. Rev. Lett. **66**, 357 (1991).

[11] P. L. Garrido, J. L. Lebowitz, C. Maes, and H. Spohn, Phys. Rev. A **42**, 1954 (1990).

[12] K. Kawasaki, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2.

[13] Although this symmetry is referred to in Ref. 1 as charge conjugation, we prefer to reserve that term for the operation of particle-antiparticle interchange only. In this language, an external "electric" field serves as an explicit breaking of charge conjugation, in much the same way that a uniform "magnetic" field explicitly breaks the Ising symmetry. Since "antiparticles" are just holes, charge conjugation is just the usual Ising symmetry in a lattice-gas model.

[14] B. I. Halperin, P. C. Hohenberg, and S-k. Ma, Phys. Rev. B **10**, 139 (1974). For a review, see P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[15] H. K. Janssen, Z. Phys. B **23**, 377 (1976); R. Bausch, H. K. Janssen, and H. Wagner, Z. Phys. B **24**, 113 (1976); C. DeDominicis, J. Phys. (Paris), Colloq. **37**, C1-247 (1976); H. K. Janssen, in *Dynamic Critical Phenomena and Related Topics,* edited by Ch. Enz (Springer, Berlin, 1979), p. 25.

[16] H. K. Janssen and B. Schmittmann, Z. Phys. B **63**, 517 (1986).

[17] R. K. P. Zia, Nucl. Phys. **B251**, 676 (1985), and references therein.

[18] K. Hwang, B. Schmittmann, and R. K. P. Zia (to be published).

[19] L. Onsager, Phys. Rev. **65**, 117 (1944).

[20] K.-t. Leung, Phys. Rev. Lett. **66**, 453 (1991).

[21] K. Hwang (unpublished). For a related system, see Z. Cheng, P. L. Garrido, J. L. Lebowitz, and J. L. Vallés, Europhys. Lett. (to be published).

[22] H. L. Frisch and J. McKenna, Phys. Rev. **139**, A68 (1965); R. S. Riffine and D. A. de Wolf, J. Geophys. Res. **70**, 4313 (1965); H. J. Raveché and R. D. Mountain, J. Chem. Phys. **57**, 3987 (1972); P. A. Egelstaff, in *Advances in Chemical Physics,* edited by I. Prigogine and S. A. Rice (Interscience, New York, 1983), Vol. 53, p. 1; P. Jacobaeus, J. U. Madsen, F. Kragh, and R. M. J. Cotterill, Philos. Mag. **41**, 11 (1980).