

Long-Range Correlations in Stationary Nonequilibrium Systems with Conservative Anisotropic Dynamics.

Z. CHENG(*), P. L. GARRIDO(*)^(§), J. L. LEBOWITZ(*) and J. L. VALLÉS(**)^(§§)

(*) *Departments of Mathematics and Physics, Rutgers University
New Brunswick, NJ 08903*

(**) *School of Physics and Astronomy, University of Minnesota
Minneapolis, MN 55455*

(received 30 October 1990; accepted in final form 30 January 1991)

PACS. 05.40 – Fluctuation phenomena, random processes, and Brownian motion.

PACS. 46.10 – Mechanics of discrete systems.

PACS. 05.70F – Phase transitions: general aspects.

Abstract. – We present results of computer studies of the spatial correlations in two nonequilibrium model systems. These are lattice gases on Z^2 described by (apparently) non-Gibbsian probability measures which are stationary with respect to simple, anisotropic, particle-conserving stochastic dynamics. The translation-invariant pair correlation functions $G(\mathbf{r})$ are found to decay like a quadrupole field, *i.e.* for $\mathbf{r} = (x, y)$, $G(\mathbf{r}) \sim (ax^2 - by^2)/r^4$, over a range of parameter values corresponding to «weak coupling» in the dynamics. This gives the strongest evidence to date of the generic nature of long-range correlations in conservative anisotropic nonequilibrium systems—in accord with some recent theoretical predictions. Some other properties of these models are also calculated. In particular it is found that, despite the slow decay of the correlations, the fluctuations in particle number look Gaussian.

1. Introduction.

In equilibrium systems long-range spatial correlations usually occur only for special values of the system parameters. For example, in the standard ferromagnetic Ising model, long-range correlations appear only at zero magnetic field and $T = T_c$, the critical temperature. Quite generally, high-temperature phases of Gibbs measures with finite-range interactions have exponentially decaying correlations[1]. In contrast to this there is growing evidence that long-range spatial correlations in nonequilibrium systems are the norm instead of the exception[2-6]. In particular, it was argued in ref. [3, 5], on the basis of perturbation expansions and renormalized fluctuating hydrodynamics, that the density-

^(§) Supported in part by Grant DGICYT, PB85-OC0062, Spain. Permanent address: Dept. Física Moderna, Univ. de Granada. E-18071 Granada, Spain.

^(§§) Supported in part by Grant DGICYT, PB85-OC0062, Spain. Permanent address: Dept. Física Fundamental, Univ. de Barcelona, 08028 Barcelona, Spain.

density correlation in the stationary state of systems with anisotropic conservative dynamics should decay generically as a quadrupole field. This corresponds, in two dimensions with proper rescaling of x and y , to

$$G(\mathbf{r}) \sim \frac{ax^2 - by^2}{r^4} \quad (r \gg 1), \quad (1)$$

where $\mathbf{r} \equiv (x, y)$, and a and b are constants which may depend on ρ , the average particle density, and other parameters of the system.

In this paper we study via computer simulation two simple two-dimensional lattice gas models whose dynamics are conservative, anisotropic and reflection invariant with respect to the principal axes. The density-density correlation $G(\mathbf{r})$ in the translation-invariant stationary state is defined as

$$G(\mathbf{r}) \equiv \langle n(0)n(\mathbf{r}) \rangle - \rho^2, \quad \rho \equiv \frac{1}{N} \sum_{\mathbf{r}} n(\mathbf{r}), \quad (2)$$

where $n(\mathbf{r})$ is the site occupation number, N the total number of sites and $\langle . \rangle$ means the ensemble average with respect to the stationary measure. We find long-range spatial correlations consistent with (1). We also examine some other properties of the models.

2. Model I: Anisotropic zero-range process.

This is a discrete-time version of the anisotropic zero-range process [7] studied by van Beijeren [4]. Let $n(\mathbf{r})$ be the occupation number of particles at site $\mathbf{r} \equiv (x, y)$, $n(\mathbf{r})$ a non-negative integer. The dynamics at every time step consists of two parts. First, one particle from each occupied site \mathbf{r} , $n(\mathbf{r}) > 0$, jumps to one of its four second-nearest-neighbor sites with equal probability; then each of the remaining particles at \mathbf{r} jumps independently to one of its two nearest-neighbor sites in the $\pm x$ directions, also with equal probability. We expect that the nature of the correlations in this model is qualitatively the same as in van Beijeren's model which involves a continuous time evolution with anisotropic local density-dependent jump rates, *i.e.* the rate for each particle at a site $\mathbf{r} \equiv (x, y)$ with an occupation number $n(\mathbf{r})$ jumping to $(x, y \pm 1)$ is $n^{-1}(\mathbf{r})$, while the rate for jumping to $(x \pm 1, y)$ is one, independent of $n(\mathbf{r})$.

To carry out the simulation, we used a lattice of size $L \times L$ with conventional periodic boundary conditions in the $\pm y$ directions. In the $\pm x$ directions, we used shifted periodic boundary conditions in which site $(L+1, y)$ is identified with site $(1, y+1)$. With these boundary conditions, the two-dimensional lattice can be treated as a one-dimensional array in the computer simulations, so that the updating can be vectorized. In this model, particles alternately occupy the sites consisting of the odd and even x columns, respectively. We eliminated this repetition by properly redefining the lattice.

Correlation function. – We performed simulations for systems of size $L = 32, 64$ and 128 with an average particle density per site $\rho = 1$. We also did simulations on systems of size $L = 32$ with $\rho = 0.25, 0.5, 2, 3$ and 4 . All simulations started with the particles randomly distributed. To reach the stationary state, we ran for about 10 000 initial time steps. Then we took data of $n(\mathbf{r})$ after every 10 time steps to compute the correlation function.

Figure 1 is a 3D plot of $G(\mathbf{r})$ for a system of size $L = 128$ and $\rho = 1$. The 2×2 region around $(0, 0)$ is excluded from this plot. Generating the data in this plot typically takes 30 to 60 hours

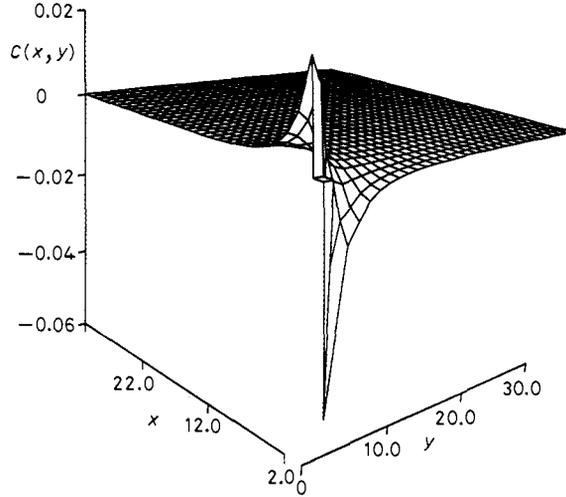


Fig. 1. - 3D plot of $G(\mathbf{r})$ for $\rho = 1$ and $L = 128$.

of CPU time on a Cyber 205. It is apparent that $G(\mathbf{r})$ follows qualitatively the quadrupole form given in eq. (1). To obtain quantitative results, we plotted $G(x, 0)$ and $-G(0, y)$ in log-log scale in fig. 2. The relative statistical error of the data at r can be estimated via the formula $\pm r^2/(L\sqrt{N})$, where N is the number of samples of the data. For r near one this gives an error bar $< 10^{-4}$ and around the tails the error bars are about 1/30, 1/10 and 1/2 for $L = 32$, $L = 64$ and $L = 128$, respectively. The results agree with a $1/r^2$ decay over the range from about 2 or 3 lattice spacings up to almost half of the system size, the maximum possible distance.

To obtain a formula of type (1) for $G(\mathbf{r})$ we used a general three-parameter fit obtained by minimizing

$$I(a, b, c) = \sum_{\mathbf{r} \neq 0}^{L/2'} \left(G(\mathbf{r}) - \frac{ax^2 - by^2}{(x^2 + cy^2)^2} \right)^2, \tag{3}$$

where the prime on the sum means that the 2×2 region around $(0, 0)$ is excluded. A relative error is defined as

$$\text{error} = I(a, b, c) / \sum_{\mathbf{r} \neq 0}^{L/2'} G^2(\mathbf{r}). \tag{4}$$

For $\rho = 1$, where we have the most extensive data, we find $a \approx b \approx 0.2$, and $c \approx 1.5$. This value of a, b and c can be compared with the results derived from fluctuating hydrodynamics by van Beijeren [4]. Following the same procedure for our dynamics, we obtain an explicit dependence of a, b and c on ρ and on $p(0)$, the probability of a site being empty. In particular, we have $c = a/b$, which seems to disagree with our data. However, we note that our fitting is somewhat insensitive to the value of c over a range of order one. Thus our data may still be consistent with the formula.

Our data for other values of ρ gives $a \sim b \sim \rho^\gamma$, $\gamma \approx 1.7$ with large error bars for ρ much smaller or much larger than one. To compare with van Beijeren's formula, we need to determine the dependence of $p(0)$ on ρ . The simulation data is unfortunately not good enough

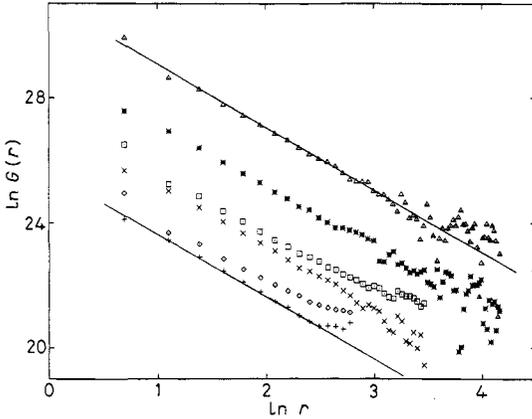


Fig. 2.

Fig. 2. - Plot of $\ln[G(x, 0)]$ vs. $\ln x$ and $\ln[-G(0, y)]$ vs. $\ln y$ for $L = 128$ (*: x -axis, Δ : y -axis) (80 000 samples), $L = 64$ (\times : x -axis, \square : y -axis) (400 000 samples), and $L = 32$ (+: x -axis, \diamond : y -axis) (1 200 000 samples). The solid lines indicate slope -2 . Data has been vertically shifted to avoid overlappings. The error bars go from less than $< 10^{-4}$ for r near one to about $1/30$, $1/10$ AND $1/2$ around the tails for $L = 32$, $L = 64$ and $L = 128$, respectively.

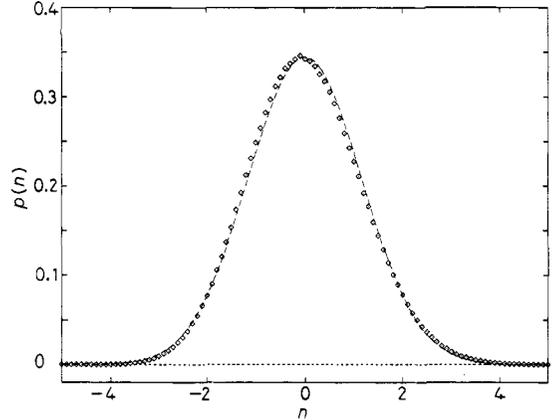


Fig. 3.

Fig. 3. - Distribution of particle numbers in a 10×10 block. The solid curve is the Gaussian distribution with same mean and variance.

for this purpose. Using however the mean-field approximation to $p(0)$ described below, van Beijeren's formula for small ρ goes like ρ^2 which is consistent with our data. For large ρ the simulation results apparently disagree with the formula.

We interpret the large error bars in our data for ρ much smaller or much larger than one as follows: for small ρ , most of the sites are occupied by either one particle or no particles, for which the x -dynamics and the y -dynamics do not differ. The stationary state is then close to that of a system with symmetric dynamics which is just a simple product measure [7]. For large ρ , the particles have a much larger probability to move in the $\pm x$ direction than in the $\pm y$ direction. The stationary state is then, in some sense, close to a one-dimensional system with only x -dynamics, which again has no long-range spatial correlations. Thus, we expect to have more difficulties seeing the long-range spatial correlations in the simulations for small or large ρ 's.

Numbers of particles per site. - The site number distribution $p(n)$ for various average densities was also collected in the simulations. We compared it with the probability distributions of site occupation numbers obtained by assuming no correlations between the sites as would be the case if the dynamics were isotropic. In that case it is easy to see [7] that for rates like those used by van Beijeren in the x -direction, the site number distribution is a Poisson distribution, $(\rho^n/n!) \exp[-\rho]$, while for the dynamics in the y -direction, it is a geometrical distribution, $(1/(1+\rho))(\rho/(1+\rho))^n$.

The simulations show that $p(n)$ for small values of n follows the corresponding Poisson distribution closely; while for larger values of n , $p(n)$ is between the distributions for x -dynamics and y -dynamics. As ρ gets small ($\rho \leq 0.5$), the range of n for which $p(n)$ follows the Poisson distribution increases. This is consistent with the comments made earlier about the nature of the stationary state for low and high densities.

Fluctuations. – It is well known [1] that in systems with rapid decay of all correlations the suitably normalized fluctuations in the number of particles in a region Λ ,

$$\eta_\Lambda = \frac{1}{\sqrt{|\Lambda|}} \sum_{r \in \Lambda} [n(r) - \rho],$$

will approach for $|\Lambda| \gg 1$ a Gaussian distribution with variance $|\Lambda|^{-1} \sum_{r, r' \in \Lambda} G(r - r')$, where $|\Lambda|$, the numbers of sites in Λ , is assumed very small compared to the size of the system. We were interested in seeing whether this will still be true for our system which has such long-range correlations. In fact this is necessary for consistency with the derivation of (1) from fluctuating hydrodynamics [3, 5].

We therefore computed η_Λ for Λ a rectangle of size $l \times l'$ with $l = 1, \dots, 10$ and $l' = 1, \dots, 10$ for a system of size $L = 128$ and density $\rho = 1$. The result for $l = l' = 10$ is given in fig. 3 where the data is compared to the appropriate Gaussian distribution. The agreement is seen to be very good. Similar agreement is obtained for $l \neq l'$ with $1 \ll l, l' \ll L$. We note that in fig. 3 the data has a small but systematic shift to the left of the corresponding Gaussian. This shift is similar to the shift which occurs when a Poisson distribution with a large parameter is approximated by a Gaussian distribution. We thus expect this to disappear as $l \rightarrow \infty$.

3. Model II: Anisotropic two-temperature Kawasaki dynamics.

We also investigated numerically another conservative anisotropic, nonequilibrium, 2D lattice gas. In this model, studied in [5], the occupation variables $n(\mathbf{r})$ take on only the values 0 or 1 (spin down or up). The configurations evolve according to the following stochastic mechanism. A lattice bond is chosen at random with rate one: if the bond is along the x -axis, an exchange of the values of the occupation variables on the adjoining sites is always performed; if the bond is along the y -axis, the exchange is accepted according to a transition probability $c = \min(1, \exp[-\beta\Delta H])$, where $\beta\Delta H$ is the change in

$$\beta H = -4\beta J \sum_{|r-r'|=1} n(\mathbf{r})n(\mathbf{r}') \quad (J > 0), \quad (5)$$

that would occur if the attempt is successful. We note that H is the energy of a ferromagnetic Ising system with isotropic interactions. We can thus think of our system as an Ising system which evolves according to Kawasaki [8] exchange dynamics (with Metropolis rates [9]) having an infinite temperature along the x -axis and $T = (k_B \beta)^{-1}$ along the y -axis. This model has some similarities with the driven diffusive system (DDS) studied in recent years [2, 10-12]. The difference with DDS resides in the symmetry here between the $\pm x$ -directions. In the DDS with strong field only jumps in $+x$ -direction are performed.

We performed a Monte Carlo study of this system for the case of a half-filled lattice, $\rho = 1/2$, of size 50×50 with periodic boundary conditions and a range of temperatures measured in units of $T_0 = 2.27J/k_B$. Once the stationary state had been reached, we took 200 measurements in an interval of 20 000 MCS.

Correlation function. – We computed the pair correlations $G(x, 0)$ and $G(0, y)$ along the x and y directions, respectively. To analyze the power law decay characteristic of this model, we plotted in fig. 4 $\log G(x, 0)$ vs. $\log r$. One can observe that at high temperature the curves have a slope of -2 , in agreement with (1). For T close to T_c , finite-size effects become

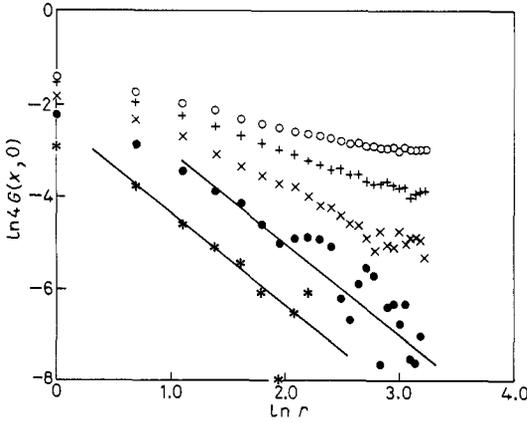


Fig. 4.

Fig. 4. - Plot of $\ln 4G(x, 0)$ vs. $\ln r$. The temperature are: 1.5 (\circ), 1.6 ($+$), 2.0 (\times), 3.0 (\bullet), and 6.0 ($*$). The solid lines have a slope -2 .

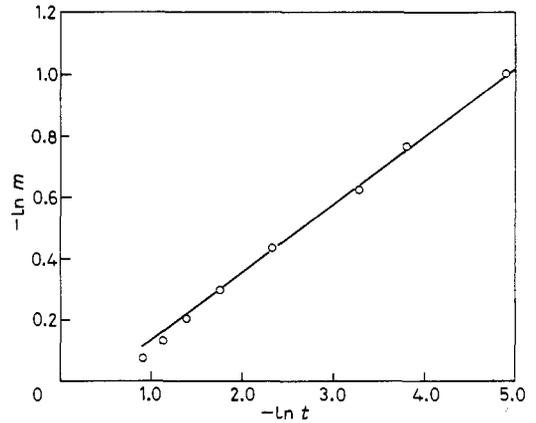


Fig. 5.

Fig. 5. - Plot of $-\ln m$ vs. $-\ln t$, where $t \equiv 1 - T/T_c$ is the reduced temperature with $T_c = 1.33$.

important, the corresponding curves do not fit to a slope -2 , though we expect [13] that the asymptotics for an infinite system still follows (1).

Nearest-neighbor correlations. - In [5] a high-temperature expansion of the master equation was developed. This gives to first order in β , for the case $\rho = 1/2$,

$$4G(1, 0)/\beta J = \frac{4 - \pi}{\pi - 2} \approx 0.7519, \quad 4G(0, 1)/\beta J = 2 \frac{\pi - 3}{\pi - 2} \approx 0.2481. \quad (6)$$

In table I we present a comparison between these high-temperature expansion results and the Monte Carlo simulations for several temperatures in the high-temperature regime. The fact that the value for the ratio $G(1, 0)/G(0, 1)$ for $T/T_0 = 6.0$ compares not so well with the asymptotic ratio is probably due to statistical error. We also show there the corresponding values for DDS taken from [2]. For our model the values of the correlation function at high temperatures appear to be significantly smaller than those for the DDS in both principal directions.

TABLE I. - Monte Carlo results of the nearest-neighbor correlations and high-temperature analytical results. In parentheses are the corresponding data for DDS taken from [2].

T/T_0	$4TG(1, 0)$	$4TG(0, 1)$	$G(1, 0)/G(0, 1)$
1.5	0.822	0.431	1.907
1.6	0.776 (0.857)	0.357 (0.436)	2.174 (1.966)
2.0	0.732 (0.830)	0.302 (0.379)	2.422 (2.190)
3.0	0.733 (0.824)	0.257 (0.358)	2.857 (2.302)
6.0	0.725 (0.822)	0.199 (0.365)	3.639 (2.252)
∞	0.752 (0.844)	0.248 (0.360)	3.031 (2.345)

Phase transition and comparison with DDS. – In analogy with DDS [2], we consider the order parameter

$$m = (\langle M_x^2 \rangle_T - \langle M_y^2 \rangle_T)^{1/2} \quad (7)$$

with

$$M_{z(y)}^2 = \frac{1}{L} \sum_{y(x)} \left\{ \frac{1}{L} \sum_{x(y)} (2n(\mathbf{r}) - 1) \right\}^2, \quad (8)$$

where x, y stand for indices over the x and y directions, respectively.

The data present a linear behavior of the order parameter when fitted to $m = A(T - T_c)^b$, with $T_c = 1.33$, $A = 0.88 \pm 0.015$ and $b = 0.235 \pm 0.006$. We show this fitting in a log-log plot in fig. 5.

We observe that similar to DDS [11], there is an increase in the «critical temperature» with respect to that of equilibrium. Our best-fitting result for the critical temperature is $T_c = 1.33$ which coincides with that of DDS within error bars. This is somewhat surprising since the critical temperature is generally model dependent. The result $b = 0.23$ is also apparently the same as the simulation result for DDS in [11]. This suggest that the critical behaviors of these two models may be in the same universality class. We note however that Schmittmann and Zia [12, 14] have suggested that for DDS in $d = 2$, b should be close to its mean-field value, $1/2$, with small, presumably logarithmic corrections. They further suggested that our model is in the same universality class as the «random field» DDS which has $b = 0.29$ in their field-theoretical calculations. More analytic and simulation works are needed to resolve this issue.

* * *

We thank H. VAN BEIJEREN, G. EYINK, H. SPOHN, R. VARADHAN and R. K. P. ZIA for helpful discussions. We also thank the NSF Supercomputing Center for computing support. This work has been supported in part by NSF grant DMR 86-12369.

REFERENCES

- [1] THOMPSON C., *Mathematical Statistical Mechanics* (Princeton University Press, Princeton) 1980.
- [2] ZHANG M. Q., WANG J.-S., LEBOWITZ J. L. and VALLÉS J. L., *J. Stat. Phys.*, **52** (1988) 1461.
- [3] GRINSTEIN G., LEE D. H. and SACHDEV S., *Phys. Rev. Lett.*, **64** (1990) 1927.
- [4] VAN BEIJEREN H., to appear in *J. Stat. Phys.*
- [5] GARRIDO P. L., LEBOWITZ J. L., MAES C. and SPOHN H., to appear in *Phys. Rev. A*.
- [6] BAK, P., TANG C. and WEISENFELD K., *Phys. Rev. A*, **38** (1988) 364.
- [7] LIGGETT T. M., *Interacting Particle Systems* (Spinger, New York, N. Y.) 1985.
- [8] KAWASAKI K., in *Phase Transitions and Critical Phenomena*, edited by C. DOMB and S. GREEN, Vol. 4 (Academic Press, London) 1972.
- [9] METROPOLIS M., ROSENBLUTH A. W., ROSENBLUTH M. M., TELLER A. H. and TELLER E., *J. Chem. Phys.*, **21** (1953) 1087.
- [10] KATZ S., LEBOWITZ J. L. and SPOHN H., *Phys. Rev. B*, **28** (1983) 1655; *J. Stat. Phys.*, **34** (1984) 497; VALLÉS J. L. and MARRO J., *J. Stat. Phys.*, **49** (1987) 89.
- [11] VALLÉS J. L. and MARRO J., *J. Stat. Phys.*, **43** (1986) 441.
- [12] SCHMITTMANN B., *Int. J. Mod. Phys. B*, **4** (1989) 2269.
- [13] WANG J., BINDER K. and LEBOWITZ J. L., *J. Stat. Phys.*, **56** (1989) 783.
- [14] SCHMITTMANN B. and ZIA R. K. P., preprint.