Spontaneous Fluctuation Correlations in Thermal Lattice-Gas Automata

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We construct a 19-bit lattice-gas model which is shown to exhibit spontaneous fluctuation correlations as produced in a thermal fluid system. Thus the lattice gas can be considered—in the same sense as a real fluid—as a reservoir of excitations with wavelengths and frequencies ranging from the microscopic level to the hydrodynamic scale. In particular the dynamic structure factor obtained from lattice-gas simulations is in agreement with the classical Rayleigh-Brillouin spectrum of real fluids.

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A most important function in the statistical mechanical study of fluid systems is the dynamic structure factor $S(k,\omega)$, the space and time Fourier transform of the density fluctuation autocorrelation function [1]. The importance of $S(k,\omega)$ stems from its content reflecting the dynamics of the fluid system as a reservoir of excitations over a wide range of wavelengths and frequencies, from the molecular level to the hydrodynamic scale. The susceptibility $S(k,\omega)$ can be computed from statistical mechanical theories and measured by scattering experiments and by numerical computations, e.g., molecular-dynamics simulations [1]. Recently, a new computational approach to fluid dynamics has developed: the lattice-gas automata (LGA) method [2]. LGA's have proved very efficient and powerful, e.g., for 2D and 3D weakly turbulent flows, for low-Reynolds-number complex flows, as well as for reactive systems [3]. In statistical mechanics a remarkable accomplishment of the LGA method has been the measurement of the non-Boltzmann persistence of long-time correlations evidenced with unprecedented accuracy [4]. These and the above-mentioned phenomena are well described by athermal models, i.e., single-speed LGA's without, or with trivial, energy conservation.

Obviously in order to have a full fluid-dynamics description, we must associate temperature to the lattice gas. Therefore we need a multispeed model (ideally a model with velocity distribution). A complete description fulfilling the conditions necessary to define the thermodynamic state requires (i) that mass conservation, momentum conservation, and energy conservation be satisfied by the LGA collision rules; (ii) that each conservation law hold independently (e.g., collisional energy transfers must redistribute energy among particles in a nontrivial way); and (iii) that there be no additional conserved quantities (susceptible to produce spurious invariants in LGA's [5]). Furthermore the LGA should exhibit correct hydrodynamic behavior, that is, the symmetry of the lattice must be sufficient to guarantee the correct form of the hydrodynamic equations [2]. In addition we require that, for a single-species system, all particles have the same (unit) mass, and that rest particles (particles with zero velocity) have zero energy [6]. These conditions impose that there be more than two nonzero velocities. When all these criteria are taken into account, none of the "thermal" LGA models so far proposed is fully satisfactory [7].

Here our concern is to construct a lattice-gas model with the philosophy of a classical hard-sphere fluid. We consider a two-dimensional LGA with hexagonal symmetry. Particles with unit mass undergo displacements with velocity moduli 1, $\sqrt{3}$, and 2 (in lattice unit length per time step), and have energy $\frac{1}{2}$, $\frac{3}{2}$, and 2, respectively, and rest particles have zero energy. Velocities 1 and 2 correspond to displacements by one and two lattice unit lengths, respectively, in one time step along any of the six lattice directions, and velocity $\sqrt{3}$ corresponds to displacements to the next-nearest-neighboring nodes along any of the six directions bisecting the lattice directions [see Fig. 1(a)]. Thus we have a 19-bit model residing on a triangular lattice. Within this lattice, particles obey the exclusion principle [2] and undergo collisions according to mass, momentum, and energy conservation laws. Some of the most elementary collisions are shown in Figs. 1(b)–1(e). The 19-bit model is a probabilistic LGA with symmetrical transition probability matrix and all transitions between input and output configurations are set to be equally probable for all compatible states according to basic conservations.

The microscopic evolution of the lattice gas is expressed by a set of microdynamical equations [2] which are the formal representation of the two-step sequence of collision and propagation. In the LGA implementation, the collision table is the operational realization of the collisional part of the microdynamical equations. The procedure consists of classifying all configurations according to the values of the invariants. In the collisional transitions we randomly choose an output state among all states belonging to the same class as the input state (in-

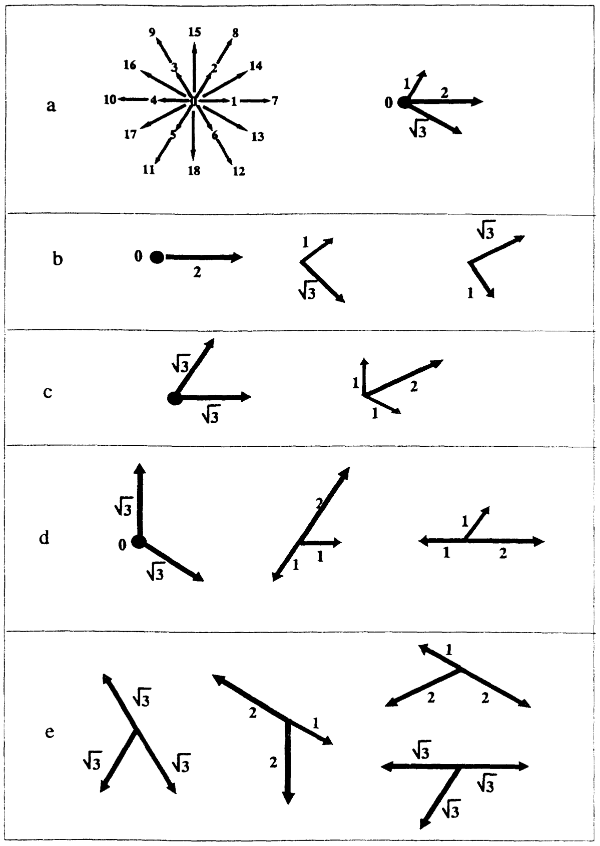

FIG. 1. The 19-bit model for thermal LGA. (a) Channel labeling and velocities on the triangular lattice. (b)-(e) Elementary configurations yielding collisions with energy transfer.

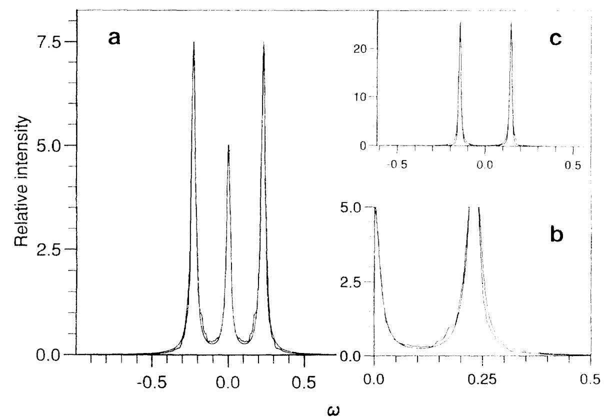

FIG. 2. The dynamic structure factor $S(k,\omega)$ as measured from spontaneous fluctuation correlations (lattice size 512 $\times$512). (a) 19-bit LGA ($k/k_0=14.422$, density per channel $n=0.317$; energy density per node, 6.74). (b) Enlargement of part of the spectrum with Lorentzian fit, Eq. (1). (c) FHP-I model ($k/k_0=14.422$, $n=0.389$): The Lorentzian fit is slightly above the measured spectrum. Horizontal scale: ω is given in reciprocal time-step units; vertical scale: relative intensity, $S(k,\omega)/\sum_{-\pi}^{\pi} S(k,\omega)\Delta\omega$, with $\Delta\omega=2\pi/2048$.

cluding the input state itself, as there is a large number of states—up to 257—in most classes) [8].

The main goal in the present work is to establish the existence of spontaneous thermal fluctuations in the 19-bit LGA model. Such fluctuations are most convincingly evidenced by the line shape of the dynamic structure factor $S(k,\omega)$. To obtain $S(k,\omega)$, we measure the space and time density fluctuations $\delta\rho(\mathbf{r},t)$ in the lattice gas based on the 19-bit model collision rules, and then we construct the density autocorrelation function. Computations are carried out under the following conditions: The system has periodic boundary conditions and is initialized with zero total momentum; thus the system is at rest and measurements are performed when the equilibrium state is reached [9]. The autocorrelation function $\langle \delta\rho_k^*(\omega) \times \delta\rho_k(\omega)\rangle$ is computed by space and time Fourier transformation of the original data over the whole lattice with angular integration over wave vectors with the same modulus and over 2048 time steps. The susceptibility $S(k,\omega)$ is treated as a spectral function, i.e., as a function of ω at fixed values of the wave number k. For each value of k, noise reduction is obtained by averaging over 400 spectra.

A typical spectrum is given in Fig. 2(a). It shows the characteristic line shape as found in real fluids where the spectral function derived from the linearized hydrodynamic equations reads (to good approximation) [1]

$$\frac{2\pi}{N}\frac{S(k,\omega)}{S(k)}=\frac{\gamma-1}{\gamma}\frac{2\chi k^2}{\omega^2+(\chi k^2)^2}+\frac{1}{\gamma}\sum_{\pm}\frac{\Gamma k^2}{(\omega\pm c_s k)^2+(\Gamma k^2)^2}, \qquad (1)$$

where $S(k)=\langle|\delta\rho_k|^2\rangle$ is the static structure factor (see comments below) and N is the number of particles. Here χ is the thermal diffusivity; $\Gamma=\frac{1}{2}[\nu+(\gamma-1)\chi]$, where ν is the longitudinal viscosity; c_s is the adiabatic sound velocity; and γ is the ratio of specific heats. Equation (1) is the long-wavelength limit of the susceptibility $S(k,\omega)$ and is expected to hold also for lattice gases in the same limit [10]: The fit of this approximation to the measured LGA $S(k,\omega)$ is shown in Fig. 2(b). We observe that the fluctuation correlations are well described by the full Rayleigh-Brillouin spectrum showing the central peak characteristic of the energy density fluctuations and the two shifted peaks characteristic of the sound modes. Similar measurements performed with the FHP-I model [11] show, as expected, that the spectrum contains only sound mode peaks [Fig. 2(c)]. We also performed fluctuation correlation measurements for the two-speed square lattice (8-bit) model [12] and for the two-speed triangular lattice ("double FHP," 12-bit) model: None of these models possesses intrinsic temperature fluctuations as evidenced by the absence of heat peak in $S(k,\omega)$ [13].

We tested the validity of the 19-bit LGA model by measuring the wave-number dependence of the frequency shift ω_s, i.e., the position of the sound peaks, and of the linewidth of both the central peak and the sound peaks. A test with the FHP-I model for the k dependence of the sound peak frequency shift was found to give excellent agreement with the theoretical prediction $\omega_s = c_s k$, with $c_s = 2^{-1/2}$ [2], as shown in Fig. 3(a). The same figure shows that the correct linear k dependence is obtained for the 19-bit model where the measured value of the sound velocity is $c_s = 1.1$. In the linearized hydrodynamic domain the half-widths of the peaks in $S(k,\omega)$ are given to good approximation by $\Delta\omega_0 = \chi k^2$ and $\Delta\omega_s = \Gamma k^2$ for the central peak and the sound peak, respectively. Thus the k^2 dependence of the linewidths, shown in Fig. 3(b),

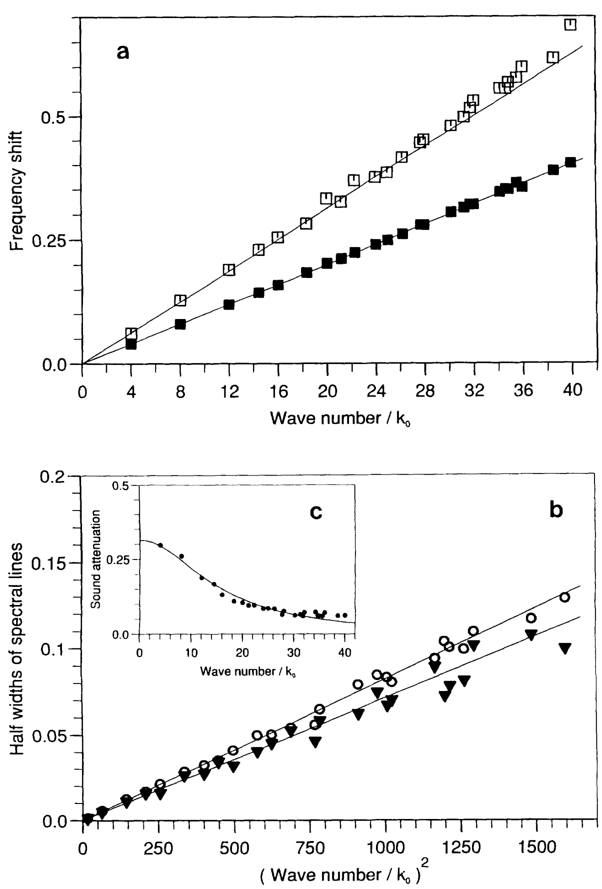

FIG. 3. k dependence of the $S(k,\omega)$ spectral features. (a) Sound peak frequency shift $\omega_s = c_s k$ (open squares, 19-bit model; solid squares, FHP-I). The lower solid line has slope $c_s = 2^{-1/2}$; the slope of the upper solid line is obtained from Eq. (1) fitted to the simulation data yielding $c_s = 1.1$. (b) Linewidth of the sound peak $\Delta\omega_s = \Gamma k^2$ (open circles) and the central peak $\Delta\omega_0 = \chi k^2$ (solid triangles). Slopes of the linear fit yield $\Gamma = 0.408$ and $\chi = 0.354$ for the 19-bit model. (c) Sound attenuation coefficient for FHP-I (solid circles); the solid curve is $\Gamma_0(1+\xi^2 k^2)^{-1}$ with $2\Gamma_0 = \nu(k=0) = 0.625$ and $\xi = 4.6$. Values are expressed in lattice units.

corroborates the validity of the 19-bit model. Furthermore the values of the transport coefficients and of the sound speed (see caption of Fig. 3) are compatible with the Boltzmann level values [10]. However, the linewidth of the FHP-I spectrum yields a value for the damping coefficient which is lower than the data obtained from sound attenuation measurements of a forced perturbation [14], indicating that the present k domain [here $4 < k/k_0 < 40$, with $k_0 = (2\pi/512)2/\sqrt{3}$ in reciprocal-lattice units] is outside the long-wavelength hydrodynamic regime. For large values of k (in real fluids, when $k\sigma$, with σ the interaction potential range, is no longer much smaller than 1) deviations from classical hydrodynamics become important: Nonlocal response renders the transport coefficients k and ω dependent [1]. Evidence of nonhydrodynamic behavior for the FHP-I model in the present wave-number range is illustrated in Fig. 3(c) showing the k dependence of the sound attenuation coefficient.

Static properties in real fluids also become k dependent at high k values, e.g., the sound velocity which is related to the reciprocal static structure factor $S(k)$. However, in the lattice gas there are no static correlations, $\langle\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')\rangle \propto \delta(\mathbf{r}-\mathbf{r}')$, and $S(k\neq 0) = \text{const}$. [Note that at $k=0$, $S(k)=0$ [15].] One has [7]

$$S(k) = \rho^{-1}\sum_j \langle(\delta n_j)^2\rangle[1-\delta(k)]\,, \tag{2}$$

with ρ the average density per node, and δn_j the density fluctuation in channel j. $S(k)$ is easily obtained by summing $S(k,\omega)$ over frequencies [16]; for both the FHP-I model and the 19-bit LGA, we find agreement with Eq. (2). We also evaluate the Landau-Placzek ratio [1] from the fit of Eq. (1) to the simulation data: The estimated value of γ is ~ 1.37.

For low k values, the situation is somewhat delicate for the lattice gas as compared to the real fluid where one assumes that a large reservoir thermalizes the sampling domain in the thermodynamic limit such that the grand ensemble applies [17]. The lattice-gas universe is finite by construction (with box-type conditions or periodic boundary conditions). Consequently the lowest k value is set by the reciprocal size of the lattice, $\sim L^{-1}$, and when k approaches this lower bound, finite-size effects can manifest and produce "unphysical" dynamical recorrelations with periodic boundary conditions. Therefore the validity of the k domain investigated here has a lower limit set at $k/k_0 = 12$ [18].

In conclusion, within the limits of the criteria imposed to comply with the requirements of a simple thermal LGA, we have constructed a minimal 2D model which can be shown to be free of known spurious invariants [19]. The 19-bit model presented exhibits actual thermohydrodynamic fluctuations as evidenced by the dynamic structure factor $S(k,\omega)$. So the LGA can be viewed—in the same sense as a real fluid—as a reservoir of excitations over a wide range of wavelengths from the *microscopic* level (the lattice mesh) to the *macroscopic* scale (the size of the lattice). The correlations dynamics is correctly described by the hydrodynamic structure factor $S(k,\omega)$; the corresponding wave-number range sets the limits of validity of the classical collective-mode behavior of the LGA.

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