Fourier's Law and the Green-Kubo Formula in a Cellular-Automaton Model

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The properties of energy transport are numerically investigated with the use of a one-dimensional cellular-automaton model called 26*R*. The validity of Fourier's law and the Green-Kubo formula for thermal conductivity κ is demonstrated for this model in the limit of large systems. Nonlinear correction to Fourier's law and the recovery of left-right symmetry are also discussed.

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To derive Fourier's law of heat conduction from dynamics remains an outstanding problem in statistical mechanics.[1] In a rigorous sense, it has been satisfactorily performed only for the Lorentz gas in the Boltzmann-Grad limit.[2] Perturbation theories to harmonic crystals failed to reproduce a thermal conductivity independent of system size. Only recently some numerical investigations appeared to suggest the convergence of a thermal conductivity in a thermodynamic limit or the validity of the Green-Kubo formula for some models with large nonlinearity.[3-5] Since these models are rather complicated, it is valuable to find a simple model system of heat conduction.

In this Letter, I present a cellular-automaton model called 26*R*, which manifests Fourier's law and the Green-Kubo formula. This model is apparently simple and purely deterministic. Neither a random nor a stochastic element enters into the definition of the dynamics except a possible contact with heat baths at the ends of the system. Moreover, all constituents involved in the model take discrete values. Hence, it is handled easily with a digital computer and errors by truncation or roundoff cannot occur. The study of heat conduction properties in cellular automata was first suggested by Pomeau.[6] In this respect, the present study may be viewed as a realization of his proposal. In general, cellular automata can be very good models to examine how statistical-mechanical concepts arise from microscopic dynamics.

Rule 26*R* is one which belongs to a family of one-dimensional cellular automata called elementary reversible cellular automata (ERCA).[7,8] An ERCA has two Boolean variables per site which evolve according to a rule written in the form

$$\sigma_i^{t+1}=f(\sigma_{i-1}^t,\sigma_i^t,\sigma_{i+1}^t)\ \mathrm{XOR}\ \hat{\sigma}_i^t\,, \tag{1a}$$

$$\hat{\sigma}_i^{t+1}=\sigma_i^t\,, \tag{1b}$$

where σ_i^t and $\hat{\sigma}_i^t$ denote the state of site i at time t each of which takes values in the set $\{0,1\}$, XOR is the "exclusive OR" operation, namely $\mu\ \mathrm{XOR}\ \nu=\mu+\nu-2\mu\nu$, and $f:\{0,1\}^3\to\{0,1\}$ is a Boolean function of three variables. This function f determines the rule, and in particular $f(\lambda,\mu,\nu)=\lambda+\nu-\mu\nu-2\lambda\nu+\lambda\mu\nu$ for rule 26*R*; indeed $\sum_{\lambda,\mu,\nu}2^{4\lambda+2\mu+\nu}f(\lambda,\mu,\nu)=26$. The reversibility of the dynamics is evident.

Energy is introduced for rule 26*R* as the additive conserved quantity Φ defined by

$$\Phi^t=\sum_i F(\sigma_i^t,\sigma_{i+1}^t,\hat{\sigma}_i^t,\hat{\sigma}_{i+1}^t) \tag{2a}$$

$$=\sum_i\{(\sigma_i^t-\hat{\sigma}_{i+1}^t)^2+(\sigma_{i+1}^t-\hat{\sigma}_i^t)^2\}\,. \tag{2b}$$

This quantity is not only conserved but also satisfies the equation of continuity:

$$F_{i,i+1}^{t+1}=F_{i,i+1}^t+J_i^t-J_{i+1}^t\,, \tag{3}$$

where $F_{i,i+1}^t=F(\sigma_i^t,\sigma_{i+1}^t,\hat{\sigma}_i^t,\hat{\sigma}_{i+1}^t)$ is the energy at time t at bond $(i,i+1)$ and

$$J_i^t=(1-2\hat{\sigma}_i^t)(\sigma_{i-1}^t-\sigma_{i+1}^t)f(\sigma_{i-1}^t,\sigma_i^t,\sigma_{i+1}^t) \tag{4}$$

is the energy flux at time t at site i. The preservation of phase-space volume is verified from the reversibility of the dynamics and the discreteness of the states. Therefore, regarding Φ as a Hamiltonian, one can construct the statistical mechanics of the model. As a result, the relation between energy per site ϕ and inverse temperature β is obtained as

$$\beta=\ln[(2-\phi)/\phi]\,. \tag{5}$$

Consider a chain of rule 26*R* with N sites under the periodic boundary condition. It has already been confirmed that this system realizes equilibrium thermodynamic behavior when N is large.[7] If one divides the chain into the sum of a subsystem consisting of a number ($\ll N$) of sites and the remaining part, which is regarded as a heat bath, the energy distribution of the subsystem becomes a canonical one. Thus, temperature is experimentally defined for this system and its values agree well with those given by Eq. (5). It has also been observed that time and ensemble averages yield the same results within the accuracy of calculations. Moreover, relaxation to the equilibrium state occurs in a short time.[9] Thus, this system shows good microcanonical properties.

In the numerical experiments of energy transport, sto-

chastic heat baths are attached to both ends of the chain in place of the periodic boundary condition. At every time step, after the updating of sites 1 through N according to the rule (1), sites 0 and $N+1$ choose their values with the conditional probabilities such that

$$P(\sigma_0,\hat{\sigma}_0 \mid \sigma_1,\hat{\sigma}_1) \propto \exp[-\beta_L F(\sigma_0,\sigma_1,\hat{\sigma}_0,\hat{\sigma}_1)], \quad (6a)$$

$$P(\sigma_{N+1},\hat{\sigma}_{N+1} \mid \sigma_N,\hat{\sigma}_N) \propto \exp[-\beta_R F(\sigma_N,\sigma_{N+1},\hat{\sigma}_N,\hat{\sigma}_{N+1})], \quad (6b)$$

where β_L $(=T_L^{-1})$ and β_R $(=T_R^{-1})$ denote the inverse temperature at the left and right ends, respectively. If one sets $\beta_L=\beta_R$, the equilibrium behavior is again realized in almost the same manner as in the periodic chain. The only difference is that the present case is canonical with given β, whereas the case of the cyclic chain is microcanonical with given ϕ. This realization of the equilibrium behavior guarantees that the above heat-bath procedure works well. In these equilibrium situations, there is, of course, no temperature gradient and the energy flux vanishes on the average. On the other hand, if $\beta_L \neq \beta_R$, after some transient the system comes to a stationary state where the transport of energy occurs. Figure 1 illustrates the temperature gradient formed in the system under such a condition. Here the temperature T $(=\beta^{-1})$ at bond $(i,i+1)$ has been determined via Eq. (5) from the observed value of the mean energy at the bond. The energy distribution at each bond is only slightly deformed from the canonical distribution of corresponding temperature to support the heat current. Thus, local equilibrium holds for this system. Remarkable in Fig. 1 is the fact that the temperature jump at the ends of the system is very small. It can be observed in the system of $N=100$, but is hardly seen when $N=200$. This property is a distinctive characteristic of rule 26R. Other rules in ERCA's do show a temperature jump, if they can form a temperature gradient. Indeed, most of the rules cannot so much as form a temperature gradient. Figure 1 also shows that the profile of the local temperatures is not a straight line and that it varies when T_L and T_R are interchanged. The former implies a strong temperature dependence of the thermal conductivity: The lower the temperature is, the larger the conductivity is. The latter is an outcome of the lack of reflection invariance in rule 26R.

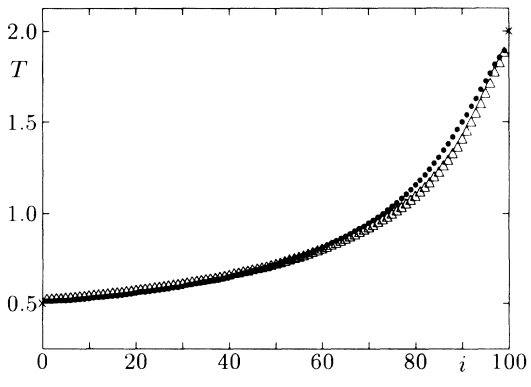

FIG. 1. Temperature gradient formed in the system. Solid circles indicate local temperatures when $T_L=0.5$ and $T_R=2.0$ (shown by the crosses). Triangles are the result with the temperature values of the heat baths interchanged, which are displayed left-right inverted for convenience. These data were obtained by time average with 10^7 iterations. The system size is $N=100$.

Using the above implements, I have checked the validity of Fourier's law

$$\langle J \rangle = -\kappa \nabla T. \quad (7)$$

The temperature gradient ∇T has been evaluated locally around points showing local temperature $T \simeq 1.0$ under various imposed temperature values of the heat baths. At the same time, the average energy flux $\langle J \rangle$ has been calculated as the time average of Eq. (4). The result thus obtained is displayed in Fig. 2, which exhibits a finite slope at the origin. The negative of this slope yields the thermal conductivity, estimated at $\kappa=0.214 \pm 0.010$. Away from the origin, one can observe a certain systematic deviation from linearity. This indicates the existence of a higher-order nonlinear correction to Eq. (7), e.g., terms proportional to $(\nabla T)^2$, $(\nabla T)^3$, etc. The figure is not symmetric with respect to the origin because rule 26R has no reflection invariance as has been stated. However, this symmetry is macroscopically restored in the linear regime, namely in the limit of large systems for fixed values of the boundary temperature. This is quite analogous to the recovery of isotropy at low Mach number in lattice-gas automata on a hexagonal lattice.[10]

It is necessary to study the N dependence of the energy flux in order to certify that a system has normal heat conduction properties. Equation (7) is equivalent to

$$N\langle J \rangle = -\int_{T_L}^{T_R} \kappa(T) dT. \quad (8)$$

Thus, if Eq. (7) is exact, the left-hand side of the above

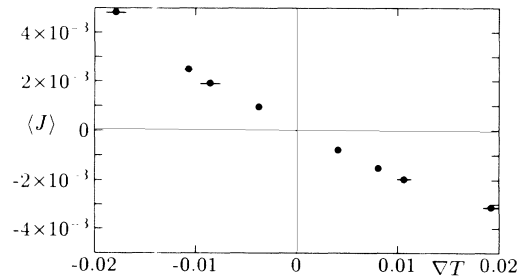

FIG. 2. Average energy flux $\langle J \rangle$ as a function of the local temperature gradient ∇T at the point with $T=1.0$. Five trials each of 2×10^6 iterations for the system of size $N=101$ have been done for each point.

equation should not depend upon N when T_L and T_R are fixed. However, if nonlinear correction exists, $N\langle J\rangle$ should vary as const$+O(|T_R-T_L|/N)$. I have computed this quantity for a set of values T_L and T_R and the values interchanged. Because of the lack of left-right inversion symmetry in rule 26R, these two cases generally yield different magnitudes of the flux. However, as observed from Fig. 3, in both cases the absolute values of the flux converge to the same value in the limit of large N. This result establishes the validity of Fourier's law in the large-N limit. Most of the deviation at relatively small N is attributed to the nonlinear correction to Eq. (7). That is, the flow $\langle J\rangle$ converges rapidly into intrinsic bulk behavior represented by a function of T and ∇T but not of N. When N is made large with fixed boundary temperature values, there only remains the first term of the function expanded with respect to ∇T, which is just Fourier's law (7). In Fig. 2, actual finite-size effects are distinguishable only for $N \leq 20$ and the bulk behavior dominates the system even for $N \simeq 50$.

The Green-Kubo formula expresses transport coefficients as integrals of autocorrelation functions in equilibrium states. Applied to the present case, the thermal conductivity is represented as

$$\kappa=\frac{1}{NT^2}\sum_{t=0}^{\infty}\langle J(0)J(t)\rangle\left(1-\frac{\delta_{t0}}{2}\right), \tag{9}$$

where $J(t)=\sum_{i=1}^{N}J_i^t$, angular brackets denote an equilibrium average, and the factor $1-\delta_{t0}/2$ is necessary because of the full discreteness of time.

To evaluate Eq. (9), I have calculated the energy-flux autocorrelation function $\langle J(0)J(t)\rangle$ for two types of chains, one with the periodic boundary condition and the other with heat baths at its ends. In the cyclic or microcanonical case, the total energy has been chosen so as to make the inverse temperature β determined by Eq. (5) closest to 1.0. In the canonical system in contact with the heat baths, the inverse temperatures of the heat baths have been set as $\beta_L=\beta_R=1.0$ at both ends. These two cases have yielded the same result for the autocorrelation function within the accuracy of the calculation. However, fluctuation in the data obtained is large for the system with the heat baths compared with the cyclic chain. This is just a general distinction between canonical and microcanonical ensembles. In regard to the N dependence, the normalized autocorrelation function $N^{-1}\langle J(0)J(t)\rangle$ obtained for $N=100$ is almost unchanged for larger N in both types of systems. This rapid convergence provides further evidence that bulk behavior is predominant even for relatively small N. The result for the microcanonical case with $N=2000$ is displayed in Fig. 4. The energy-flux autocorrelation function shows a fast damp for small t and a negative exponential tail for large t, which is manifested by the semilogarithmic plot of the inset in Fig. 4. Consequently, the convergence of the series in Eq. (9) is satisfactory, which results in $\kappa=0.213\pm0.005$. This result agrees in an excellent manner with the value determined via Fourier's law mentioned earlier. Thus, the validity of the Green-Kubo formula has been confirmed for rule 26R.

The fact that the Green-Kubo formula holds for rule 26R means the realization of thermodynamic fluctuations in this model. Since equilibrium and relaxation properties have already been established for this model, rule 26R exhibits all of what is generally called the thermodynamic behavior.[11] Thus, this model will provide a valuable example for the investigation of the origin of

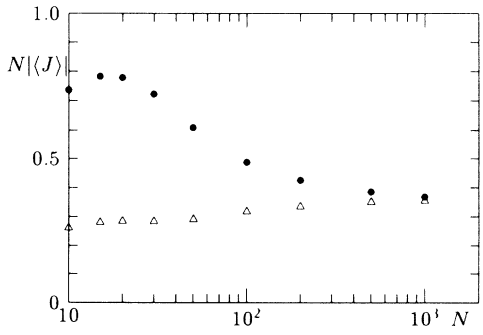

FIG. 3. Absolute values of the average energy flux multipled by the system size, $N|\langle J\rangle|$, as a function of N. Temperatures of the heat baths are fixed to $T_L=2.0$ and $T_R=0.5$ (solid circles) and $T_L=0.5$ and $T_R=2.0$ (triangles).

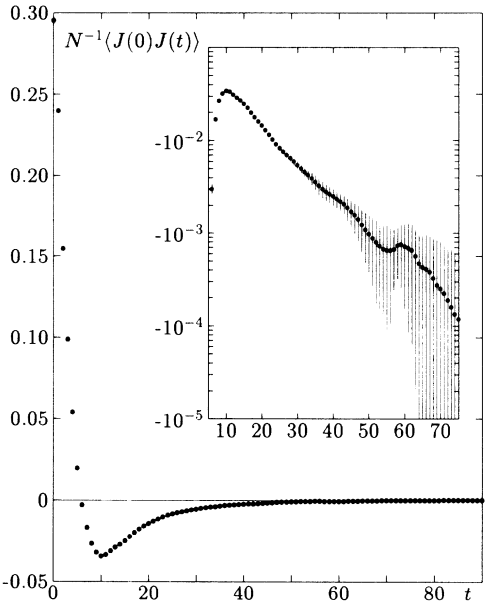

FIG. 4. The normalized energy-flux autocorrelation function calculated for the system with the periodic boundary condition. The solid circles denote the average values over twenty trials each of 10^6 iterations for the system with $N=2000$ and $\Phi=1076$, which yields $\beta=0.9997$ via Eq. (5). Inset: Semilogarithmic plot of the same quantities.

the thermodynamic behavior. In rule 26R, the energy can be regarded as particles. Such a particle propagates with a constant speed by itself, and its velocity varies through collisions with other particles. Because there is no quantity corresponding to momentum in rule 26R, a collision changes not only the velocity of each particle but also the total velocity. This is in contrast to the fact that a solitonlike solution can hardly change its motion in Hamiltonian systems.[12] This may be the reason why rule 26R can show such beautiful properties of the thermal conductivity. A detailed analysis of the scattering rule will be reported elsewhere.

In summary, I have numerically proved that the cellular-automaton model 26R manifests normal heat conduction properties. The energy flux is proportional to the local temperature gradient in the stationary local equilibrium states, which is Fourier's law. The thermal conductivity at $\beta=1.0$ was calculated as the negative of the slope at the origin of the energy flux versus the local temperature gradient. In the large-N limit, the energy flux was shown to be proportional to N^{-1}. This is evidence that the thermal conductivity depends only upon temperature in the thermodynamic limit. Moreover, it was shown that convergence to bulk behavior is achieved in a relatively small system. The thermal conductivity was independently calculated via the Green-Kubo formula from the equilibrium energy-flux autocorrelation functions and the value shows excellent agreement with that from Fourier's law. It is concluded from these observations that this model is a thermodynamic system.

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