Anomalous heat conductivity induced by finite size and non-Markovian dynamics

Xiao-Peng Zhang and Jing-Dong Bao*
Department of Physics, Beijing Normal University, Beijing 100875, China
(Received 9 January 2006; published 23 June 2006)

Heat conduction in a one-dimensional non-Markovian damping channel between two heat baths separated by a finite distance is studied numerically. It is found that the Fourier heat law is not obeyed for a finite-size underdamped channel under a Gaussian white noise and the coefficient of heat conductivity is a nonmonotonic function of the channel length in the sub-Ohmic damping case. The key dynamic feature is that the system does not approach the stationary state when it arrives at the cold bath for the former, and the system exhibits different diffusive behaviors from ballistic diffusion to subdiffusion at initial and asymptotic periods of time for the latter. We evaluate a damping-dependent critical separation size between two heat baths above which the heat conductivity becomes independent of the separation.

DOI: 10.1103/PhysRevE.73.061103 PACS number(s): 05.20.−y, 44.10.+i, 05.45.−a

I. INTRODUCTION

An excellent situation for linking the stochastic process with thermodynamics is heat conductivity [1–5]. It is interesting to seek which systems obey the Fourier heat law, i.e., the coefficient of heat conductivity is independent of the channel length as if the temperature difference between the hot and cold heat baths is small [5–14]. The two typical models have been proposed such as the two-dimensional (2D) billiard gas channel and the one-dimensional (1D) dynamical heat channel, where the kinetic energy of system is conserved anywhere within the channel and changes only at collisions with heat baths. Previous works for the billiard gas channel have predicted that the linear instability in the polygonal billiards is sufficient for energy transport, obeying the Fourier heat law [1,4–6,11]. Some authors suggested that nonintegrability was necessary but not sufficient to guarantee normal heat conductivity in the 1D lattices model [12]. Moreover, it has been proved that the momentum conservation leads to anomalous heat conductivity in the 1D lattice model [7].

In the studies of anomalous heat conduction based on the dynamical heat channel model, the diffusive behavior of energy carriers within the channel is usually assumed to be either subdiffusion or superdiffusion. The mean first passage time from the hot bath to cold one is used to calculate heat current as energy exchange in unit time. Nevertheless, the time-dependent transport process has not been presented yet in detail, and the possible mechanism of anomalous heat conductivity needs to be investigated. In recent years, there has been great interest in anomalous diffusion, which has been found in many situations [15]; therein, non-Markovian memory damping and its corresponding thermal colored noise play a critical role in the transport. Application to the heat conductivity should be a subject of interest.

In this paper we would like to explore a possible origin of anomalous heat conductivity in view of the time-dependent transport process. The coefficient of heat conductivity is calculated via Langevin simulation, and the effects of finite size and non-Ohmic memory damping are discussed. A relation between the channel length and the damping strength is proposed in order to distinguish normal and anomalous heat conductivities.

II. THERMAL CHANNEL DESCRIBED BY GENERALIZED LANGEVIN EQUATION

We consider each energy carrier with mass m starting from the warm heat bath and stopping at the cold one, the motion of carrier in the channel is assumed to obey a 1D generalized Langevin equation (GLE) [15–20],

$$m\ddot{x}(t) + m\int_0^t \gamma(t-t')\dot{x}(t')dt' = \xi(t), \tag{1}$$

where $\gamma(t)$ is the memory damping kernel, $\xi(t)$ is a stationary thermal noise with zero-mean $\langle\xi(t)\rangle=0$ and obeys the fluctuation-dissipation theorem $\langle\xi(t)\xi(t')\rangle=m\gamma(t-t')k_BT(x)$, k_B is the Boltzmann constant, and $T(x)$ is the local temperature of the heat channel. The memory damping kernel function reads

$$\gamma(t) = \frac{1}{m}\frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega}\cos\omega t, \tag{2}$$

where $J(\omega)$ is connected to the frequency-dependent damping coefficient of the environmental oscillators $\gamma(\omega)$ and is given by $J(\omega)=m\omega\gamma(\omega)$ [19]. For the Ohmic or Markovian damping, spectral density is expressed as $J(\omega)=m\gamma\omega$ and then the damping kernel is reduced to $\gamma(t)=2\gamma\delta(t)$. In the non-Ohmic damping environment, $J(\omega)=m\gamma_\delta(\omega/\tilde{\omega})^{\delta-1}\omega$ [19], where $\tilde{\omega}$ denotes a reference frequency allowing for the damping constant $m\gamma_\delta$ to have the dimension of a viscosity for any power exponent δ. In the force-free case, the mean square displacement of the particle reads $\langle x^2(t)\rangle \propto t^\delta$ with subdiffusion for $0<\delta<1$, normal diffusion for $\delta=1$, superdiffusion for $1<\delta<2$, and ballistic diffusion for $\delta=2$.

Let us consider a situation where the particle is initially located at the hot end of the 1D channel with a positive velocity distribution as

*Corresponding author. Electronic address: jdbao@bnu.edu.cn

$$P(v) = \frac{m|v|}{k_B T} \exp\left(-\frac{mv^2}{2k_B T}\right), \tag{3}$$

where the absolute value of v is conveniently taken to eject back the particle to heat channel after a one-time collision with the warm bath. The transport process will be stopped when the test particle reaches the cold bath. The thermodynamic limit is obtained upon taking a long channel length and the number density of test particles is kept to be fixed.

In order to investigate the thermodynamic properties of heat transport in a convenient way, we fix the temperatures of two heat baths as T_0 and $T_1=T_0+\Delta T$, where the temperature difference ΔT is assumed to be small. The linear temperature field applicable for small temperature differences [2,11] is then taken as

$$\nabla T = \frac{T_0 - T_1}{L} = -\frac{\Delta T}{L}, \tag{4}$$

$$T(x) = T_1 - \frac{x}{L}(T_1 - T_0), \tag{5}$$

where L is the length of heat channel. Since the kinetic energy of the particle exchanges only at collision with each bath, we define the heat transfer by the ith collision with the cold bath,

$$Q_i = \Delta E_i = E_i^{in} - E_i^{out}, \tag{6}$$

where E_i^{in} and E_i^{out} are the energies of the ith particle before and after collision with the cold bath. The average heat flux and the coefficient of heat conductivity [1,2,4–6] are

$$J = \frac{\langle Q(t)\rangle}{t}, \tag{7}$$

and

$$\kappa = -\frac{J}{\nabla T}, \tag{8}$$

where $\langle Q(t)\rangle$ is the ensemble average over the heat transfer $Q(t)$ during the period t of time.

For an ensemble of noninteracting particles, the heat flux is written as $J_{ens}=NJ(L)$ [4]. It is reasonable to assume that the number of energy carriers is proportional to the system's size, so we take into account the number of carriers N being also proportional to L. According to the Fourier heat law, the coefficient of heat conductivity κ is independent of the temperature gradient ∇T when the applied temperature difference is small. This requires the heat flux J to be proportional to the temperature gradient.

In the Langevin simulations, the test particle starts from the hot bath and will be reflected by it (reflecting boundary) with an inverse velocity if it returns to the hot bath; the process is stopped as the test particle arrives at the cold end (absorbing boundary) of thermal channel. This implies that the heat transfer should be influenced strongly by the channel length during a finite period of time. The parameters used in this work are $m=1$, $k_B=1$, $T_0=1$, $T_1=1.05$, $\gamma_\delta=0.1$, the number density of test particles is $N/L=10^3$, and the time step $\Delta t=0.01$. In order to verify whether the heat conductivity is normal, we have to look at the heat conduction scaling with the channel length. The heat flux $J(L)$ of a single test particle and then the coefficient of heat conductivity $\kappa=-J_{ens}/\nabla T$ requires numerical calculation.

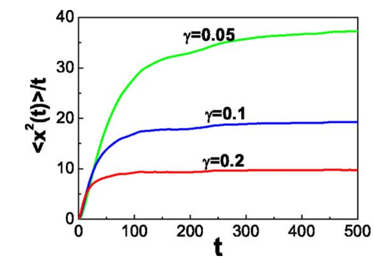

FIG. 1. (Color online) Mean square displacement of a normal diffusing particle divided by time for various damping strengths.

III. EFFECTS OF FINITE SIZE AND NON-MARKOVIAN MEMORY

A. Transient heat conductivity due to finite size

First we study the influence of finite size of thermal channel on the heat conductivity where the noise is considered to be a Gaussian white one. The GLE (1) reduces to a Markovian Langevin equation with $\gamma(t)=2\gamma\delta(t)$. It is well known that the diffusive behavior of a free Brownian particle driven by the Gaussian white noise is normal at long times, i.e., the mean square displacement (MSD) reads $\langle x^2(t)\rangle=2Dt$, where D is the diffusion coefficient. It is expected that the normal heat conductivity appears in the thermodynamic limit ($L\to\infty$), because the system can relax to the stationary state in this case.

All quantities plotted here and below are dimensionless. In Fig. 1, we plot the MSD of a force-free particle divided by time for various damping strengths. This quantity is used to check whether the system has arrived at the stationary state. At the initial period of time, the MSD increases with time faster than the linear law and shows ballistic diffusion; moreover, normal diffusion is realized in the long time limit. The time required for the system arriving at the stationary state is defined as the relaxation time, which is proportional to the inverse of damping strength for the regular Brownian dynamics.

Figure 2 shows the coefficient of heat conductivity κ as a function of the channel length L for various damping

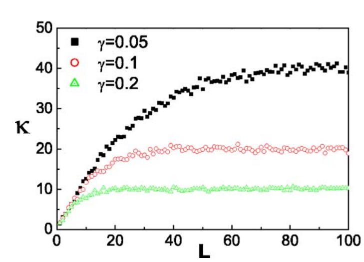

FIG. 2. (Color online) The heat conductivity κ as a function of channel length L for various damping strengths.

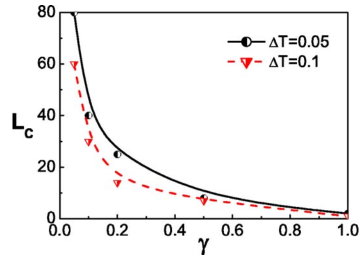

FIG. 3. (Color online) The critical channel length L_c as a function of the damping strength γ.

strengths. It is seen that the heat conductivity increases with increasing channel length in the case of small L and approaches a constant when the value of L is large enough. Furthermore, the coefficient of heat conductivity increases with decreasing damping strength. This implies that the dissipation is obstructive to the heat conductivity. Here we define a critical length L_c above which the heat conductivity is independent of the channel length. It is remarkable that the critical length needs to be large in the underdamped cases. Our results show that the Fourier heat law is not valid, even for a normal diffusing system, if the channel's size is finite and the normal heat conductivity exhibits only in the thermodynamic limit.

In Fig. 3, we plot the critical length L_c as a function of the damping strength γ at fixed temperature difference between two heat baths. It is seen that the value of critical length decreases with increasing damping and becomes short when the temperature difference increases. From this figure we can estimate the behavior of heat conduction, which is normal above the curve, indicating the thermodynamic limit, and might be anomalous one below the curve, exhibiting finite size effect.

Let us consider the heat conduction in the presence of ratchet potential [21,22] between two heat baths,

$$V(x) = \begin{cases} \dfrac{V_0}{\alpha L_0}x, & x \in [0, \alpha L_0) \\ \dfrac{V_0}{(1-\alpha)L_0}(L_0 - x), & x \in [\alpha L_0, L_0), \end{cases}$$

where L_0, V_0, and α denote the periodic length, the barrier height, and the asymmetrical parameter of the ratchet potential, respectively.

In Fig. 4(a), we plot the coefficient of heat conductivity as a function of the channel length L for various barrier heights V_0 at fixed $L_0=1$ and $\alpha=0.8$. It is seen that the effect of finite size is still exhibited in the ratchet channel. Namely, the transient heat conductivity increases with increasing the channel length and the coefficient of heat conductivity approaches a constant in the case of large L. Figure 4(b) shows the dependence of heat conductivity on V_0. Upon inspection, we find a prominent result: κ is a nonmonotonic function of V_0. As it is known that the effective potential should be tilted along the slow direction of the ratchet if the multiplicative noise (position-dependent temperature here) is changed into an additive noise [23], there exists a directed current between the hot and cold baths. This is called the ratchet effect. The

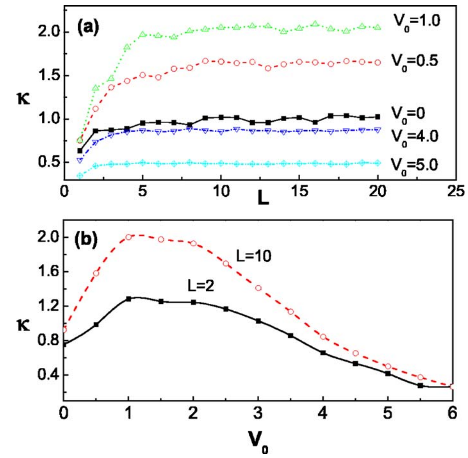

FIG. 4. (Color online) The heat conductivity κ in the presence of ratchet potential with $\alpha=0.8$ vs the channel length L in (a) and the barrier height V_0 in (b).

selective role of the ratchet potential is weak for small V_0; however, the carrier requires the potential for large V_0 to be overcome and thus the directed current is decreased. Therefore, the directed dynamical transport helps the heat conductivity at a finite barrier of ratchet and thus the coefficient of heat conductivity varies nonmonotonously with the ratchet's barrier.

B. Influence of non-Markovian dynamics on heat conduction

One of the dynamical sources of anomalous diffusion is due to nonlocality in time, such as the velocity of the particle having a memory effect. The non-Ohmic damping mechanism is frequently used to discuss anomalous diffusion. Here we consider the behavior of heat conduction in the non-Ohmic damping environment for a finite thermal channel.

We apply the inverse Fourier transform technique [24] to simulate numerically GLE (1) with the non-Ohmic memory damping. In the ω Fourier space, the correlation function of noise reads

$$\langle \xi(\omega)\xi(\omega')\rangle = 2\pi\gamma(\omega)\delta(\omega+\omega'), \tag{9}$$

where $\xi(\omega)$ and $\gamma(\omega)$ are the Fourier transforms of $\xi(t)$ and $\gamma(t)$, respectively. We discretize first the time in $N=2^n$ intervals of mesh size Δt. This mesh size can be taken to be the smallest time scale associated with the problem at hand. The discrete Fourier version of the correlation is given by

$$\langle \xi(\omega_\mu)\xi(\omega_\nu)\rangle = \gamma(\omega_\mu)N\Delta t\,\delta_{\mu+\nu,0}. \tag{10}$$

Then the noise term in the Fourier space is written as

$$\xi(\omega_\mu) = \sqrt{N\Delta t\,\gamma(\omega_\mu)}\,\alpha_\mu, \quad \mu = 1, \ldots, N-1$$

$$\xi(\omega_0) = \xi(\omega_N), \tag{11}$$

where α_μ are the Gaussian random numbers with zero mean and correlation $\langle\alpha_\mu\alpha_\nu\rangle = \delta_{\mu,-\nu}$.

In Fig. 5, we plot the coefficient of heat conductivity as a function of the channel length for two kinds of power exponents $\delta=0.5$ and $\delta=0.3$. The result shows a nonmonotonic

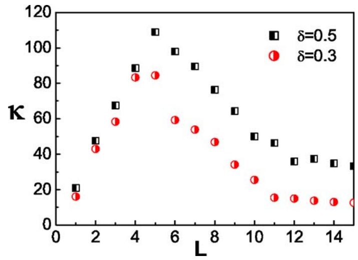

FIG. 5. (Color online) The heat conductivity κ as a function of the length L of sub-Ohmic damping channel with two kinds of power exponents $\delta=0.3$ and $\delta=0.5$.

varying behavior with the channel length. For a finite-size channel, the heat conductivity increases with the increase of channel length, because the diffusion is faster than the linear behavior due to the transient process. If the size of dynamical channel is large enough, the heat conductivity should show a convergent behavior, i.e., $\kappa \propto L^{\beta}$ with $\beta<0$. The smaller the value of δ is, the faster the heat conductivity decreases. As L goes to infinity, the heat conductivity approaches vanishing. This is interesting that the present dynamical channel becomes a thermal insulator in the thermodynamic limit of $L \to \infty$.

The size-dependent heat conductivity is shown in Fig. 6 for $\delta=1.3$ and $\delta=1.5$. The finite size effect is observed clearly in the case of small L, which originates from the diffusive behavior of the particle at the transient process. If the size of the thermal channel is large enough, the heat conductivity increases with channel length in the power form $\kappa \propto L^{\beta}$. Here the exponent β is connected to the non-Ohmic exponent δ with an approximate formula $\beta=2-2/\delta$ [3]. Anomalous heat conduction with a divergent behavior L^{β} $(0<\beta<1)$ has been proved in the 1D billiard models with triangles whose interangles are rational multiples of π [6].

Ballistic diffusion can be realized in the non-Markovian Brownian dynamics driven by either a broad-band colored noise [16] or a harmonic velocity noise [18]. The MSD increases with the square of time, which is the limit of thermal superdiffusion. The heat conductivity is shown in Fig. 7. The finite size effect is still shown in the case of small L. Note that the heat conductivity increases linearly with channel length when L is large enough. Such behavior has been observed in the harmonic lattice [27], because the phonon transports ballistically in the lattice. The heat conductivity diverges in the thermodynamic limit.

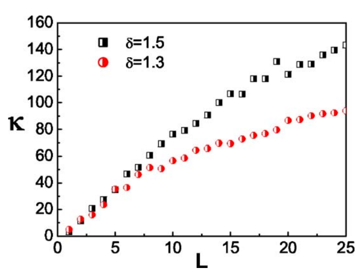

FIG. 6. (Color online) The heat conductivity κ as a function of channel length L with two kinds of power exponents $\delta=1.3$ and $\delta=1.5$.

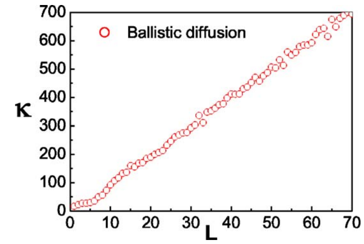

FIG. 7. (Color online) The heat conductivity κ as a function of channel length L in the case of ballistic diffusion.

The motion of the present energy carriers should mainly be thermal diffusion, since the temperature difference between two heat baths is considered to be small. In order to analyze the dependence of the heat conductivity on the channel length, we write the mean square displacement of the particle subjected to a non-Ohmic damping, i.e.,

$$\langle \Delta x^2(t) \rangle = 2\frac{k_B \bar{T}}{m} t^2 E_{2-\delta,3}[-(\omega_\delta t)^{2-\delta}], \tag{12}$$

where $\bar{T}$ is the average temperature, and we have used the generalized Mittag-Leffler function defined by the series expansion $E_{\alpha,\beta}(x)=\sum_{n=0}^{\infty} x^n/\Gamma(\alpha n+\beta)$ [25]. All the above results can be understood well from the concept of the mean first passage time from the hot bath to the cold bath.

If the thermal channel is short, the particle arrives quickly at the cold bath. During a very short period of time, Eq. (12) is approximately rewritten as

$$\langle \Delta x^2(t) \rangle \simeq 2\frac{k_B \bar{T}}{m\Gamma(3)} t^2, \tag{13}$$

and then the mean first passage time is given by $\langle t_{LR} \rangle \simeq [m\Gamma(3)/(2k_B\bar{T})]^{1/2} L$. According to the definition of the heat conductivity, $\kappa=-NJ/\nabla T$ with the current $J=\Delta T/(2\langle t_{LR}\rangle)$, we obtain the coefficient of heat conductivity as $\kappa=cL$, where c is a constant. This implies that the coefficient of heat conductivity increases linearly with channel length for a short thermal channel.

On the other hand, the test particle should require long times to arrive the cold bath if the thermal channel is long. At long times, we have

$$\langle \Delta x^2(t) \rangle \simeq 2\frac{k_B \bar{T}}{m} \frac{\omega_\delta^{\delta-2}}{\Gamma(1+\delta)} t^{\delta}, \tag{14}$$

and $\langle t_{LR} \rangle \simeq [m\Gamma(1+\delta)/(2k_B\bar{T}\omega_\delta^{\delta-2})]^{1/\delta} L^{2/\delta}$, so that $\kappa=cL^{2-2/\delta}$. This leads to a divergent result for the heat conductivity if $\delta>1$. More importantly, it is shown that the coefficient of heat conductivity is a nonmonotonic function of the channel length if $\delta<1$.

IV. CONCLUSION

We have investigated the effects of finite size and non-Markovian memory damping on the heat conduction in the one-dimensional dynamical thermal channel. Our results have shown that the Fourier law for the heat conduction cannot be obeyed even for a normal diffusing system and which is valid only in the thermodynamic limit, i.e., the infinite size of thermal channel. This is due to the fact that the nature of time-dependent diffusive behavior for Langevin dynamics varies when the damping strength changes. We have defined a critical length above which the heat conductivity is independent of channel length. Moreover, we have found that the directed transport of energy carrier can help heat conduction in the presence of ratchet potential. Indeed, anomalous heat conductivity also exhibits in a non-Markovian memory damping channel with non-Ohmic form even in the thermodynamic limit; the heat conductivity is a nonmonotonic function of channel length in the sub-Ohmic damping case. It is reported that the anomalous heat transport process has been observed in many real physical systems, such as the binary hard sphere model [26], the harmonic lattice [27], and in single wall nanotubes [28]. Furthermore, anomalous heat conduction should have an extensive application in the innovation of novel thermal devices.

ACKNOWLEDGMENTS

This work was supported by the Specialized Research Fund under Grant No. 20050027001 and the National Natural Science Foundation of China under Grant No. 10235020.

[1] For a review, see S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[2] D. Alonso, R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. Lett. **82**, 1859 (1999).
[3] B. Li and J. Wang, Phys. Rev. Lett. **91**, 044301 (2003).
[4] D. Alonso, A. Ruiz, and I. deVega, Phys. Rev. E **66**, 066131 (2002).
[5] S. Denisov, J. Klafter, and M. Urbakh, Phys. Rev. Lett. **91**, 194301 (2003).
[6] B. Li, L. Wang, and B. Hu, Phys. Rev. Lett. **88**, 223901 (2002).
[7] O. Narayan and S. Ramaswamy, Phys. Rev. Lett. **89**, 200601 (2003).
[8] P. L. Garrido, P. I. Hurtado, and B. Nadrowski, Phys. Rev. Lett. **86**, 5486 (2001).
[9] O. V. Gendelman and A. V. Savin, Phys. Rev. Lett. **92**, 074301 (2004).
[10] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998).
[11] B. Li, G. Casati, and J. Wang, Phys. Rev. E **67**, 021204 (2003).
[12] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **61**, 3828 (2000).
[13] J. S. Wang and B. Li, Phys. Rev. E **70**, 021204 (2004).
[14] G. Casati and T. Prosen, Phys. Rev. E **67**, 015203(R) (2003).
[15] For a review, see R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).
[16] J. D. Bao and Y. Z. Zhuo, Phys. Rev. Lett. **91**, 138104 (2003).
[17] J. D. Bao, Phys. Rev. E **69**, 016124 (2004).
[18] J. D. Bao, Y. L. Song, Q. Ji, and Y. Z. Zhuo, Phys. Rev. E **72**, 011113 (2005).
[19] U. Weiss, *Quantumn Dissipative Systems*, 2nd ed. (World Scientific, Singapore, 1999).
[20] J. D. Bao, H. Y. Wang, Y. Jia, and Y. Z. Zhuo, Phys. Rev. E **72**, 051105 (2005).
[21] P. Reimann, Phys. Rep. **361**, 57 (2002).
[22] J. D. Bao and Y. Z. Zhuo, Phys. Lett. A **239**, 238 (1998).
[23] M. Büttiker, Z. Phys. B: Condens. Matter **68**, 161 (1987); J. D. Bao, Y. Z. Zhuo, and X. Z. Wu, Phys. Lett. A **217**, 241 (1996).
[24] K. Lü and J. D. Bao, Phys. Rev. E **72**, 067701 (2005).
[25] N. Pottier, Physica A **317**, 371 (2002).
[26] P. Grassberger, W. Nadler, and L. Yang, Phys. Rev. Lett. **89**, 180601 (2002).
[27] A. J. O'Connor and J. L. Lebowitz, J. Math. Phys. **15**, 692 (1974).
[28] S. Maruyama, Physica B **323**, 193 (2002); P. Grassberger and L. Yang, e-print cond-mat/0204247.