Anomalous Heat Conduction and Anomalous Diffusion in One-Dimensional Systems

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We establish a connection between anomalous heat conduction and anomalous diffusion in one-dimensional systems. It is shown that if the mean square of the displacement of the particle is $\langle \Delta x^2 \rangle = 2Dt^\alpha (0 < \alpha \leq 2)$, then the thermal conductivity can be expressed in terms of the system size L as $\kappa = cL^\beta$ with $\beta = 2 - 2/\alpha$. This result predicts that normal diffusion ($\alpha = 1$) implies normal heat conduction obeying the Fourier law ($\beta = 0$) and that superdiffusion ($\alpha > 1$) implies anomalous heat conduction with a divergent thermal conductivity ($\beta > 0$). More interestingly, subdiffusion ($\alpha < 1$) implies anomalous heat conduction with a convergent thermal conductivity ($\beta < 0$), and, consequently, the system is a thermal insulator in the thermodynamic limit. Existing numerical data support our results.

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Does heat conduction in one-dimensional (1D) systems obey the Fourier law? If it does, what are the necessary and sufficient conditions? If it does not, then what is the reason for this and how does the thermal conductivity diverge or converge with the system size L? These questions have attracted increasing attention in recent years [1–21]. Although some progress has been achieved, many puzzles remain. For example, in an attempt to establish a connection between heat conduction and the underlying microscopic dynamics, some controversial examples exist. In their model Casati *et al.* [2] show that at onset of global chaos heat conduction crosses over from an abnormal one to a normal one obeying the Fourier law. It is thus concluded that chaos is a deciding factor. Later on, in order to show that exponential instability is a necessary condition, Alonso *et al.* [12] studied the heat conduction in a Lorentz gas channel, a quasi-1D billiard with circular scatterers, and found that heat conduction obeys the Fourier law. However, the results from 1D Ehrenfest gas channels [15], in which the Lyapunov exponent is zero, show that the Fourier heat law might not have any direct connection to the underlying dynamical chaos, because heat conduction can be normal and abnormal, depending on whether or not disorder is introduced.

Recently, a quasi-1D triangle billiard model, which consists of two parallel lines of length L at distance d and a series of triangular scatterers, has been introduced and studied[16]. In this model, no particle can move between the two reservoirs without suffering elastic collisions with the triangles. Therefore this model is analogous to the Lorentz gas channel studied in [12] with triangles instead of disks, and the essential difference is that in the triangular model the dynamical instability is linear and therefore the Lyapunov exponent is zero. It is found that the motion inside the irrational triangle channel (the internal angles are irrational multiples of π) is diffusive and has a normal heat conduction. Therefore deterministic diffusion and normal heat transport, which are usually associated to full hyperbolicity, can take place in systems without exponential instability. Another example is the Fermi-Pasta-Ulam (FPU) model [4], which has nonzero Lyapunov exponent; however, the heat conduction in this model does not obey the Fourier law.

The heat conduction in the rational triangle model (the internal angles are rational multiples of π) and in the FPU model is anomalous and does not obey the Fourier law; the thermal conductivity κ diverges with system size L as L^β with $\beta = 0.22$ for the rational triangle model [16] and $0.34 < \beta < 0.44$ for the FPU model [4]. Indeed, similar divergent behavior has been observed in many 1D systems. For example, in the binary hard sphere model [19,20], $0.22 < \beta < 0.35$, in single wall nanotubes $0.22 < \beta < 0.37$ [18], and in many classical lattices such as the harmonic lattice, $\beta = 1$ [22], disordered harmonic lattice, $\beta = 1/2$ [23], and the Frenkel-Kontorova (FK) model under the condition of $T/K \gg 1$, $0 < \beta < 1$ [14], where T is temperature and K is the effective amplitude of a sinusoidal on-site potential.

Obviously, a universal value of β does not exist; it differs from model to model. Most recently, Narayan and Ramaswamy [21] show theoretically that in a 1D momentum-conserving continuous system, the heat conduction is anomalous, and the thermal conductivity diverges with system size L as $L^{1/3}$. Up to now, in all available numerical results only the heat conduction in a (5,5) single wall nanotube [18] shows an exponent ($\beta \approx 0.32$) close to this $1/3$ [24]. Despite the fact that the conduction mechanism is similar, a (10,10) single wall nanotube shows a different value [18] for unknown reasons. The numerical results from other models such as the FPU model, the harmonic model, and other billiards models deviate largely from this value for reasons to be investigated.

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On the other hand, even if the momentum conservation breaks down, the heat conduction can be anomalous such as that in the Frenkel-Kontorova model [14]. The question becomes how to explain this anomalous heat conduction, in particular, the value of the exponent β in the thermal conductivity. A general theory is still lacking. The only existing theory is for the 1D harmonic chain [22], in which the phonons transport along the chain ballistically and the thermal conductivity, κ, diverges as L, i.e., $\beta = 1$.

In this Letter, we would like to find the microscopic origin of the anomalous heat conduction observed in many 1D models. We are not restricted to any specific model. This should give us a more general way to understand the heat conduction in 1D systems.

As is well known, depending on the value of exponent α in the mean square of displacement of the particle, $\langle \Delta x^2 \rangle = 2Dt^\alpha$ with $0 < \alpha \leq 2$, 1D microscopic motion can be classified into ballistic motion, $\alpha = 2$, superdiffusion, $1 < \alpha < 2$, normal diffusion, $\alpha = 1$, and subdiffusion $\alpha < 1$. Ballistic transport is observed in the harmonic lattice. Normal diffusion shows up in the FK model in a certain parameter regime [5], the disordered FPU model [10], the Lorentz gas channel [12], the disordered Ehrenfest gas channel [15], the irrational triangle channel [16], and the alternative mass hard-core potential model [17]. In some billiard models, superdiffusion [15,16,25–27] and subdiffusion [25] are observed. Superdiffusion and subdiffusion can be studied from the fractional Fokker-Planck equation; for detailed theoretical investigation and discussion about the anomalous diffusion, please refer to review articles [27,28] and the references therein.

To establish a connection between the microscopic process and the macroscopic heat conduction, let us consider a 1D model of length L whose two ends are put into contact with thermal baths of temperature T_L and T_R for the left end and the right end, respectively. Suppose the energy is transported by energy carriers (they are phonons in lattices and particles in billiard channels) from the left heat bath to the right heat bath and vice versa. If the mean square of displacement of the carrier, with velocity v, inside the system can be described by

$$\langle \Delta x^2 \rangle = 2Dv^\alpha t^\alpha; \tag{1}$$

then the so-called "mean first passage time" (MFPT) is [29]

$$\langle t_{LR} \rangle = \frac{4\gamma}{\alpha \pi v}\left(\frac{2L}{\pi\sqrt{D}}\right)^{2/\alpha}, \qquad \gamma = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^{1+2/\alpha}}. \tag{2}$$

Obviously, if the 1D system is isotropic, the MFPT for the carrier traveling from the right to the left end $\langle t_{RL} \rangle$ is the same as $\langle t_{LR} \rangle$.

If the heat bath is a stochastic kernel of Gaussian type, namely, the probability distribution of velocities is $p(v, T) = 4\pi v^2 \exp(-v^2/2T)/(2\pi T)^{3/2}$, the MFPT becomes

$$\langle t_{LR} \rangle = \frac{16T\gamma}{\alpha(2\pi T)^{3/2}}\left(\frac{2L}{\pi\sqrt{D}}\right)^{2/\alpha}. \tag{3}$$

We define the heat current as the energy exchange between two heat baths in unit time. Thus the current induced by a carrier ($m = 1$) with velocity v moving from left to right and coming back is

$$j = \frac{\int_0^\infty \frac{v^2}{2}[p(v, T_L) - p(v, T_R)]}{\langle t_{LR} \rangle + \langle t_{RL} \rangle} = \frac{T_L - T_R}{2\langle t_{LR} \rangle}. \tag{4}$$

If the temperature difference between the two baths is sufficiently small so that $\nabla T = (T_R - T_L)/L$, then the thermal conductivity, $\kappa = -Lj/\nabla T$, is

$$\kappa = cL^\beta, \qquad \beta = 2 - 2/\alpha, \tag{5}$$

and the constant is $c = 3\pi\sqrt{2\pi}\alpha(\pi\sqrt{D}/2)^{2/\alpha}\sqrt{T}/(32\gamma)$.

Equation (5) is the central result of this Letter [30]. It connects heat conduction and diffusion quantitatively. The main conclusion is that an anomalous diffusion indicates an anomalous heat conduction with a divergent (convergent) thermal conductivity. More precisely, our result tells us that ballistic motion means thermal conductivity proportional to the system size L, normal diffusion means a normal heat conduction obeying the Fourier law, superdiffusion means a divergent thermal conductivity, and subdiffusion means a zero thermal conductivity in the thermodynamic limit. In the following, we compare our results with the existing analytical and numerical results.

Ballistic motion, $\alpha = 2$, leads to a divergent thermal conductivity $\kappa \propto L$. The only existing analytical result is heat conduction in a 1D harmonic lattice. It is known that heat is transported by phonons in the lattice model. Because there are no resistance and umklapp process, the phonons transport ballistically in the harmonic lattice model; thus $\alpha = 2$. From our formula (5), the thermal conductivity in the 1D harmonic lattice diverges as L^β with $\beta = 1$; this is exactly what was shown by Lebowitz and co-workers [22] ("*" in Fig. 1).

Normal diffusion, $\alpha = 1$, means that the thermal conductivity is a size independent constant, $\beta = 0$; i.e., the heat conduction obeys the Fourier law. For example, in the 1D Frenkel-Kontorova model [5], in a certain range of parameter such as $T/K \ll 1$ [31], the phonons transport diffusively [7]; thus the thermal conductivity is finite and independent of the system size L. The disordered FPU model also has a finite thermal conductivity due to the random walklike scattering process in the chain [10]. Other 1D models showing normal diffusion and normal thermal conduction are the 1D Lorentz gas channel [12], the 1D disordered Ehrenfest gas channel [15], the 1D irrational triangle channel [16], the alternative mass hard-core potential model [17], and some 1D polygonal

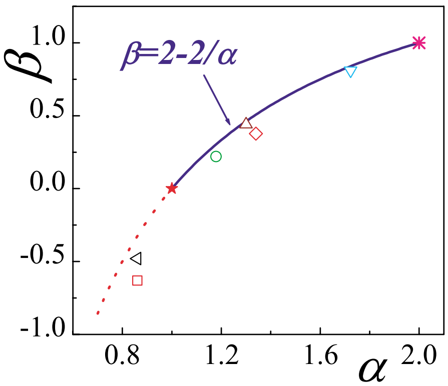

FIG. 1 (color online). The $\alpha - \beta$ plot. *Normal diffusion:* ★ represents models with a normal diffusion and a normal heat conduction, i.e., $\alpha = 1$ and $\beta = 0$, such as the Lorentz gas channel [12], the Frenkel-Kontorova model [5], the ϕ^4 model [9], the disordered FPU model [10], the disordered Ehrenfest gas channel [15], the irrational triangle channel [16], the alternative mass hard-core potential model [17], and some rational polygonal channel[25], etc. *Ballistic motion:* * represents the ballistic transport, i.e., $\alpha = 2$ and $\beta = 1$, such as the 1D harmonic lattice model. *Superdiffusion:* ▽, 1D Ehrenfest gas channel with right angle triangle scatterers[15]; ○, 1D channel with rational triangle scatterers[16]; △, polygonal billiard channel with one irrational $[(\sqrt{5}-1)\pi/4]$ and one rational $(\pi/3)$ triangle; ◇, a 1D triangle-square channel [26]. *Subdiffusion:* the polygonal billiard channel with one irrational angle $[(\sqrt{5}-1)\pi/4]$ and one rational angle $(\pi/4)$ [25], □, from the channel length $1 \leq L \leq 40$; ◁, from the channel of length $40 \leq L \leq 80$.

billiard channels with certain rational triangles [25]. "★" in Fig. 1 represents all models with normal diffusion.

Superdiffusion, $1 < \alpha < 2$, implies an anomalous heat conduction with a divergent thermal conductivity L^β. The exponent $0 < \beta < 1$ differs from model to model. Here we take the billiard models as our examples because they are very clean, and both the diffusion and thermal conductivity in these models can be calculated very accurately. The first example is the 1D Ehrenfest gas channel in which the scattering obstacles are isosceles right triangles periodically posted along the channel [15]. In this model one has $\alpha = 1.672$. From our analytical result (5), the thermal conductivity should diverge as L^β with $\beta = 2 - 2/\alpha = 0.804$ which agrees with the result from the simulation of heat conduction $\beta = 0.814$ [15] ("▽" in Fig. 1). The second example is the 1D channel with triangles whose interangles are rational multiples of π [16]. This model shows a superdiffusion with $\alpha = 1.178$. The divergent exponent of thermal conductivity is $\beta = 0.302$. This exponent is slightly larger than the one obtained from thermal conductivity simulation $\beta = 0.22$ ("○" in Fig. 1). This deviation is due to the finite size effect in the heat conduction simulation.

Subdiffusion, $\alpha < 1$, results in an anomalous heat conduction with a convergent thermal conductivity, i.e., $\kappa \propto L^\beta$, with $\beta < 0$. This is an interesting result implying that the system becomes a thermal insulator in the thermodynamic limit $L \to \infty$. Although there are many examples showing subdiffusion [32–36], a systematic study on the heat conduction in such a system is still lacking. The only existing example is the heat transport in a polygonal billiard which supports our conclusion [25]. Most recently, Alonso *et al.* [25] show that in a very special configuration, $\alpha = 0.86$, and the thermal conductivity goes as $\kappa \sim L^{-0.63}$ ("□" in Fig. 1). As L goes to infinity, the thermal conductivity goes to zero. According to our formula (5), if $\alpha = 0.86$, $\beta = -0.33$ which is larger than the one obtained by Alonso *et al.* [25]. This is not a surprise, because the channel length in their study of thermal conductivity is too small ($L \leq 40$). If the channel is longer, the value of β will become much closer to our theoretical estimation ($\beta = -0.33$). To demonstrate this, we extend the thermal conductivity simulation from $L \in [1, 40]$ used by Alonso *et al.* [25] to $L \in [40, 80]$, and we find that $\beta = -0.48$ ("◁" in Fig. 1), which is closer to $\beta = -0.33$ than the one obtained by Alonso *et al.* If $L \to \infty$, one can expect β goes to -0.33.

All numerical results are summarized and represented in Fig. 1, where we draw β versus α, and compare with Eq. (5). As is shown, Eq. (5) is exact for both normal diffusion and the ballistic motion. The agreement with most existing numerical data is good. However, discrepancies remain for some models mainly due to the limited numerical simulations. The best data close to curve $\beta = 2 - 2/\alpha$ are the simulation from the 1D Ehrenfest gas channel [15]. This is because the channel length used in the simulation is the longest one ($L \sim 10^3$) among all the available data.

In summary, we have established a connection between anomalous heat conduction and anomalous diffusion in 1D systems. Our central result Eq. (5) includes all possible cases observed in different classes of 1D models, ranging from subdiffusion, normal diffusion, and superdiffusion to ballistic transport. Several conclusions can be drawn: (i) A normal diffusion leads to a normal heat conduction obeying the Fourier law. (ii) A ballistic transport leads to an anomalous heat conduction with a divergent thermal conductivity $\kappa \propto L$. (iii) A superdiffusion leads to an anomalous heat conduction with a divergent thermal conductivity in a thermodynamic limit. (iv) More importantly, our result predicts that a subdiffusion system will be a thermal insulator. Existing numerical data support our results.

We should mention that the subdiffusion process has been observed in many real physical systems such as highly ramified media in porous systems [32], percolation clusters [33], exact fractals [34], the motion of a bead in a polymer network [35], and charge carrier transport in amorphous semiconductors [36]. Any numerical simulation or real experimental measurement of thermal conductivity in these systems will be very interesting and will allow one to test the theory given in this Letter. More importantly, it will have a wide application in designing novel thermal devices.

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[30] Alternatively, Eq. (5) can be derived from the fractional Fokker-Planck equation by replacing time t by t^α, and other simple ways; see Ref. [26] for more information.

[31] It is worth mentioning that heat conduction in the Frenkel-Kontorova model obeys the Fourier law only in an intermediate regime of parameter T/K. It is clear that in the two extremes, $T/K \ll 1$ and $T/K \gg 1$, heat conduction violates the Fourier law. The reason is that, in the case of $T/K \ll 1$, the sinusoidal on-site potential can be approximated by a harmonic on-site potential. In this case a temperature gradient cannot be set up; the heat conduction is much like the case of a harmonic chain. In the case of $T/K \gg 1$, the thermal fluctuation is so large that the on-site potential is smeared out; namely, the on-site potential will not be an effective barrier for the phonon transport. Thus the role of on-site potential can be neglected. For more quatitative analysis of the crossover from a normal to an anomalous heat conduction in the Frenkel-Kontorova model, please see Ref. [14].

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