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Heat conduction in two-dimensional disk models

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We study the heat conduction problem in two-dimensional (2D) lattice models of disk shape consisting of two circular heat baths with radius r_1 and r_2 ($r_1<r_2$), located concentrically at the center and the edge of the disk. Compared with the lattice models of rectangle shape adopted in previous studies, the main advantage of the disk models is that they have an unambiguous 2D dimensionality. The Fermi-Pasta-Ulam interaction of β type and the ϕ^4 system are considered, respectively, as momentum conserving and nonconserving prototypes. In the former we find that in the range of the system size investigated, the heat conductivity κ depends on the system size $L=r_2-r_1$ as $\kappa\sim(\ln L)^\alpha$ with α being a function of r_1/r_2. In particular, in the limit of $r_1/r_2\to 1$ we have $\alpha\to 1$, i.e., a logarithmic dependence of κ on L, which is in agreement with the prediction of existing theories. In the momentum nonconserving ϕ^4 system the heat conductivity converges to a finite value as the system size is increased.

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Spatial constraints caused by the dimensionality are important in many physical issues, such as phase transitions, specific heat, and various localization phenomena of photons, phonons, and electrons. However, in spite of many efforts, the dimensionality dependence of the energy transport is still a challenge [1,2]. The "standard" energy transport law, i.e., the Fourier law of heat conduction, states that the heat flux is proportional to the temperature gradient: $\boldsymbol{J}=-\kappa\nabla T$, where κ, the heat conductivity, is a constant at a given temperature. During the past 200 years the Fourier law has been witnessed a great success. Nevertheless, almost all the experimental studies and applications have been performed with bulk [three-dimensional (3D)] materials. Whether the Fourier law depends on the dimensionality, and if yes in what a way, has not been exposed yet.

In recent years, as low dimensional materials have been widely fabricated and studied in laboratories, such as nanowires, single-walled nanotubes and graphene flakes [3–7], much attention has been attracted to this topic. Moreover, the rapid development of computing technology nowadays has made it possible to check the law in systems of reduced dimensions via the simulations of their dynamics. On the other hand, theoretically, based on either the hydrodynamics approach [8] or the mode-coupling theory [9], it has been conjectured that for the momentum conserving systems the heat conductivity diverges with the system size in a power (logarithmic) law in one-dimensional (1D) [two-dimensional (2D)] but remains finite in 3D systems. In 2006, this theoretical prediction was analytically verified by Basile *et al.* [10] in an explicitly solvable model of stochastic dynamics.

Another paradigm of momentum conserving systems is the Fermi-Pasta-Ulam (FPU) system, whose dynamics is deterministic. After decades of intensive studies, there have been strong evidence that in the 1D FPU system the heat conductivity would diverge in a power law and the divergent exponent is 0.3–0.4 [11–13]. Meanwhile, in the experiments the breakdown of the Fourier law has been reported with the divergence exponent being 0.6–0.8 for 1D carbon nanotubes and 0.4–0.6 for 1D boron-nitride nanotubes [3]. Though the accurate value (values) of the divergent exponent is (are) to be determined, the power-law divergence of the heat conductivity in 1D momentum conserving systems has been well accepted. Recently, Saito and Dhar [14] numerically studied 3D FPU lattices and found a nondiverging heat conductivity. This result, together with the previous ones [10], has dramatically enhanced our confidence in the theoretical predictions [8,9]. However, as being pointed out in Ref. [14] and some earlier Refs. [15,16], the theoretical predictions for the 2D case has not been confirmed yet in deterministic systems; In fact, the existing studies are quite contradictory [14–16].

The controversies on the 2D FPU system may arise from the lattice model adopted in previous studies. It consists of N_x columns and N_y rows of identical atoms, and the atoms in the left- and right-most columns are coupled to two heat baths at different temperatures T_+ and T_- ($T_+>T_-$), respectively. See Fig. 1(a) for a schematic illustration. The periodic boundary condition is imposed in y direction and the problem studied is the size dependence of the heat conductivity in

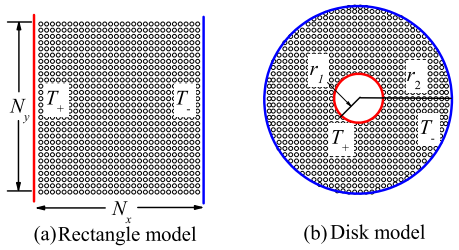

FIG. 1. (Color online) Two lattice models used for 2D heat conduction problems. Open dots represent the atoms residing on the lattice. (a) The rectangle model adopted in previous studies; the left (right) vertical solid line represents the hot (cold) heat bath of temperature T_+ (T_-). (b) The disk model investigated in this work. The center (edge) solid circle has a radius of r_1 (r_2), representing the hot (cold) heat bath of temperature of T_+ (T_-).

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x direction. In the following we refer to this model as the *rectangle* model. Note that a crucial control parameter employed is the ratio $\sigma=N_y/N_x$. Lippi and Livi [17] performed the simulations and observed a logarithmic divergence of the conductivity. Later Grassberger and Yang [18] studied the problem with larger system sizes, but instead, they found the heat conductivity depends on the system size in a power law. In particular, by varying the parameter σ from $\sigma \ll 1$ to $\sigma=1$ they observed a crossover of the heat conduction behavior from 1D to 2D; i.e., the power-law exponent varies from 0.37 to 0.22. But in their further studies [19] they reclaimed a logarithmic divergence for $\sigma=1$. A recent study [20] retrieved the power-law divergence again with a fixed ratio of $\sigma=1/2$, and obtained a power-law exponent $\alpha \simeq 0.268$. Meanwhile, some authors have declared that the heat conductivity in the 2D rectangle model depends on the system size logarithmically even for the Frenkel-Kontorova system [21]. Noting that the Frenkel-Kontorova system is a typical momentum nonconserving system and the normal heat conduction behavior has been well verified in its 1D counterpart [22], this result seems unusual. In summary, the size dependent behavior of the heat conduction in 2D systems is still far away from being clear.

We note that a crucial disadvantage of the rectangle model lies in the inherent ambiguity of its dimensionality. Physically the model will reduce to an effective 1D model as $\sigma \to 0$, and as σ is increased from zero, one may expect the transition from 1D to quasi-1D first, and then that from quasi-1D to 2D eventually. Hence the parameter σ is closely related to the dimensionality. But, however, at what values of σ these transitions may occur has not been understood yet. One may hence conjecture that the confusions arose in previous studies are due to the different effective dimensions implied by various values of σ considered in those studies. It should be pointed out that in principle an ideal 2D model can be achieved by resorting to an infinite, or large enough value of σ; but in practice this is impossible: it could be prohibitively expensive for numerical studies.

In order to overcome this difficulty, in this Communication we consider a variant lattice model. It is not only 2D exactly, but also convenient to deal with numerically. Instead of the rectangle geometry, our model is a disk, as shown schematically in Fig. 1(b). The center (edge) heat bath has a higher (lower) temperature T_+ (T_-); it is composed of the nearest neighboring atoms whose bonds cross the center (edge) circle of radius r_1 (r_2). The fixed boundary conditions are applied to our model; i.e., the inner (outer) layer of the neighboring atoms next to the center (edge) heat bath is set to be fixed. The two heat baths are arranged to be concentric. In this setup the effective heat current flows along the radial direction, and the problem to be studied is how the radial heat conductivity depends on the radial scale of the system. The radial scale of the system is given by $L=r_2-r_1$.

We refer to this model as the "disk model;" it has also another advantage: by adjusting the parameter r_1/r_2, one can use it to model a broad spectrum of heat conduction problems. For example, in the limit of $r_1/r_2 \to 1$ it gives a variant of the ideal rectangle model, while in that of $r_1/r_2 \to 0$ it models the heat conduction problem with point-to-surface contact. As the point-to-surface contact is common in many real-world situations, the disk model may have practical implications as well. One interesting example is experimental investigations of the heat conduction behavior of the graphene flakes [4–7]; in experiments as such the point-to-surface contact is a frequently used technique to inject the heat into the sample.

In the next we will investigate the size dependence of κ in the disk model. The Hamiltonian of the lattice is $H=\Sigma_{i,j}[\frac{\mathbf{p}_{i,j}^2}{2m}+V(|\mathbf{q}_{i+1,j}-\mathbf{q}_{i,j}|)+V(|\mathbf{q}_{i,j+1}-\mathbf{q}_{i,j}|)+U(\mathbf{q}_{i,j})]$, where $\mathbf{q}_{i,j}$ is the displacement of the atom on the site (i,j) from its equilibrium position and $\mathbf{p}_{i,j}$ is the corresponding momentum. Note that only nearest neighboring interactions are considered, and the dimensionless mass m is fixed to be unity. We consider both the momentum conserving and nonconserving cases, represented by the 2D FPU and ϕ^4 systems, respectively. Here we diskuss the ϕ^4 system instead of the Frenkel-Kontorova system because it has a simpler on-site potential, which can facilitate the numerical simulations considerably [23,24]. To be concrete, we will focus on the FPU-β system with $V(x)=\frac{1}{2}x^2+\frac{1}{4}x^4$, $U(x)=0$, and the ϕ^4 system with $V(x)=\frac{1}{2}x^2$, $U(x)=\frac{1}{4}x^4$. The role of the on-site potential $U(x)$ in the latter is to destroy the conservation of the momentum.

The Nose-Hoover heat baths [25] are implemented. Therefore the motions of particles in heat baths are governed by

$$\dot{\mathbf{q}}_{i,j}=\mathbf{p}_{i,j},$$

$$\dot{\mathbf{p}}_{i,j}=-\frac{\partial V}{\partial \mathbf{q}_{i,j}}-\varsigma_{\pm}\mathbf{p}_{i,j}, \quad \dot{\varsigma}_{\pm}=\frac{\mathbf{p}_{i,j}^2}{2T_{\pm}}-1, \tag{1}$$

and the motions of other particles in between the heat baths are described by

$$\dot{\mathbf{q}}_{i,j}=\mathbf{p}_{i,j}, \quad \dot{\mathbf{p}}_{i,j}=-\frac{\partial V}{\partial \mathbf{q}_{i,j}}. \tag{2}$$

The Boltzmann constant is set to be $k_B=1$ and the local temperature is defined as $T_{i,j}=[\langle (p_{i,j}^x)^2\rangle+\langle (p_{i,j}^y)^2\rangle]/2$ with $\langle\cdot\rangle$ denoting the average. The heat flux reads

$$j_{i,j}^x=-[f_{i,j}^{xx}(p_{i,j}^x+p_{i+1,j}^x)+f_{i,j}^{yx}(p_{i,j}^y+p_{i+1,j}^y)]/4,$$

$$j_{i,j}^y=-[f_{i,j}^{xy}(p_{i,j}^x+p_{i,j+1}^x)+f_{i,j}^{yy}(p_{i,j}^y+p_{i,j+1}^y)]/4. \tag{3}$$

In above definitions $p_{i,j}^x$ and $p_{i,j}^y$ are the x and y components of the momentum vector $\mathbf{p}_{i,j}$, $j_{i,j}^x$ and $j_{i,j}^y$ are the x and y components of the local heat flux, and $f_{i,j}^{xx}=-\frac{\partial V(|\mathbf{q}_{i+1,j}-\mathbf{q}_{i,j}|)}{\partial q_{i,j}^x}$, $f_{i,j}^{yx}=-\frac{\partial V(|\mathbf{q}_{i+1,j}-\mathbf{q}_{i,j}|)}{\partial q_{i,j}^y}$, $f_{i,j}^{xy}=-\frac{\partial V(|\mathbf{q}_{i,j+1}-\mathbf{q}_{i,j}|)}{\partial q_{i,j}^x}$, $f_{i,j}^{yy}=-\frac{\partial V(|\mathbf{q}_{i,j+1}-\mathbf{q}_{i,j}|)}{\partial q_{i,j}^y}$.

As the disk model is rotationally symmetric, the heat flux has only the radial component, hence the problem reduces to a 1D problem. Given the 2D Fourier law, in our disk model it reads $J_r=-2\pi\kappa r\frac{dT}{dr}$ with $J_r=2\pi\langle \mathbf{j}_\mathbf{r}\cdot\mathbf{r}\rangle$ being the total heat flux in the radial direction. Here $\mathbf{j}_\mathbf{r}$ is the local heat flux at the position $\mathbf{r}$ [26], whose Cartesian components are given in Eq. (3). Based on this, the heat conductivity can be calculated with

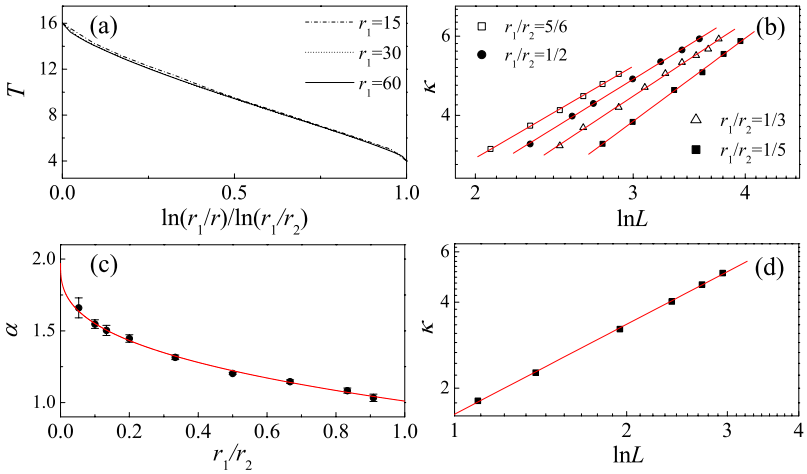

FIG. 2. (Color online) Numerical simulation results for the 2D disk model of the momentum conserving FPU-β interaction. (a) Temperature profiles in the radial direction for different values of r_1 with fixed $r_1/r_2=1/2$. (b) Dependence of the heat conductivity κ on the system size L for $r_1/r_2=1/5$, 1/3, 1/2 and 6/5. (c) Divergence exponent α versus r_1/r_2. The solid (red) curve is for the best fitting $\alpha=\alpha_0-A(r_1/r_2)^\beta$ with $\alpha_0=2.06\pm0.21$, $A=1.05\pm0.21$, and $\beta=0.32\pm0.10$. (d) Dependence of the heat conductivity κ on the system size L with $r_1=100$ and $r_2=103$, 104, 107, 111, 115, and 119 (from left to right). Note that in (b) and (d) the error bars (not shown) are smaller than the symbol size, and the (solid) red lines are for the best linear fittings.

$$\kappa \approx -J_r \frac{\ln(r_1/r_2)}{2\pi\Delta T}, \tag{4}$$

where $\Delta T=T_+-T_-$, if

$$\frac{dT}{d\ln r} \approx \frac{\Delta T}{\ln(r_1/r_2)}. \tag{5}$$

Equivalently, Eq. (5) implies that the temperature profile between two heat baths reads $T(r)\approx T_-+\Delta T\frac{\ln(r/r_2)}{\ln(r_1/r_2)}$; this will be checked in the first place to justify the calculations of κ with Eq. (4).

Now we present the numerical results for the 2D FPU-β system. The temperatures of the heat baths are fixed to be $T_+=16$ and $T_-=4$; initially all the atoms reside on their equilibrium positions and take a random velocity generated from the Maxwellian distribution at temperature $T=(T_++T_-)/2$, then the motion equations are integrated with the velocity-Verlet algorithm [27] with a time step 0.005. The transient stage of 10^6 evolution time is diskarded (This time has been verified to be long enough for the system to reach the stationary state); then the next evolution of time 10^7 is performed for the time average. We have also checked other values of parameters and verified that our results do not qualitatively depend on the their particular values taken here.

The results are summarized in Fig. 2. First of all in Fig. 2(a) the temperature T as a function of $\ln(r_1/r)/\ln(r_1/r_2)$ are shown for $r_1=15$, 30, and 60 with fixed $r_1/r_2=1/2$. It can be seen that all the three curves are close to the temperature profile implied by Eq. (5), i.e., T depends on $\ln r$ linearly. This result suggests that the heat conductivity can be obtained via Eq. (4) immediately. With this facility, in Fig. 2(b) the size dependence of the heat conductivity is shown, from which a linear relation between $\ln\kappa$ and $\ln(\ln L)$ can be clearly recognized. A further careful study suggests that $\kappa\sim(\ln L)^\alpha$, where the exponent α is a function of r_1/r_2, and its value can be evaluated conveniently by linearly fitting $\ln\kappa$ against $\ln(\ln L)$ in Fig. 2(b). We find that α decreases from 1.45 to 1.15 as r_1/r_2 increases from 1/5 to 5/6, indicating a definite trend of $\alpha\to1$ as $r_1/r_2\to1$.

In order to have a close look at this trend, in Fig. 2(c) we plot α against r_1/r_2, therein four data points are extracted from Fig. 2(b) while others are calculated additionally in the same way. Applying the best fitting, we find α versus L can be fitted with $\alpha=\alpha_0-A(r_1/r_2)^\beta$, yielding $\alpha_0=2.06\pm0.21$, $A=1.05\pm0.21$, and $\beta=0.32\pm0.10$. Within the range of error it suggests that $\alpha\to1$ for $r_1/r_2\to1$ and α tends to a value close to 2 for $r_1/r_2\to0$. This is the main result of this work. Note that the limit $r_1/r_2\to1$ corresponds to the ideal rectangle model; hence $\alpha\to1$ extrapolated here is in agreement with the theoretical predictions [8,9] for the 2D rectangle model.

Due to the importance and subtlety of this issue, the evidence of $\kappa\sim\ln L$ for the ideal rectangle model is desired. Though a direct investigation is numerically too expensive (which requires to deal with large system size), some hints consistent with the logarithmic divergence of κ can be extracted in the range of the system size accessible to us: We fix r_1 to be $r_1=100$ and calculate κ with r_2 being a close value such that $r_1/r_2\approx1$; As shown in Fig. 2(d), $\kappa\sim(\ln L)^\alpha$ still holds, and the best fitting suggests $\alpha=1.02\pm0.02$.

Finally, in Fig. 3 we present the results of the 2D ϕ^4 system. The heat baths with $T_+=12$ and $T_-=8$ are applied. The temperature profiles share the similar features of the

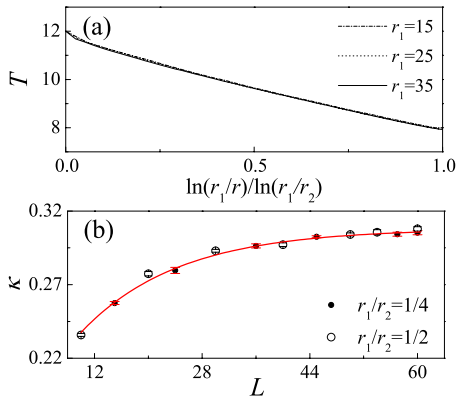

FIG. 3. (Color online) Heat conduction behavior of the 2D disk ϕ^4 system. (a) Temperature profiles in radial direction for $r_1/r_2=1/3$. (b) The heat conductivity versus the system size for $r_1/r_2=1/4$ and 1/2. The (solid) red line is the best fitting $\kappa=\kappa_\infty-\nu\exp(-L/\gamma)$ with $\kappa_\infty=0.308\pm0.001$, $\nu=0.14\pm0.01$, and $\gamma=14.56\pm0.08$.

FPU-β system, as seen in Fig. 3(a), but the size dependent behavior of κ is quite different. Indeed, as can be seen in Fig. 3(b) κ saturates at a constant regardless of r_1/r_2. It shows that the 2D disk ϕ^4 system still obeys the Fourier law as its 1D counterpart does [22].

In summary, the disk model reveals some essential features of heat conduction in 2D crystals. While the momentum nonconserving ϕ^4 system obeys the Fourier law, the momentum conserving FPU-β system has a divergent heat conductivity $\kappa \sim (\ln L)^{\alpha}$ in the range of the system size studied. This divergent behavior has one important limit, i.e., $\alpha \to 1$ as $r_1/r_2 \to 1$; the logarithmic divergence in this case is coincident with the theoretical prediction for 2D lattice systems. In addition, α has been shown to depend on r_1/r_2 monotonically in $0 < r_1/r_2 < 1$. It implies that the boundaries introduced by the heat baths may govern the heat conductivity divergent behavior in 2D systems disobeying the Fourier law, and hence should be taken into account necessarily in studies. These results may also have experimental implications. For example, if the logarithmic heat conductivity divergence is observed in laboratories with 2D lattice systems of rectangle shape and two heat baths applied at two opposite ends, the heat conductivity divergence measured instead with a point-to-surface heat bath, just as being widely adopted in the present experimental studies [4–7], may take a distinct form.

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