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Logarithmic divergent thermal conductivity in two-dimensional nonlinear lattices

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Heat conduction in three two-dimensional (2D) momentum-conserving nonlinear lattices are numerically calculated via both nonequilibrium heat-bath and equilibrium Green-Kubo algorithms. It is expected by mainstream theories that heat conduction in such 2D lattices is divergent and the thermal conductivity κ increases with lattice length N logarithmically. Our simulations for the purely quartic lattice firmly confirm it. However, very robust finite-size effects are observed in the calculations for the other two lattices, which well explain some existing studies and imply the extreme difficulties in observing their true asymptotic behaviors with affordable computation resources.

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Heat conduction induced by a small temperature gradient in the stationary state in a macroscopic material is expected to satisfy Fourier's law: $\boldsymbol{j} = -\kappa \nabla T$. This is a well-known empirical law, while a complete understanding of the microscopic mechanism that determines such a law remains a challenging problem of nonequilibrium statistical mechanics [1,2]. Fourier's law implies that a fixed temperature difference ΔT that is applied to a homogeneous material with length N induces a steady-state heat current j that should be inversely proportional to N: $j = -\kappa \Delta T/N$. On the other hand, j is found, by numerical simulation, to decay as $N^{-1+\alpha}$ with a positive α in many one-dimensional (1D) models [1,2]. This implies an infinite κ which diverges with N as N^{α}. It has been generally accepted that global momentum conservation is a key factor to induce such an anomalous heat conduction. Most of the theories, e.g., the renormalization group analysis [3] and the mode-coupling theories [4] support such a power-law divergence. However, a well-accepted conclusion for the value of α is still not reached [2,5–7]. For three-dimensional (3D) momentum-conserving systems, all the above-mentioned theories predict that the heat current autocorrelation function decays with the time lag τ as τ^{β}, where $\beta = -3/2$, which suggests a finite κ. The finiteness of κ in 3D nonlinear lattice models has been recently confirmed by both nonequilibrium heat-bath [8] and equilibrium Green-Kubo [9] calculations. It should be noted, however, that in Ref. [9] the calculated value of β is -1.2, which is less negative than $-3/2$.

As for two-dimensional systems, the theoretically predicted value of β is -1, which leads to a logarithmically divergent κ. However, existing numerical simulations are still far from conclusive. Such a logarithmic divergence is reported by numerical simulation in the Fermi-Pasta-Ulam (FPU)-β rectangle [10] and the disk [11] lattices with vector displacements. However, a power-law divergence is observed in the FPU-β lattices with scalar displacements [12]. Up to now, the size dependence of the thermal conductivity and the role of the details of interparticle interactions in 2D systems are still unclear.

Such a study is not only of theoretical importance. Progress in nanotechnology has enabled us to measure experimentally the size dependence of the thermal conductivity in some 1D [13] and 2D [14] nanoscale materials. Furthermore, the study may also help in fabricating building blocks of nanoscale phononic devices [15].

In this paper we study heat conduction in two-dimensional square lattices with a scalar displacement field $u_{i,j}$. In those lattices, each particle interacts with its nearest neighbors only. The Hamiltonian reads

$$H = \sum_{i=1}^{N_X} \sum_{j=1}^{N_Y} \left[\frac{\dot{u}_{i,j}^2}{2} + V(u_{i+1,j} - u_{i,j}) + V(u_{i,j+1} - u_{i,j}) \right],$$

where the interparticle potential takes the form of $V(x) = \frac{1}{2}k_2x^2 + \frac{1}{3}k_3x^3 + \frac{1}{4}k_4x^4$. The mass of all the particles has been set to unity. To examine carefully the validity of the logarithmic divergence and also study the role of interparticle coupling, we systematically study three types of lattices, i.e., the FPU-$\alpha\beta$ lattice: $k_2 = k_4 = 1, k_3 = 2$; the FPU-β lattice: $k_2 = k_4 = 1$, $k_3 = 0$; and the purely quartic lattice: $k_2 = k_3 = 0$, $k_4 = 1$. The purely quartic lattice can be regarded as the high-temperature limit of the other two. Due to its simplicity and high nonlinearity, one would expect that its asymptotic behaviors could be displayed in shorter time and space scales.

We first calculate the thermal conductivity κ_{NE} in nonequilibrium stationary states. To this end, fixed boundary conditions are applied in the X direction, while periodic boundary conditions are applied in the Y direction. The left- and right-most columns are coupled to Langevin heat baths with temperatures $T_L = 1.5$ and $T_R = 0.5$, respectively. Heat currents flowing along the X direction are measured. A number of independent runs (16 for 2048×64 lattices and 8 for others) starting from different randomly chosen initial states are performed. The simulation time depends on the model and the lattice size. For each largest lattice (2048×64), the average

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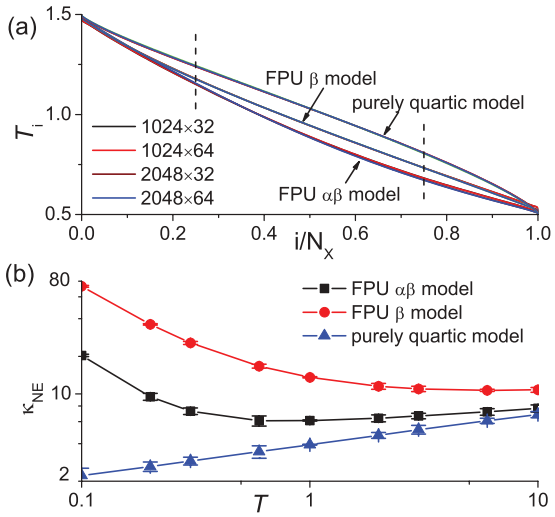

FIG. 1. (Color online) (a) Temperature distributions of different models for various lattice size $N_X \times N_Y$. Curve groups from down top correspond to the FPU-$\alpha\beta$, FPU-β, and purely quartic lattices, respectively. Only the data in the central region between the two vertical dashed lines are taken into account in calculating the temperature gradient ∇T, i.e., the left and right 1/4 of the lattices are excluded. (b) $\kappa_{\rm NE}$ vs temperature T in 1024×32 lattices. They tend to be identical in the high-temperature limit.

is performed over $2 \sim 4 \times 10^7$ dimensionless time units after enough transient time units. The simulation for each largest lattice costs several months' wall time in our high-performance parallel computing cluster. The temperature of each column is defined as the average over this column, i.e.,

$$T(i) \equiv \frac{1}{N_Y} \sum_{j=1}^{N_Y} \langle \dot{u}_{i,j}^2 \rangle,$$

where the symbol $\langle\rangle$ stands for the time average. We have carefully confirmed that the heat currents along the lattices and the temperature distribution approach constants independent of time. The temperature distributions of different models for various N_X and N_Y are plotted in Fig. 1(a). Those for the same model with various lattice sizes well overlap each other, which indicates that temperature profiles can be established. The thermal conductivity $\kappa_{\rm NE}$ is calculated by

$$\kappa_{\rm NE} = -\frac{\langle J \rangle}{N_Y \nabla T},$$

where J stands for the total heat current, and the temperature gradient ∇T is along the X direction. To reduce boundary effects, ∇T is calculated by a linear least-squares fitting of the temperature profiles in the central region where the left- and right-most 1/4 of the lattices are excluded. As shown in Fig. 1(a), the temperature profiles are evidently nonlinear, and that is why such a procedure is necessary. Such a nonlinearity is not caused by the temperature dependence of the thermal conductivity but by boundary effects. This can be realized by studying the temperature dependence of $\kappa_{\rm NE}$ for different lattices, as shown in Fig. 1(b). The data for the purely quartic lattice fit the theoretical prediction that $\kappa \sim T^{1/4}$ exactly.

The thermal conductivity $\kappa_{\rm NE}$ versus lattice length N_X for different lattices with various lattice widths is shown in Fig. 2.

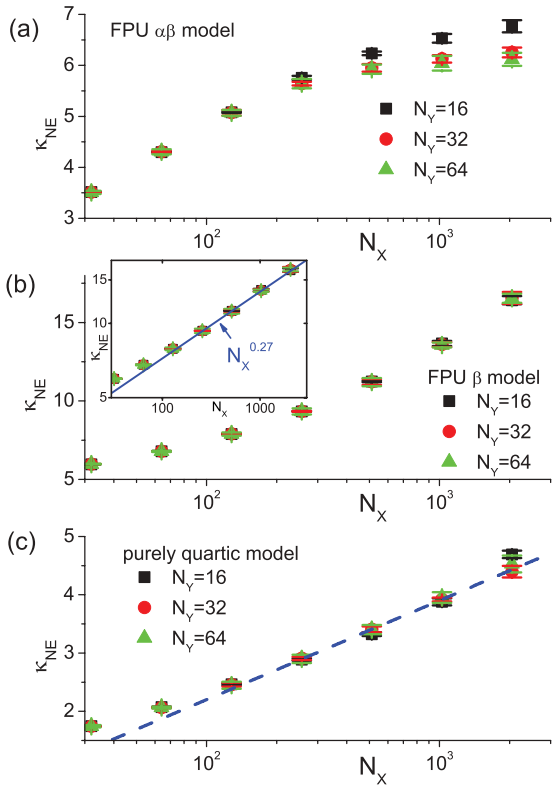

FIG. 2. (Color online) Thermal conductivity $\kappa_{\rm NE}$ in 2D (a) FPU-$\alpha\beta$, (b) FPU-β, and (c) purely quartic lattices vs lattice length N_X for various N_Y. The dashed line that indicates logarithmic growth is drawn for reference. Inset of (b): data for the FPU-β lattice but in double logarithmic scale. Solid line corresponds to the power-law divergence $N^{0.27}$.

We see in Fig. 2(a) that in the long N_X regime, the smaller the N_Y the higher the $\kappa_{\rm NE}$. It is reasonable since the finite width effect makes a 2D lattice behave close to a 1D lattice. The data for $N_Y = 64$ present a flat curve, i.e., $\kappa_{\rm NE}$ increases much more slowly than logarithmically in this regime. In contrast, we see in Fig. 2(b) that $\kappa_{\rm NE}$ increases evidently faster than logarithmically. In the inset, the same data are plotted in double logarithmic scale. The power exponent estimated from the best fit of the last four points is 0.27 ± 0.02. The data for the purely quartic lattices are shown in Fig. 2(c). In at least one order of magnitude, $\kappa_{\rm NE}$ shows a logarithmic growth very well.

Similar to the situation in 1D lattices [7], finite-size effects of the nonequilibrium method are quite considerable due to the presence of heat baths and the fixed boundaries,. Furthermore, the temperature gradient in the lattice must not be too small, otherwise net heat currents cannot be distinguished from background statistical fluctuations. Thus the lattice is far from an ideal close-to-equilibrium states. To reduce further those effects, simulations of a much longer lattice are necessary. However, that demands a huge computational resource, which is beyond our means. We will therefore calculate the heat current autocorrelation function in order to make a more convincing verification. Based on the Green-Kubo formula, this provides an alternative way to determining α independently [16]. This method has been proven to have much better efficiency [7,9].

In the Green-Kubo simulation, periodic boundary conditions are applied in both the X and Y directions, since they provide the best convergence to the thermodynamic limits. The interactions between a particle labeled (i,j) and its nearest right and up neighbors are $f^X_{i,j} = -dV(u_{i+1,j} - u_{i,j})/du_{i,j}$ and $f^Y_{i,j} = -dV(u_{i,j+1} - u_{i,j})/du_{i,j}$. The local instantaneous heat currents in the two directions are defined as $j^X_{i,j} = \dot{u}_{i,j}(f^X_{i,j} + f^X_{i-1,j})/2$ and $j^Y_{i,j} = \dot{u}_{i,j}(f^Y_{i,j} + f^Y_{i,j-1})/2$, respectively.

The rescaled heat current autocorrelation function in the X direction for a given lattice size is defined as

$$c^X_{N_X,N_Y}(\tau) \equiv \frac{1}{k_B T^2 N_X N_Y} \langle J^X(t) J^X(t+\tau) \rangle_t, \qquad (1)$$

where $J^X(t) \equiv \sum_{i,j} j^X_{i,j}(t)$ is the instantaneous global heat current in the X direction, and the Boltzmann constant k_B is set to unity. For the sake of simplicity, the subscripts of c are omitted hereafter except in case of necessity. Microcanonical simulations are performed with zero total momentum [1] and identical energy density ϵ which corresponds to the same temperature $T = 1$. ϵ equals 0.887, 0.892, and 0.75 for the FPU-$\alpha\beta$, FPU-β, and purely quartic lattices, respectively. An embedded 8(6)th-order Runge-Kutta-Nystrom algorithm [17], which provides very high accuracy, is used in such a deterministic energy-conserving system. A number of independent runs (64 for 1024×1024 and fewer for smaller lattices) are performed. Simulations of the largest lattices (1024×1024) are carried out for about 10^7 dimensionless time units.

The rescaled heat current autocorrelation function in the X direction, $c^X(\tau)$, for different types of lattices is plotted in Fig. 3. To avoid finite-size effects, we perform simulations by varying N_X and N_Y and consider only the asymptotic behavior shown in the part of curves overlapping with each other. To avoid confusion, data for only two typical lattice sizes, 1024×1024 and 512×512, are plotted. Within the range of standard error, they overlap with each other. Thus no data for the intermediate size are necessary. Since $N_X = N_Y$, we actually plot $[c^X(\tau) + c^Y(\tau)]/2$ instead. This greatly reduces statistical errors without performing any more simulations. Not surprisingly, $c^X(\tau)$ in 2D FPU-$\alpha\beta$ lattices decays much faster than τ^{-1} in a wide regime of (τ), just like what has been found in 1D FPU-$\alpha\beta$ lattices [7]. This explains well the flat $\kappa_{\rm NE}$ that is observed in Fig. 2(a). The decay tends to slow down for yet longer τ. Due to large fluctuations, we are not able to confirm its asymptotic behavior. The simulation for each 1024×1024 lattice costs a few months' wall time with a 64-CPU parallel computational workstation. In Fig. 2(b), we see that $c^X(\tau)$ in the 2D FPU-β lattice decays evidently more slowly than τ^{-1}. This also agrees with the power-law divergence of $\kappa_{\rm NE}$ shown in Fig. 2(b). In Fig. 2(c), we see, in nearly three orders of magnitude of τ, $c^X(\tau)$ in the purely quartic lattice decays as τ^{-1}. This strongly supports a logarithmically divergent thermal conductivity κ and is also in agreement with the finding in Fig. 2(c).

The length dependence of the thermal conductivity $\kappa_{\rm GK}(N)$ can be determined by putting a cutoff time instead of infinity as the upper limit of the Green-Kubo integral [16]

$$\kappa_{\rm GK}(N) \equiv \lim_{N_X\to\infty} \lim_{N_Y\to\infty} \int_0^t c^X(\tau) d\tau, \qquad (2)$$

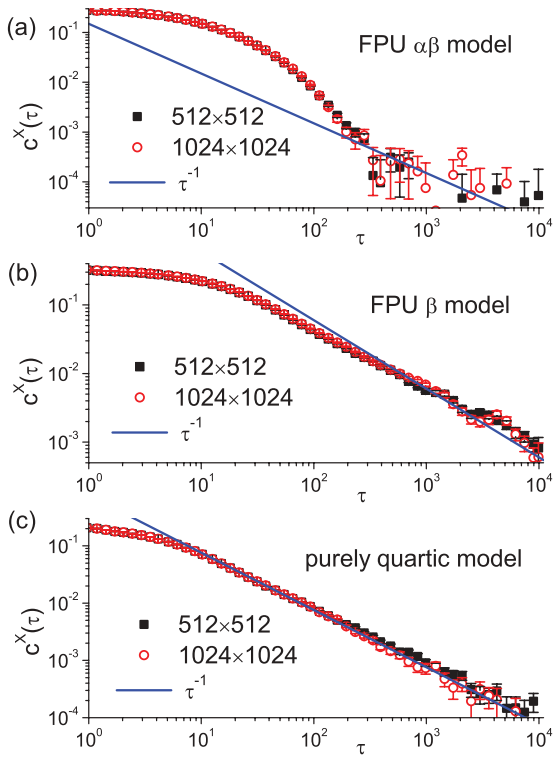

FIG. 3. (Color online) Rescaled heat current autocorrelation function $c^X(\tau)$ vs the time lag τ in $N_X \times N_Y$ lattices. Data binning over contiguous τ regimes has been performed to reduce statistical fluctuations. Lines correspond to τ^{-1} are drawn for reference. (a) FPU-$\alpha\beta$ lattice. $c^X(\tau)$ decays much faster than τ^{-1} when $\tau < 300$, while the decay tends to slow down for yet longer τ. (b) FPU-β lattice. In a quite wide regime of τ, $c^X(\tau)$ decays obviously slower than τ^{-1}. This explains some existing numerical results that suggest a power-law divergent thermal conductivity κ. (c) Purely quartic lattice. In nearly three orders of magnitude of τ, $c^X(\tau)$ follows τ^{-1} very well. This strongly supports a logarithmically divergent thermal conductivity κ.

where $t = N/v_s$ with at most a constant-factor difference as $N \to \infty$. Therefore, if $c(\tau)$ decays asymptotically as τ^{-1}, then the thermal conductivity $\kappa_{\rm GK}$ should diverge asymptotically as $\log N$. The speed of sound v_s can be obtained by simulating the heat diffusion process [18]. It is of the order of magnitude of one in the models that we have studied. Since we are interested in the divergence exponent of $\kappa_{\rm GK}$ only, this value does not affect our conclusion. We thus simply regard it as unity. The length dependence of the thermal conductivity $\kappa_{\rm GK}(N)$ is displayed in Fig. 4. Since the integral operation largely reduces the statistical error, the difference between different lattice sizes can be observed. We thus plot the data for lattice sizes 512×1024 and 1024×512 also. Because $c^X_{512,1024}(\tau) = c^Y_{1024,512}(\tau)$, the simulations for the two lattices can be carried out by the same run. In all the lattices, the tendency of $\kappa_{\rm GK}(N)$ is in good agreement with that of $\kappa_{\rm NE}(N_X)$, as shown in Fig. 2. For the FPU-$\alpha\beta$ lattice, a flattened $\kappa_{\rm GK}$ is again observed. In the FPU-β lattice, $\kappa_{\rm GK}$ displays a power-law divergence in a wide regime. The best fit of the power exponent in the regime $N > 10^3$ is 0.25 ± 0.01. As for the purely quartic lattice, the data for the largest lattice size follow a

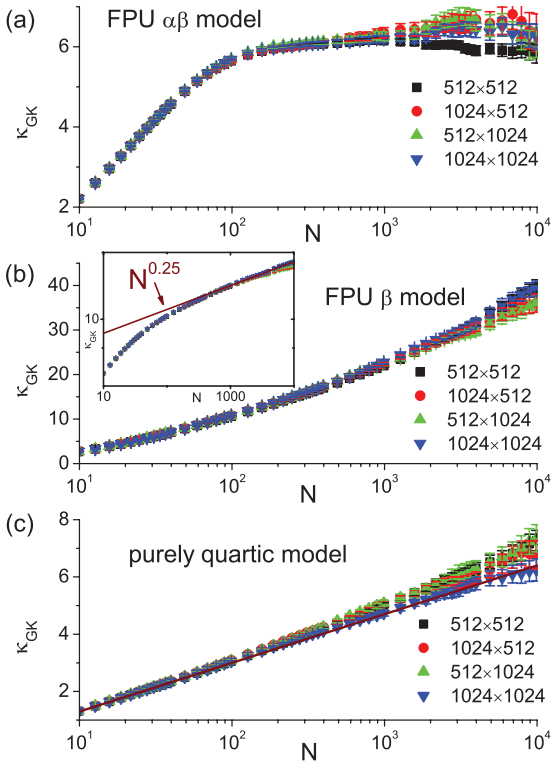

FIG. 4. (Color online) $\kappa_{\rm GK}(N)$ in the X direction vs N in $N_X \times N_Y$ lattices. (a) FPU-$\alpha\beta$ lattice. A flat $\kappa_{\rm GK}$ is again observed for $N < 2000$. Thereafter $\kappa_{\rm GK}$ tends to rise up. Mathematically it is easily understood that a slow down of the decay of $c(\tau)$ cannot instantly induce a visible rise up of $\kappa_{\rm GK}$, since $c(\tau)$ has already decayed to a too low value. (b) FPU-β lattice. In a quite wide regime of τ, c_τ decays obviously slower than τ^{-1}. Inset: data plotted in double logarithmic scale. Solid line corresponds to $N^{0.25}$. (c) Purely quartic lattices. In nearly three orders of magnitude of τ, $\kappa_{\rm GK}$ for 1024×1024 follows the straight line very well. This strongly supports a logarithmically divergent thermal conductivity. The slight rise for smaller lattices is due to the finite-size effect.

straight line very well in three orders of magnitude of N. This strongly confirms a logarithmically divergent thermal conductivity.

In summary, we have extensively studied heat conduction in three 2D typical nonlinear lattices. The roles of harmonic and asymmetric terms of the interparticle coupling are clearly observed by comparing the results for the purely quartic lattice and the other two lattices. In the purely quartic lattice, the heat current autocorrelation function $c(\tau)$ is found to decay as τ^{-1} in three orders of magnitude from 10^1 to 10^4. This strongly supports a logarithmically divergent thermal conductivity κ. For the FPU-β lattice, our nonequilibrium and equilibrium calculations suggest a power-law divergence with an exponent $\alpha = 0.27 \pm 0.02$ and 0.25 ± 0.01, respectively. They are consistent with each other and also with the finding in Ref. [12] that $\alpha = 0.22 \pm 0.03$. A very strong finite-size effect which induces a flat κ is found in the FPU-$\alpha\beta$ model whose interparticle coupling is asymmetric due to the cubic term. Such a phenomenon has also been observed in the 1D case [7]. Here we recall that most existing numerical studies on lattices with asymmetric interaction terms suggest a logarithmically divergent κ, e.g., the Fermi-Pasta-Ulam (FPU)-β rectangle [10] and disk [11] lattices with vector displacements. We suppose that the effect of the harmonic term is largely offset by that of the asymmetric term, thus a logarithmic-like divergence is obtained. This is also implied by the fact that the curve for the FPU-$\alpha\beta$ lattice, compared to that of the FPU-β lattice, is much closer to that of the purely quartic model, as shown in Fig. 1(b).

Based on the finding that in 1D lattices, κ tends to diverge in the same way in the thermodynamic limit [7], we therefore expect that in long enough FPU-$\alpha\beta$ and FPU-β lattices, κ shall also diverge as $\log L$, just like the theoretical expectation which is confirmed in the purely quartic lattice. However, our simulation also indicates that in order to see such an asymptotic divergence, lattices with lengths much longer than those that have hitherto been simulated have to be studied. The cost of computational resources is probably prohibitively high unless much more efficient algorithms are proposed.

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[1] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[2] A. Dhar, Adv. Phys. **57**, 457 (2008).
[3] O. Narayan and S. Ramaswamy, Phys. Rev. Lett. **89**, 200601 (2002).
[4] G. Basile, C. Bernardin, and S. Olla, Phys. Rev. Lett. **96**, 204303 (2006); L. Delfini, S. Lepri, R. Livi, and A. Politi, Phys. Rev. E **73**, 060201 (2006).
[5] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997).
[6] T. Mai, A. Dhar, and O. Narayan, Phys. Rev. Lett. **98**, 184301 (2007).
[7] L. Wang and T. Wang, Europhys. Lett. **93**, 54002 (2011).
[8] K. Saito and A. Dhar, Phys. Rev. Lett. **104**, 040601 (2010).
[9] L. Wang, D. He, and B. Hu, Phys. Rev. Lett. **105**, 160601 (2010).
[10] A. Lippi and R. Livi, J. Stat. Phys. **100**, 1147 (2000); L. Yang, P. Grassberger, and B. Hu, Phys. Rev. E **74**, 062101 (2006).
[11] D. Xiong, J. Wang, Y. Zhang, and H. Zhao, Phys. Rev. E **82**, 030101 (2010).
[12] P. Grassberger and L. Yang, arXiv:cond-mat/0204247.
[13] C. W. Chang, D. Okawa, H. Garcia, A. Majumdar, and A. Zettl, Phys. Rev. Lett. **101**, 075903 (2008).
[14] S. Ghosh, W. Bao, D. L. Nika, S. Subrina, E. P. Pokatilov, C. N. Lau, and A. A. Balandin, Nat. Mater. **9**, 555 (2010); X. Xu, Y. Wang, K. Zhang, X. Zhao, S. Bae, M. Heinrich,

C. Tinh Bui, R. Xie, J. T. L. Thong, B. H. Hong, K. P. Loh, B. Li, and B. Oezyilmaz, arXiv:1012.2937; Z. Wang, R. Xie, C. T. Bui, D. Liu, X. Ni, B. Li, and J. T. L. Thong, Nano Lett. **11**, 113 (2011); D. L. Nika, A. S. Askerov, and A. A. Balandin, *ibid*. **12**, 3238 (2012).

[15] N. Li, J. Ren, L. Wang, G. Zhang, P. Hänggi, and B. Li, Rev. Mod. Phys. **84**, 1045 (2012).

[16] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II, Springer Series in Solid State Sciences Vol. 31* (Springer, Berlin, 1991).

[17] J. R. Dormand, M. E. A. El-Mikkawy, and P. J. Prince, IMA J. Numer. Anal. **7**, 423 (1987).

[18] B. Li, J. Wang, L. Wang, and G. Zhang, Chaos **15**, 015121 (2005).