Heat conduction in the nonlinear response regime: Scaling, boundary jumps, and negative differential thermal resistance

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We report a numerical study on heat conduction in one-dimensional homogeneous lattices in both the linear and the nonlinear response regime, with a comparison among three prototypical nonlinear lattice models. In the nonlinear response regime, negative differential thermal resistance (NDTR) can occur in both the Frenkel-Kontorova model and the ϕ^4 model. In the Fermi-Pasta-Ulam-β model, however, only positive differential thermal resistance can be observed, as shown by a monotonous power-law dependence of the heat flux on the applied temperature difference. In general, it was found that NDTR can occur if there is nonlinearity in the onsite potential of the lattice model. It was also found that the regime of NDTR becomes smaller as the system size increases, and eventually vanishes in the thermodynamic limit. For the ϕ^4 model, a phenomenological description of the size-induced crossover from the existence to the nonexistence of a NDTR regime is provided.

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I. INTRODUCTION

Heat conduction in low-dimensional systems has become the subject of a large number of theoretical and experimental studies in recent years. An existing theoretical problem of great interest is on the validity of Fourier's law in low-dimensional classical systems. In recent years it has been found that Fourier's law is not satisfied in momentum-conserving systems such as the Fermi-Pasta-Ulam (FPU) chain [1], where the corresponding anomalous heat-conduction behavior is characterized by a size-dependent thermal conductivity $\kappa \propto N^{\nu}$. Conflicting results have been obtained for the value of the exponent ν. In the linear response regime, the renormalization group theory predicts a universal value of $\nu = 1/3$ [2] while some recent calculations [3,4] based on the mode coupling theory suggest a value of $\nu = 1/3$ for the FPU-α model and a value of $\nu = 1/2$ for the FPU-β model. In the presence of a nonlinear on-site potential, it has been generally conjectured that Fourier's law is obeyed (i.e., normal heat conduction), which has been numerically verified for the Frenkel-Kontorova (FK) model as well as the ϕ^4 model [5–7]. It should be emphasized that most of these studies focus on the linear response regime, in which only small temperature differences are applied to the system. For heat conduction in the nonlinear response regime, only relatively few studies have been carried out. For example, the existence, and uniqueness of the stationary state of an anharmonic chain coupled to two heat baths at any arbitrary temperature difference has been proven in Ref. [8]. The deviation from local equilibrium in the nonlinear response regime has also been investigated [9,10]. However, a general theoretical framework for heat conduction in the nonlinear response regime is still lacking to date.

The study of heat conduction in low-dimensional systems also has practical implications. Recently it has been found that nonlinear systems with structural asymmetry can exhibit thermal rectification [11–16], which has triggered model designs of various types of thermal devices such as thermal transistors [17], thermal logic gates [18], and thermal memory [19]. It is worth pointing out that most of these studies are relevant to heat conduction in the nonlinear response regime, where the counterintuitive phenomenon of negative differential thermal resistance (NDTR) may be observed and plays an important role in the operation of those devices [17–19]. Here, NDTR refers to the phenomenon where the resulting heat flux decreases as the applied temperature difference (or gradient) increases. It can be seen that a comprehensive understanding of the phenomenon of NDTR, which is lacking at the moment, would be conducive to further developments in the designing and fabrication of thermal devices.

So far all existing studies on NDTR have been on models with structural inhomogeneity, for example the two-segment Frenkel-Kontorova model [17,20,21] and the weakly coupled two-segment ϕ^4 model [22]. Interestingly, there has not been any NDTR study on structurally homogeneous models so far, and it is still not clear whether NDTR can occur in a structurally homogenous lattice and what role structural inhomogeneity plays in the exhibition of NDTR. For harmonic systems attached to Langevin heat baths, theoretical studies [23] have shown that the heat flux is all the way proportional to the applied temperature difference, implying the absence of a NDTR regime. For anharmonic homogeneous systems, however, there has not yet been any conclusion on whether NDTR can occur in the nonlinear response regime. In view

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of this, we have carried out an extensive investigation on the heat-conduction behavior of various prototypical homogeneous nonlinear lattice models—the FK model, the ϕ^4 model and the FPU-β model. It was found that NDTR can occur in the FK model as well as in the ϕ^4 model, but not in the FPU-β model. For the ϕ^4 model, we have developed a phenomenological model that eventually predicts the existence of a critical system size for the occurrence of NDTR.

II. METHOD OF SIMULATION

The homogeneous lattice models investigated in this study are each described by a Hamiltonian of the form

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2}+V(x_{i+1}-x_i)+U(x_i), \tag{1}$$

For the ith particle along a one-dimensional lattice chain, x_i is the instantaneous displacement of the particle from its equilibrium position, p_i is the particle's instantaneous momentum, $V(x_{i+1}-x_i)$ is the nearest-neighbor interaction potential, and $U(x_i)$ is the onsite potential. The temperatures at the two ends of the one-dimensional lattice chain are fixed at T_+ and T_-, respectively. Since exact analytic solutions to these lattice models are generally very rare, numerical simulations have turned out to be an indispensable tool of investigation. In our nonequilibrium molecular dynamics simulations, Langevin heat baths [1] were used for controlling the temperatures at the two ends of each lattice chain and the fixed-boundary conditions $x_0=x_{N+1}=0$ were employed. For each of the one-dimensional lattice models under study, the equation of motion takes the form

$$\ddot{x}_i=-\frac{\partial H}{\partial x_i}-\gamma_i\dot{x}_i+\eta_i, \tag{2}$$

where $\gamma_i=\gamma(\delta_{i,1}+\delta_{i,N})$ and $\eta_i=\eta_+\delta_{i,1}+\eta_-\delta_{i,N}$. The noise terms $\eta_\pm$ denote a Gaussian white noise that has a zero mean and a variance of $2\eta_\pm k_B T_\pm$. The heat flux is given by $j=\langle F(x_{i+1}-x_i)p_{i+1}\rangle$, where $F(x)=-V'(x)$ and the notation $\langle\ldots\rangle$ denotes a steady-state average. At steady states, the numerically computed local heat flux is always constant along the chain (i.e., independent of position), and the local temperature is given by $T_i=\langle p_i^2\rangle$. A rescaled heat flux $J=Nj$ (usually referred to as the "total heat flux" in the literature [1]) is also considered for convenience sake. Note that Langevin heat baths instead of Nosé-Hoover heat baths were chosen for the simulations because the use of Nosé-Hoover heat baths might lead to unreliable results in the nonlinear response regime [24], particularly at very low or very high temperatures.

III. RESULTS

In the language of nonequilibrium thermodynamics, it would be interesting to understand the behavior of thermodynamic systems when they are driven away from equilibrium. For heat conduction in lattice systems described by Eq. (1), it would be interesting to understand how the resulting heat flux depends on the externally applied temperature difference $\Delta T=T_+-T_-$. When ΔT is small, the system is only weakly driven by the thermodynamic force so that the system falls within its linear response regime, i.e., the resulting heat flux j is directly proportional to ΔT. But when ΔT is sufficiently large, the relation between j and ΔT can become nonlinear. An instance of this is the exhibition of NDTR [17–22], which is characterized by the existence of a negative slope in the plot of j against ΔT and reminiscent of the well-known phenomenon of negative differential electrical resistance (NDER) in tunnel diodes [25]. As mentioned above, previous NDTR studies have all been on structurally inhomogeneous systems. This paper presents a first report on the exhibition of NDTR in homogeneous nonlinear lattices.

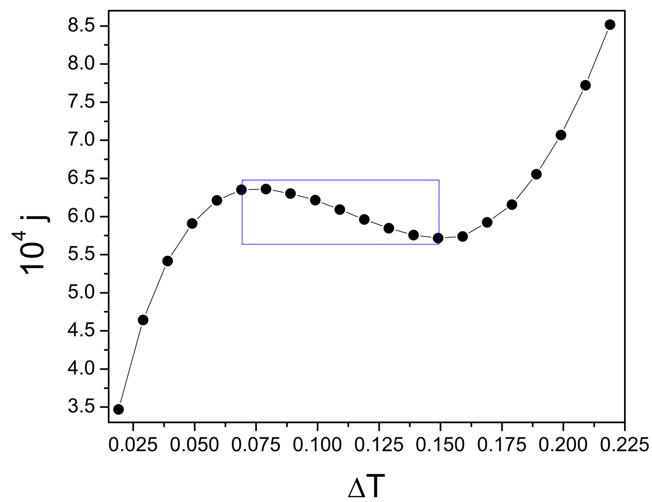

FIG. 1. (Color online) FK model: heat flux j as a function of the applied temperature difference $\Delta T=T_+-T_-$. NDTR occurs in an intermediate range of ΔT as indicated by the dotted rectangle. Here, $K=0.5$, $V=5$, $T_-=0.001$, and $N=32$.

A. FK model

The Hamiltonian of the FK model is given by

$$H_{\mathrm{FK}}=\sum_{i=1}^{N}\frac{p_i^2}{2}+\frac{K}{2}(x_{i+1}-x_i)^2-\frac{V}{(2\pi)^2}\cos 2\pi x_i. \tag{3}$$

Figure 1 shows the relation between j and ΔT at $K=0.5$, $V=5$, $T_-=0.001$, and $N=32$. When ΔT is sufficiently small, j and ΔT are proportional to each other and the system is within its linear response regime. But at larger values of ΔT, i.e., between $\Delta T=0.075$ and $\Delta T=0.15$, the system enters a nonlinear response regime where NDTR occurs. It is interesting to see that the curve in Fig. 1 mimics the typical NDER curves of tunnel diodes [25].

For the FK model, it was found that the regime of NDTR varies with the strength V of the onsite potential (Fig. 2). For decreasing V, the NDTR range of ΔT becomes smaller. This can be understood as follows: for decreasing V or increasing temperature (i.e., increasing ΔT in our case), it becomes easier for the particles to overcome the onsite potential via their thermal energy. Essentially, the system is approaching the harmonic limit where NDTR cannot occur. In addition, as

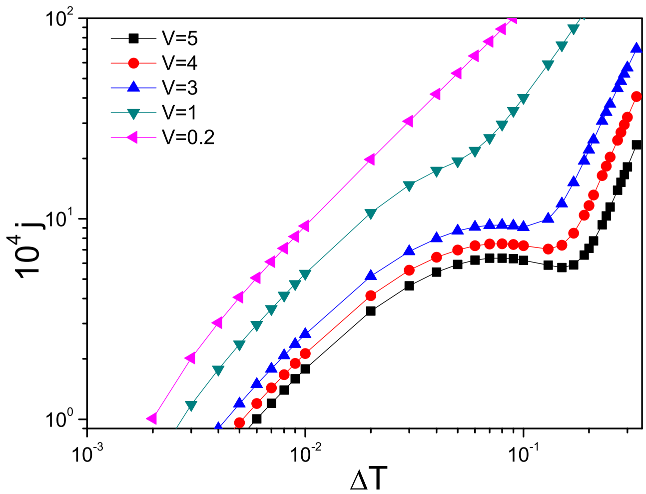

FIG. 2. (Color online) FK model: heat flux j as a function of ΔT for $V=0.2$, 1, 3, 4, and 5. Here, $K=0.5$, $T_-=0.001$, and $N=32$.

illustrated in Fig. 3, our numerical simulations show the exhibition of NDTR for a system size of $N=32$, 64, and 128 but not for the case of $N=512$. This suggests that the NDTR regime generally becomes smaller as the system size N increases. Note that there are two possibilities regarding the shrinkage of the NDTR regime for increasing system size: (a) the NDTR regime disappears at some finite critical system size N^*; OR (b) As long as the system size remains finite, the NDTR regime still exists; yet, when the system size is relatively large, e.g., $N=512$, the NDTR regime falls at very small values of ΔT which are not covered by our numerical simulations and which are possibly in the order of numerical error. Therefore, the question of whether there exists a finite critical system size N^* above which the NDTR regime no longer exists can only be answered analytically. As reported in the next section, this is exactly the case of the ϕ^4 model where our theoretical analysis predicts the existence of such a critical system size N^*. Regarding the system as equivalent to a set of equal-sized thermal resistors connected in series, the overall thermal resistivity of the system is simply the average over the local thermal resistivity everywhere in the bulk as well as the thermal resistivity at each individual boundary. As the system size N increases, the thermal resistivity at each boundary carries a smaller weight in the average thermal resistivity of the system. The coincidence of (a) NDTR occurring mainly in small-size systems and (b) the relative importance of thermal boundary resistance in small-size systems has led us to the speculation that NDTR is the result of some kind of boundary mechanisms (e.g., phonon-boundary scattering) or properties (e.g., thermal boundary resistance) that could potentially influence the spatially continuous heat flux j. This has motivated us to carry out an initial study on the relation between boundary temperature jumps and heat flow. Figure 4 shows how the heat flux j and the boundary temperature jump [9] $\delta T \equiv T(N)-T_-$ vary with the applied temperature difference ΔT. A general correlation between j and δT, which corresponds to the existence of thermal boundary resistance, can be seen.

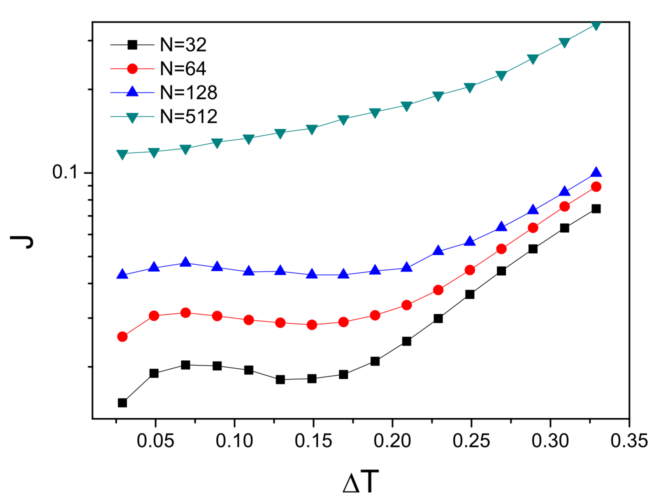

FIG. 3. (Color online) FK model: rescaled heat flux $J=Nj$ as a function of ΔT for $N=32$, 64, 128, and 512. Here, $K=0.5$, $T_-=0.001$, and $V=5$.

B. ϕ^4 model

What role does the onsite potential of a lattice model play in the occurrence of NDTR? Is the occurrence of NDTR related to the presence of a bounded onsite potential (e.g., the sinusoidal onsite potential in the FK model)? In this study, insights have been gained via a NDTR study of the ϕ^4 model, which has an unbounded onsite potential. Its Hamiltonian is given by

$$H_{\phi^4} = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1}-x_i)^2 + \frac{\lambda}{4}x_i^4, \tag{4}$$

where λ is termed the strength of the quartic onsite potential. It can be envisaged that the presence of such an "unbounded" onsite potential will contribute to a difference in conduction behavior between the ϕ^4 and the FK model. For the FK model, the particles can, at sufficiently high temperatures, overcome the "bounded" substrate potential via their thermal energy so that the system would behave like a harmonic system without the occurrence of NDTR. For the ϕ^4 model, since its onsite potential is unbounded, it is expected that such kind of "harmonic" behavior will not occur. In fact, it was found that there exists a critical temperature difference ΔT^* that separates the low-ΔT regime (i.e., low-temperature regime for T_- being fixed) of PDTR and the high-ΔT regime (i.e., high-temperature regime for T_- being fixed) of NDTR (Fig. 5). As shown in the figure, the value of ΔT^* decreases for increasing λ. Unlike the FK model, the ϕ^4 model does not have an upper bound for its NDTR range of ΔT. This is attributed to the "unboundedness" of the onsite potential of the ϕ^4 model. It was also found that the value of ΔT^* increases for increasing system size N (Fig. 6), and eventually approaches infinity in the thermodynamic limit. This is similar to the case of the FK model, where the regime of NDTR generally becomes smaller for increasing system size. Figure 7 illustrates how the temperature profile of the system changes for a variation of the system size from $N=32$ to $N=2048$ at some fixed values of T_+, T_-, and λ. As in the case

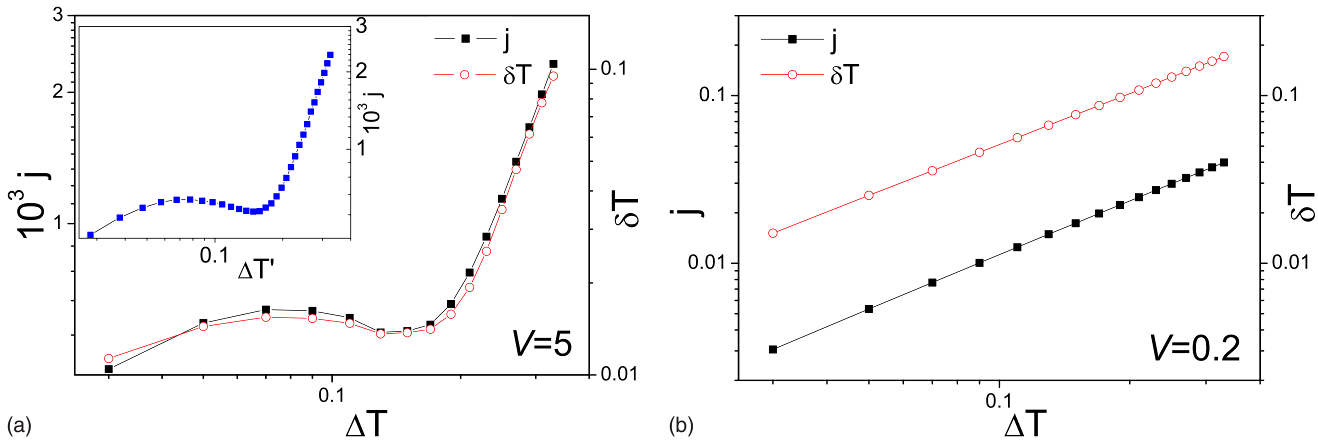

FIG. 4. (Color online) FK model: heat flux j and the corresponding boundary temperature jump δT as a function of ΔT for $V=5$ (left) and $V=0.2$ (right). Here, $K=0.5$, $T_{-}=0.001$, and $N=32$. The inset for the case of $V=5$ (left) shows a plot of j against the "inner" temperature difference $\Delta T' = T(1) - T(N)$. Note that it also displays the occurrence of NDTR and is practically the same as the plot of j against ΔT. This is because the boundary temperature jumps are typically at least one order of magnitude less than ΔT, meaning that ΔT and $\Delta T'$ are practically the same.

of the FK model, there also exists a temperature jump at each end of the ϕ^4 chain where the detailed relation of such boundary temperature jumps to the occurrence of NDTR remains to be understood.

It has been generally found that the thermal conductivity $\kappa(T)$ of the ϕ^4 model follows a power-law relation $\kappa(T) = AT^{-\alpha}$ with the temperature T [10]. The phenomenological parameters A and α can be evaluated by numerical fitting, e.g., $A=2.83$ and $\alpha=1.35$ for $\beta=1$ [10]. In the continuum limit, one can incorporate this power-law dependence of the thermal conductivity into the equation $j(x) = -\kappa(T)\nabla T(x)$ to obtain [7,9,10]

$$j = \frac{A(T_{+}^{1-\alpha} - T_{-}^{1-\alpha})}{(1-\alpha)N} \tag{5}$$

and

$$T(x) = T_{+}\left\{1 - \left[1 - \left(\frac{T_{-}}{T_{+}}\right)^{1-\alpha}\right]\frac{x}{N}\right\}^{1/1-\alpha} \tag{6}$$

through an integration along the lattice chain. The numerical results presented in Figs. 6 and 7 for the case of the largest system size, i.e., $N=2048$, are in good quantitative agreement with the curves of Eqs. (5) and (6), respectively. Note that Langevin heat baths were employed in our simulations while modified Nosé-Hoover heat baths were used in Refs. [7,10]. The agreement between the two methods suggests that the validity of the above continuum analysis is independent of the choice of heat baths. In particular, Eq. (5) predicts a saturation of the heat flux for $T_{+} \gg T_{-}$, meaning that in the continuum limit NDTR cannot occur, i.e., ΔT^{*} approaches to infinity. For increasing ΔT, such saturation is a result of the counterbalance of two competitive effects: As ΔT increases,

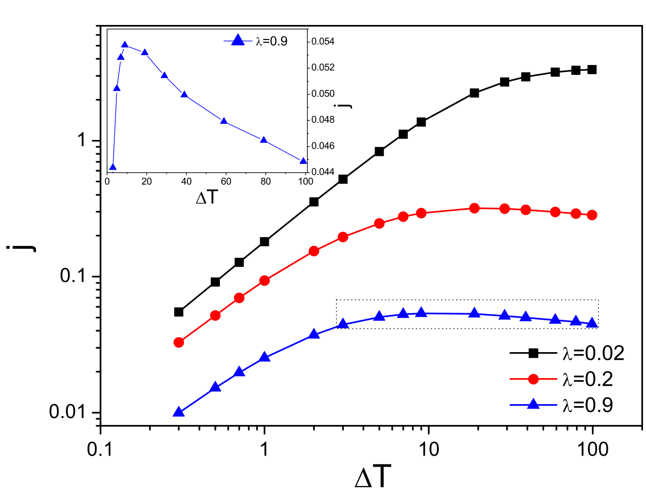

FIG. 5. (Color online) ϕ^4 model: heat flux j as a function of ΔT for $\lambda=0.02$, 0.2, and 0.9. Here, $T_{-}=1$ and $N=64$. The inset gives an enlarged view of the NDTR behavior within the dotted rectangle for $\lambda=0.9$.

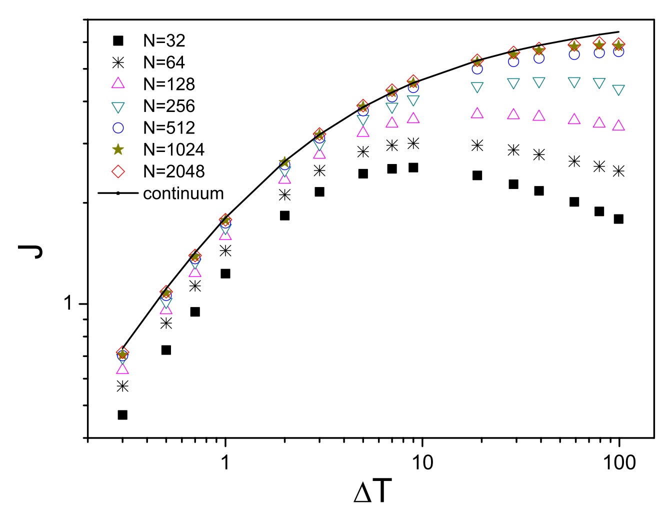

FIG. 6. (Color online) ϕ^4 model: rescaled heat flux $J=Nj$ as a function of ΔT for $N=64$, 128, 256, 512, 1024, and 2048. The solid line depicts the continuum limit as described by Eq. (5). Here, $T_{-}=1$ and $\lambda=1$.

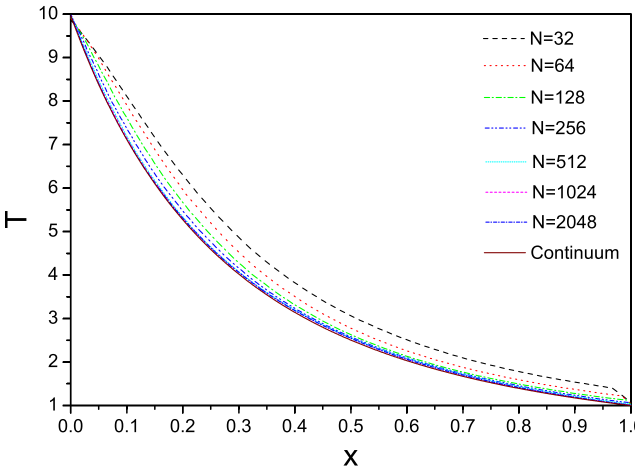

FIG. 7. (Color online) ϕ^4 model: temperature profiles (from top to bottom) for $N=32$, 64, 128, 256, 512, 1024, and 2048, where, for the ith particle, $x \equiv (i-1)/(N-1)$. The solid line depicts the continuum limit as described by Eq. (6). Here, $T_-=1$, $T_+=10$, and $\lambda=1$.

the heat flux j tends to increase due to the increase in the thermodynamic driving force. However, the corresponding decrease in the thermal conductivity of the system tends to slow down the conduction of heat.

Although the numerical data in Fig. 6 suggest a general increase in ΔT^* for increasing N, one still cannot conclude whether there exists a critical system size N^* above which NDTR cannot occur. This is because it is still possible that cases with an infinite ΔT^* (i.e., cases where NDTR can never occur) correspond only to the thermodynamic limit of an infinite N but not to any other case with a finite N. Therefore, to find out whether there exists such a critical system size N^*, addition information is needed, hence the following phenomenological model that provides a description of the size-induced crossover from the existence to the nonexistence of a NDTR regime. As mentioned above, the thermal conductivity κ follows a power-law relation with the temperature T in the linear response regime [10]. Following this, we assume a similar power-law relation

$$\kappa_{eff}(\bar{T}) = C(\bar{T}+t)^{-\gamma} \tag{7}$$

between the effective (nonlocal) thermal conductivity $\kappa_{eff} = Nj/\Delta T$ of the whole system and the average temperature $\bar{T}=(T_+ + T_-)/2$ for both the linear and the nonlinear response regimes. Here, $C>0$, $\gamma>0$, and t are fitted parameters that generally vary with the system size N. Note that this assumed power-law relation between κ_{eff} and $\bar{T}$ can be reduced to the power-law relation between κ and T for sufficiently small values of ΔT, i.e., in the linear response regime. For any fixed value of T_-, NDTR corresponds to

$$\left.\frac{\partial j}{\partial \Delta T}\right|_{T_-} < 0. \tag{8}$$

It can be easily shown that the above inequality is invalid for $\gamma \leq 1$. That is, NDTR occurs only when $\gamma > 1$ and $\Delta T > \Delta T^*$, where $\Delta T^* = 2(T_- + t)/(\gamma - 1)$.

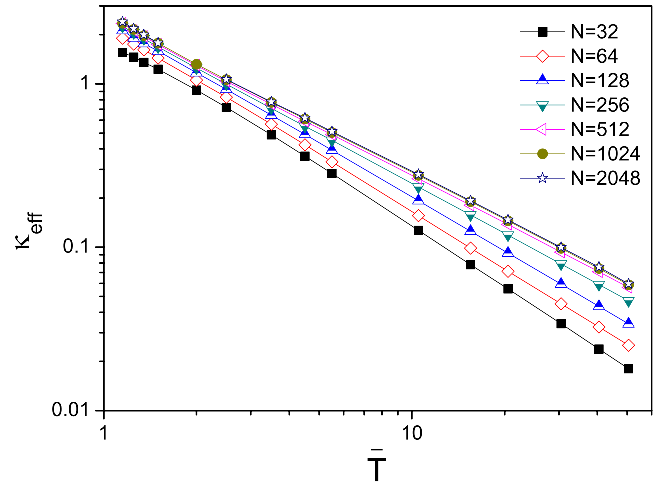

FIG. 8. (Color online) ϕ^4 model: effective thermal conductivity κ_{eff} as a function of the average temperature $\bar{T}=(T_+ + T_-)/2$ for $N=32$, 64, 128, 256, 512, 1024, and 2048. Here, $\lambda=1$ and $T_-=1$, with the covered values of T_+ corresponding to the same values of ΔT in Fig. 6. The straight curves in this log-log graph indicate that the assumed power-law relation in Eq. (7) is valid, even for the nonlinear response regime at $\Delta T \gg 0$ (i.e., $\bar{T} \gg 1$), and that the fitted parameter t is practically zero.

As shown in Fig. 8, the assumed power-law relation in Eq. (7) has been verified numerically across almost two orders of magnitude in $\bar{T}$ (i.e., also in ΔT) for a range of the system size from $N=32$ to $N=2048$. Figure 9 shows that, for increasing system size N, the scaling exponent γ decreases monotonously from $\gamma=1.23$ to $\gamma=0.96$. The critical system size N^* above which NDTR can never occur is at $N^* \approx 300$. Note that this is consistent with the numerical results in Fig. 6, where there exists a NDTR regime for the cases of $N=32$, 64, 128, and 256 but not for the cases of $N=512$, 1024, and 2048. It is worth pointing out that the conclusions from this phenomenological model can be applied to cases of any

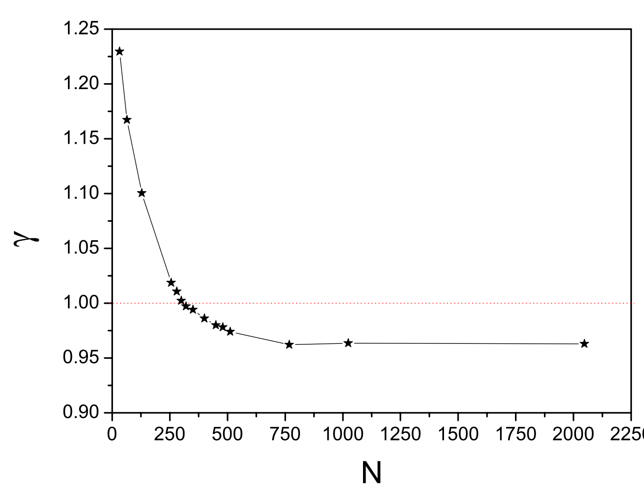

FIG. 9. (Color online) ϕ^4 model: scaling exponent γ as a function of the system size N. The crossover from the existence to the nonexistence of a NDTR regime for increasing N occurs at the critical exponent $\gamma=1$ (dotted line) where $N=N^* \approx 300$.

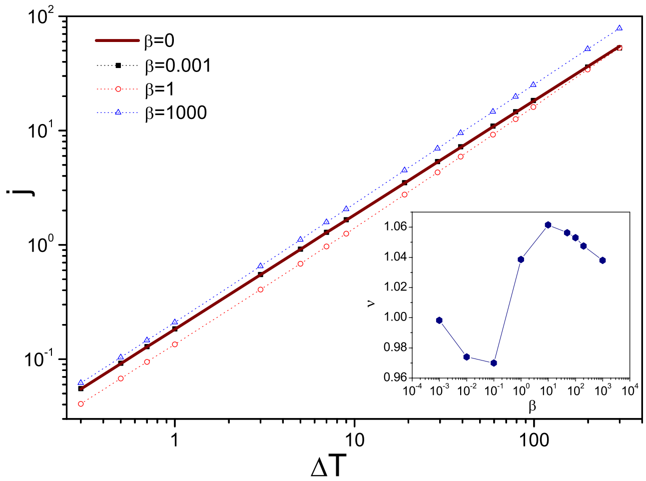

FIG. 10. (Color online) FPU-β model: heat flux j as a function of ΔT for $\beta=0.001$, 1, and 1000 in the FPU-β model. Here $T_{-}=1$. The results are fitted (dotted lines) well by $j \propto \Delta T^{\nu}$. As a reference, the bold solid line depicts the analytical solution for the heat flux in the harmonic limit ($\beta=0$), $j=\frac{1+2\chi^2-\sqrt{1+4\chi^2}}{4\chi^3}\Delta T$ (see [23]), where χ is the system-bath coupling. Here, $\chi=1$ was chosen for the numerical simulations. The inset shows that ν varies only within a relatively small range [0.97, 1.06] with the nonlinearity β of the interaction potential.

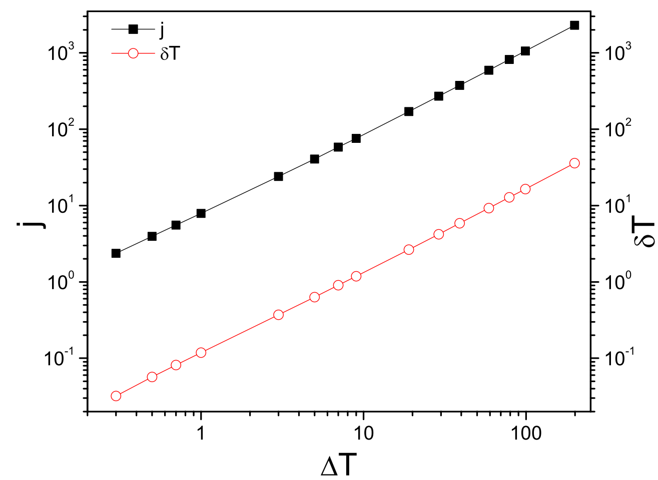

FIG. 11. (Color online) FPU-β model: heat flux j and the corresponding temperature jump δT versus ΔT. Here, $T_{-}=1$, $\beta=1$ and $N=64$.

arbitrarily large value of ΔT, and can therefore provide an answer to the question of whether NDTR can occur at values of ΔT that are too large to be considered in numerical simulations.

C. FPU-β model

The Hamiltonian of the FPU-β model is given by

$$H_{\mathrm{FPU}}=\sum_{i=1}^{N}\frac{p_i^2}{2}+\frac{1}{2}(x_{i+1}-x_i)^2+\frac{\beta}{4}(x_{i+1}-x_i)^4, \tag{9}$$

where β is referred to as the strength of the nonlinear interaction. As mentioned above, for the FK model, if the temperature is sufficiently high, the particles can overcome the onsite potential of the lattice so that the system behaves like a harmonic model. This means that the regime of NDTR, if exists, must be extremely small. The FPU-β model shares a similar situation with the harmonic model in that both of them do not have an onsite potential. Will NDTR cease to occur in the FPU-β model as in the case of a harmonic chain? As shown in Fig. 10, it was found that the heat flux j is practically proportional to the temperature difference ΔT. That is, $j \propto \Delta T^{\nu}$, where the numerically fitted exponent ν ranges only between 0.97 and 1.06 for a variation of β over six orders of magnitude from $\beta=0.001$ to $\beta=1000$. Extensive numerical simulations have also revealed the same quasilinear behavior for different values of the system size N, which suggests that NDTR generally cannot occur in the FPU-β model. Such quasilinear behavior corresponds to a similarity with the behavior of a harmonic chain ($\nu=1$), which might be due to the following reason: The FPU-β model, even in the case of strong nonlinear interactions (i.e., large values of β), can be treated as an effective weakly interacting phonon system via renormalization means [26,27]. Finally, it was also found for the FPU-β model that the boundary temperature jump exhibits a correlation with j (Fig. 11) as in the case of the FK as well as the ϕ^4 model.

IV. CONCLUSIONS AND DISCUSSION

Heat conduction in three prototypical homogeneous lattice models has been studied in both the linear and nonlinear response regime. As the applied temperature difference ΔT increases, the system undergoes a transition from the linear to the nonlinear response regime, with the latter being generally characterized by a nonuniform local temperature gradient. This study shows for the first time that NDTR can occur in homogeneous lattice models, in contrast to previous NDTR studies which all focus on inhomogeneous systems, e.g., two-segment models. It was found that NDTR can occur in the FK and in the ϕ^4 model, both of which consist of a nonlinear onsite potential. However, extensive numerical simulations suggest that NDTR cannot occur in the FPU-β model, which does not have a nonlinear onsite potential. For both the FK and the ϕ^4 model, the regime of NDTR becomes larger as the system size decreases or the strength of the nonlinear onsite potential increases. For the ϕ^4 model, the existence of a critical system size N^* above which NDTR can never occur was predicted from a theoretical analysis of the numerical data. Although the scaling assumption in Eq. (7) for the ϕ^4 model is well supported by numerical data, a first-principle derivation of this assumption is highly anticipated. In general, the observation of a larger NDTR regime at smaller systems has led us to the speculation that certain boundary mechanisms (e.g., phonon-boundary scattering) or properties (e.g., thermal boundary resistance) are related to the occurrence of NDTR, which has motivated us to carry out an initial study on the relation between boundary temperature jumps and heat flow. However, much further work is needed to identify the underlying physical mechanisms that are responsible for the occurrence of NDTR.

The presence of a nonlinear onsite potential facilitates the occurrence of phonon-lattice scattering [5], which generally becomes more significant for increasing temperature and can therefore contribute to a decrease in the thermal conductivity. In the case of the FK model, such phonon-lattice scattering is important only at sufficiently low temperatures where the dynamics of the particles is much influenced by the bounded onsite potential. As the applied temperature difference ΔT increases from zero with T_- being fixed, the increase in the thermodynamic driving force will drive an increase in the heat flux j. At higher values of ΔT (i.e., higher values of the system's average temperature), however, the effect of phonon-lattice scattering becomes so significant that NDTR occurs. But with a further increase in ΔT, the average temperature of the system has become sufficiently high such that the particles can overcome the bounded onsite potential via their thermal energy; Phonon-lattice scattering is no longer an important factor and therefore the regime of NDTR comes to an end, hence the S-shaped curves of j vs ΔT in Figs. 1–3. In the case of the ϕ^4 model, the dynamics of the particles is always influenced by the unbounded onsite potential and, for increasing temperature, the increase in phonon-lattice scattering is reflected by the power-law decrease of the thermal conductivity [Eq. (7)]. For increasing ΔT with T_- being fixed (i.e., increasing system's average temperature), the particles in the ϕ^4 model are not able to overcome the onsite potential as in the case of the FK model so that there is no upper bound of ΔT for the occurrence of NDTR (Fig. 6). In the case of the FPU-β model, the nonexistence of a NDTR regime might be due to the lack of phonon-lattice scattering in the absence of a nonlinear onsite potential.

As to the experimental fabrication of NDTR devices, the conclusion that NDTR mainly occurs in small-size systems is in line with the current trend of device miniaturization in the technological world [28]. The observation of NDTR in homogeneous systems shows that spatial inhomogeneity is not a necessary condition for the occurrence of NDTR. This implies that NDTR devices can be fabricated without involving the complicated control of interfacial properties as in the case of multisegment systems.

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