Temperature-dependent divergence of thermal conductivity in momentum-conserving one-dimensional lattices with asymmetric potential

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(Received 17 September 2018; published 1 February 2019)

In this study we used a nonequilibrium simulation method to investigate the temperature dependent divergence of thermal conductivity in a one-dimensional momentum conserving system with an asymmetric double well nearest-neighbor interaction potential. We show that across all temperatures thermal conductivity exhibits power-law divergence with the chain length and the value of the divergence exponent (α) depends on the temperature of the system. At low and high temperatures α reaches close to ~0.5 and ~0.33, respectively. Whereas in the intermediate temperature the divergence of thermal conductivity with the chain length saturates with $\alpha \sim 0.07$. Subsequent analysis showed that the estimated value of α in the intermediate temperature may not have reached its thermodynamic limit. Further calculations of local α revealed that its approach towards the thermodynamic limit is crucially dependent on the temperature of the system. At low and high temperatures local α reaches its thermodynamic limits in shorter chain lengths. On the contrary, in the case of intermediate temperature its progress towards the asymptotic limit is nonmonotonic.

DOI: 10.1103/PhysRevE.99.022103

I. INTRODUCTION

Understanding the heat conduction in finite dimensional systems has been a longstanding and much debated problem for some time. Particularly, a major focus has been establishing Fourier's law of heat conduction for low-dimensional systems. In Fourier's law the heat flux (J) becomes proportional to the temperature gradient (∇T) with thermal conductivity (κ) as the proportionality constant, $J = -\kappa \nabla T$. In pursuit of finding out the microscopic basis of the macroscopic law of heat conduction, lattice models of a one-dimensional (1D) chain of particles connected by nonlinear interaction potentials have been investigated [1,2]. These investigations concluded that in 1D momentum conserving nonlinear lattices, the heat flux follows a power-law scaling with the system size (N), $J \sim N^{\alpha-1}$ [3], which is a deviation from Fourier's law that dictates $J \sim N^{-1}$. Therefore in the thermodynamic limit of large N, the thermal conductivity diverges with the system size and it scales as $\kappa \sim N^{\alpha}$. Both theoretical calculations [1,4–15] and numerical simulations [2–4,7,16–20] of lattice models with various variants of the Fermi-Pasta-Ulam (FPU) interaction potential predicted the anomalous nature of κ in 1D momentum conserving systems. Specific values of α varied from one calculation to other [2]. However in all cases the exponent lies in the range of $0 \leqslant \alpha \leqslant 1$. The specific value of α was found to depend on the nature of nonlinearity in the interaction potential. However, generally three different values $\alpha = 2/5$ [4,21], $\alpha = 1/3$ [6,7,11,18,19], and $\alpha = 1/2$ [8,10,12,13] have been obtained in different calculations. Further momentum conserving chains with asymmetric potentials that allow bond dissociation (e.g., Lennard-Jones or Morse potential) were predicted to show convergent thermal conductivity [25,26].

However, there has been report of finite thermal conductivity in momentum conserving systems with an asymmetric interaction potential [22]. This result was in contradiction with theoretical and numerical results in 1D momentum conserving systems that was predicted to have divergent conductivity. The prediction of normal thermal conductivity for asymmetric lattice in 1D at low temperature was debated and the possibility of strong low-temperature finite-size effects were discussed by Das *et al.* [23]. Further, using the equilibrium Green-Kubo method of heat current autocorrelation, Wang *et al.* [24] predicted the length scale (N) dependence of the divergence exponent (α) for single-well asymmetric FPU-$\alpha\beta$ and LWAII [22] 1D lattices. They concluded that α reaches its asymptotic thermodynamic limit at a much longer chain length in asymmetric LWAII lattice as compared to asymmetric FPU-$\alpha\beta$ lattice. Therefore at shorter length scale α becomes a function of N. However N dependence of α may further be affected by parameters in the potential and more importantly the average temperature of a heat bath. Temperature dependent divergence was reported in the symmetric double well (DW) potential where κ diverged with $\alpha = 0.33$ at high temperature and at low temperature it showed weak divergence [19]. A similar conclusion was also made for the FPU-$\alpha\beta$ lattice with $\alpha = 0.4$ at high temperature and weak divergence at low temperature [25]. Thus temperature dependent divergence in an asymmetric momentum conserving lattice needed further systematic investigations.

In this paper we addressed the problem of temperature dependent divergence of thermal conductivity in 1D nonlinear lattice with an asymmetric nearest-neighbor interaction potential. We used an asymmetric DW potential for nearest-neighbor interaction among the particles in the lattice. We varied the heat bath temperatures and, using the nonequilibrium simulation method, we calculated κ for the lattice of various sizes with different degrees of asymmetry in the interaction

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potential to investigate the temperature dependence of the divergence of κ.

II. MODEL AND RESULTS

We have considered a one-dimensional lattice model with a nearest-neighbor interaction potential. The classical Hamiltonian for the model can be represented as

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

where x_i and p_i are the displacement from equilibrium position and momentum of the ith particle, respectively. The mass and the total number of particles on the chain are given by m and N, respectively. The nearest-neighbor interaction potential between the particle i and $i-1$ is given by $V(x_i - x_{i-1})$. As we have not considered any external potential, our lattice model becomes a momentum conserving chain. We fixed $m = 1$ for our calculations throughout. We have chosen the asymmetric double well nearest-neighbor interaction potential of the form given by

$$V(x) = -\tfrac{1}{2}k_2x^2 + \tfrac{1}{3}k_3x^3 + \tfrac{1}{4}k_4x^4, \tag{2}$$

where k_2, k_3, and k_4 are three positive constants. This potential belongs to the general class of the FPU-$\alpha\beta$ potential and due to the cubic nonlinearity the potential becomes asymmetric $[V(x) \neq V(-x)]$. In Fig. 1 we present the asymmetric nature of the double well potential for two different values of cubic nonlinear parameter k_3 that determines the degree of asymmetry of the potential. With an increase in the value of k_3 the asymmetric nature of the potential increases.

In order to study the thermal conduction through the nonlinear chain using the nonequilibrium simulation method, both ends of the lattice are connected to Langevin heat baths having different temperatures. The equation of motion of the ith particle in the chain is given by

$$\begin{aligned}\ddot{x}_i = {} & k_2(2x_i - x_{i+1} - x_{i-1}) - k_3[(x_i - x_{i-1})^2 - (x_{i+1} - x_i)^2] \\ & - k_4[(x_i - x_{i-1})^3 - (x_{i+1} - x_i)^3] - \gamma_i\dot{x}_i + \eta_i,\end{aligned} \tag{3}$$

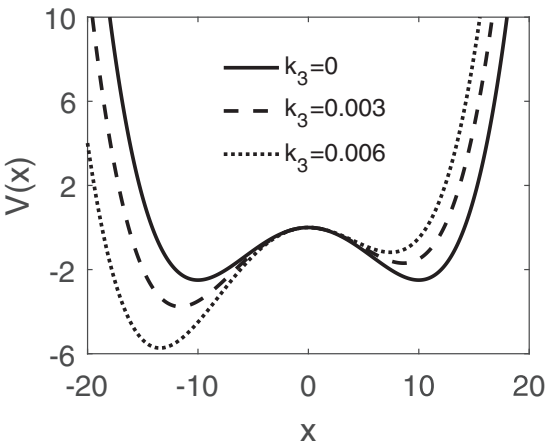

FIG. 1. Schematic representation of the double-well (DW) nearest-neighbor interaction potential, $V(x)$, with different values of asymmetric parameter k_3. $k_2 = 0.1$ and $k_4 = 0.002$.

where the fluctuation (η_i) and dissipation (γ_i) terms are defined as $\eta_i = \eta_L\delta_{i,1} + \eta_R\delta_{i,N}$ and $\gamma_i = \gamma(\delta_{i,1} + \delta_{i,N})$, respectively. The heat baths are characterized by the fluctuation-dissipation relations followed by the two Markovian heat baths, $\langle\eta_L(t)\eta_L(t')\rangle = 2\gamma k_B T_L\delta(t-t')$ and $\langle\eta_R(t)\eta_R(t')\rangle = 2\gamma k_B T_R\delta(t-t')$. The γ, k_B, T_L, and T_R are the dissipation constant, Boltzmann constant, temperatures of left and right heat baths, respectively. The values of Boltzmann constant (k_B) and the dissipation constant (γ) were chosen to be unity throughout. We varied the left and right bath temperatures (T_L and T_R) to investigate the effect of temperature on the divergence behavior of thermal conductivity. In this context we defined two relevant quantities: the temperature difference, $\Delta T = T_L - T_R$, and the average temperature, $T = (T_L + T_R)/2$.

The instantaneous local heat current between ith and $(i+1)$th is defined by

$$j_i = \frac{1}{2}(\dot{x}_i + \dot{x}_{i+1})\frac{\partial H}{\partial x_i}. \tag{4}$$

Defining the time-averaged local heat current as $J_i = \lim_{t\to\infty}\frac{1}{t}\int_0^t j_i(\tau)d\tau$, that reaches a nonequilibrium stationary state across the lattice after a long time, the global heat current in the lattice is given by

$$J = \sum_{i=1}^{N-1}\frac{J_i}{N-1}. \tag{5}$$

The thermal conductivity is related to the steady state global heat current as

$$\kappa = \frac{JN}{\Delta T}. \tag{6}$$

If the global heat current follows $J \sim N^{-1}$ scaling then the thermal conductivity becomes convergent in the thermodynamic limit (large N). However in 1D momentum conserving systems, J has been predicted to scale as $J \sim N^{\alpha-1}$. Thus κ becomes divergent with a power-law scaling relation as $\kappa \sim N^{\alpha}$.

In order to numerically integrate the dynamical equations (3), we used the fourth order Runge-Kutta method. We chose to use fourth order Runge-Kutta method to achieve higher accuracy in our calculations although it leads to a considerable increase in simulation time. We typically ran 2–5×10^{10} iterations in numerical integrations with an integration step length of 0.01. In the DW potential (2) we fixed $k_2 = 0.1$, $k_4 = 0.002$, and varied k_3 (0.003 or 0.006) in order to explore the effect of asymmetry on the nature of divergence in κ. Further to investigate the temperature dependence of divergence we chose various combinations of T and ΔT (T, ΔT). We used a fixed boundary condition (BC), $x_0 = x_{N+1} = 0$, in our calculations. Previous works highlighted the importance of boundary conditions in the heat conduction in lattice models [23,27].

In Fig. 2(a) we show the divergence of thermal conductivity for the asymmetric potential ($k_3 = 0.003$) with varying average heat bath temperatures keeping the ΔT fixed. The chosen (T, ΔT) pairs were (9.5, 1.0); (4.5, 1.0); (1.5, 1.0). For these three different values of T the system exhibits

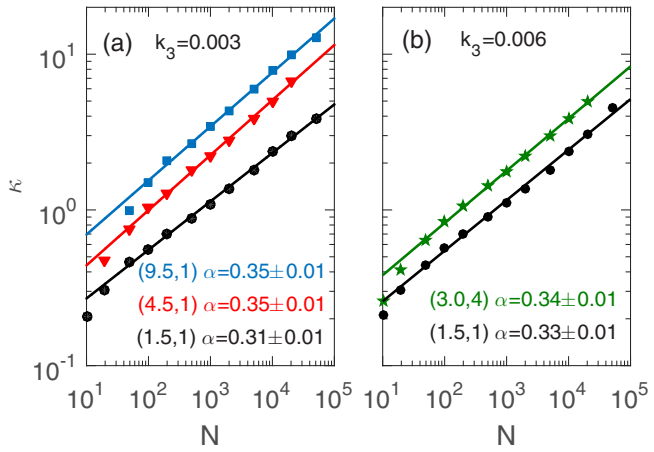

FIG. 2. Divergence of thermal conductivity, κ, as a function of chain length, N. Different colored symbols represent simulations with different average bath temperatures with fixed temperature difference, (T, ΔT); circle: (1.5,1), triangle: (4.5,1), square: (9.5,1), and star: (3.0,4). Solid lines are from power-law fitting ($\kappa \sim N^{\alpha}$). The values of α are indicated inside the plots for (a) $k3 = 0.003$ and (b) $k3 = 0.006$.

power-law divergence of thermal conductivity with α ranging between 0.31–0.35. These α values are similar to the predicted $\alpha = 1/3$ by renormalization group theory, mode coupling theory, and many numerical simulations [6,7,10,11,18,19]. We found a similar divergence of κ for the same system with higher asymmetry ($k_3 = 0.006$) in the interaction potential [Fig. 2(b)]. One important aspect of these divergence behaviors is that the average temperature of the system is large. Therefore at the high temperature limit the asymmetric-DW-momentum-conserving system behaves similar to the symmetric-FPU-$\alpha\beta$-momentum-conserving system.

We next investigated the divergence behavior of thermal conductivity for a range of average temperature values in the intermediate to low T limits again by varying the heat bath temperatures T_L and T_R. Particularly we aimed to determine the nature of divergence in the intermediate and low temperature regimes. In Fig. 3 we show the divergence of κ in different average temperatures of the system with $k_3 = 0.003$. Figure 3 indicates that the qualitative nature of divergence changes depending on the average temperature of the heat bath. The conductivity diverged sharply with $\alpha = 0.49$ at very low temperature ($T = 0.075$). With an increase of temperature ($T = 0.15$) the divergence becomes shallow with $\alpha = 0.18$ and at $T = 0.3$, the thermal conductivity appears to saturate with $\alpha = 0.07$. At high temperature ($T = 1.5$) κ shows its usual divergence behavior with $\alpha = 0.31$. The striking feature of the temperature dependent thermal conductivity here is that two different types of scaling behaviors of κ at very low ($\alpha = 0.49$) and very high ($\alpha = 0.31$) temperatures. Further, the very weak divergence of thermal conductivity (or saturation of κ with N) in the intermediate T poses a possibility of validity of Fourier's law. In addition, consistent with previous observations [23,25], we also find the weak divergence with the fixed BC even though fixed BC does not allow a thermal expansion that was known to provide additional avenue of

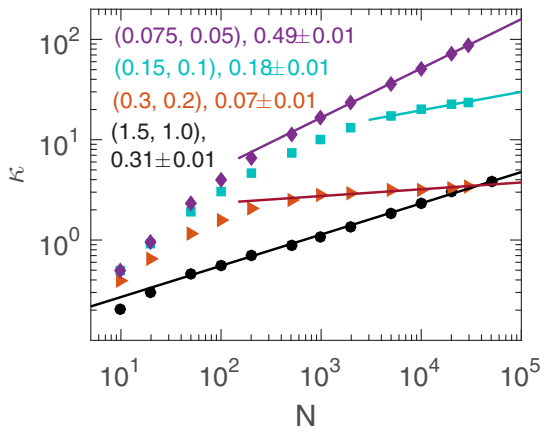

FIG. 3. Divergence of κ as a function of N for different average T and ΔT; circle: (1.5,1), triangle: (0.3,0.2), square: (0.15,0.1), and diamond: (0.075,0.05). The asymmetric parameter k_3 was 0.003. The α values are indicated inside the plot.

phonon scatterings leading to normal conductivity. Similar saturation of κ with N was first reported in an asymmetric lattice by Zhong *et al.* [22] and it was proposed by them that the system follows Fourier's law. However in an asymmetric FPU-$\alpha\beta$ potential whether the saturation was indeed due to the asymmetric nature of the interaction potential or not was discussed later [23,24]. Repeating calculations with higher asymmetry of the potential ($k_3 = 0.006$) also resulted similar observations as in $k_3 = 0.003$ (Fig. 4). Thus our simulation results indicate that the values of α depend on the temperature of the system in the asymmetric DW interaction potential.

To determine the temperature dependence of α, we plotted the α as a function of T for two different values of asymmetric parameter k_3 (Fig. 5). With an increase in T, α decreases sharply and, passing through a minimum, it increases to saturate with $\alpha = 0.35$ at high T. The weakest divergence of κ occurs at the intermediate T both for low and high asymmetries of the potential. This type of turnover behavior

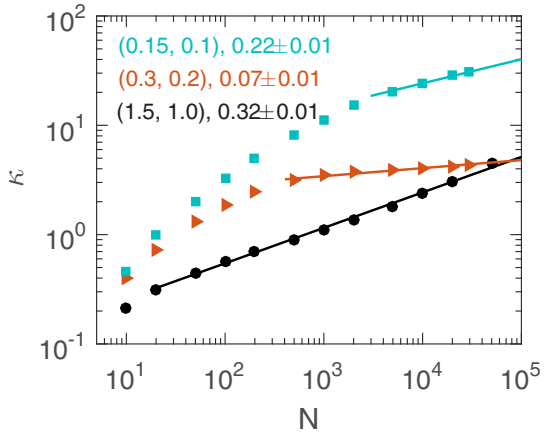

FIG. 4. Divergence of κ with N at different temperatures with asymmetric parameter $k_3 = 0.006$. (T, ΔT) pairs are: circle (1.5,1), triangle (0.3,0.2), square (0.15,0.1).

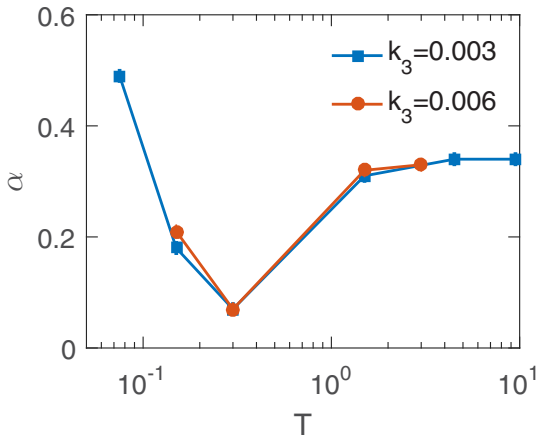

FIG. 5. Temperature dependence of α for two different values of asymmetric parameters k_3. The sizes of error bars on α are nearly the same as the sizes of the markers.

has been reported in the recent past [28,29] in the case of the 1D anharmonic chain. The comparison of α vs. T for low and high k_3 indicates that the divergence behaviors of thermal conductivity for different asymmetry values are identical. If the saturation of κ in this system was an asymmetry induced effect then there must have been a shift in α vs. T plots for the two different values of k_3. However the two curves overlap with each other. Further for the same reason, expectedly higher asymmetry would have resulted saturation of κ at lower N as compared to lower asymmetry [23]. The comparison of κ vs. N profiles for higher and lower asymmetry at different T (Fig. 6) do not indicate any such asymmetry induced early saturation of κ. These results and analyses point out that the saturation of κ may be a finite length effect occurring only at intermediate T. However our results does point out that the nature of divergence is indeed temperature dependent.

In order to determine the finite-size effect on α we calculated the local divergence coefficient, α_N, by determining the local slope in κ vs. N line. In Fig. 7 we present the α_N as a function of N estimated at various T for two different values

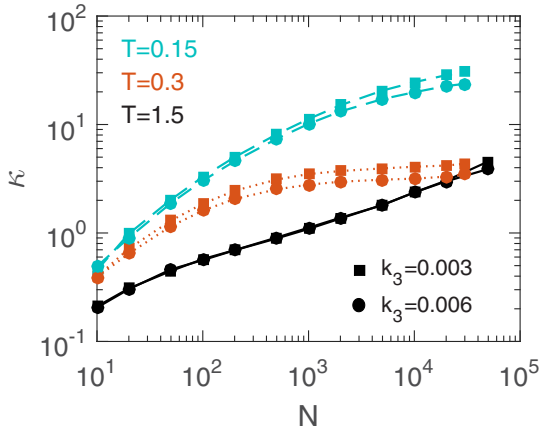

FIG. 6. Comparison of the divergence of κ with N for different values of asymmetric parameter k_3 at various average bath temperatures, T. Solid line: $T = 1.5$, dotted line: $T = 0.3$, and dashed line: $T = 0.15$.

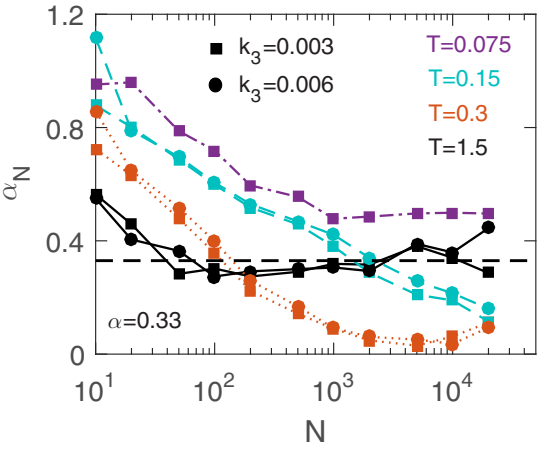

FIG. 7. Plot of local divergence coefficient α_N with N for different values of asymmetric parameter k_3 and at different average bath temperature, T. The α_N was estimated by calculating the local slope of κ vs. N plots given in Figs. 3 and 4. Solid line: $T = 1.5$, dotted line: $T = 0.3$, dashed line: $T = 0.15$, and dashed-dot line: $T = 0.075$. The horizontal dashed line represents $\alpha = 0.33$.

of asymmetry parameter. At high T ($T = 1.5$) the well-known thermodynamic limit of 0.33 is achieved at the shorter length of the chain and α_N settles nearly with that value for a large range of N. On the other hand, at very low T ($T = 0.075$), α_N appeared to settle at $\alpha \sim 0.5$ value, indicating the different scaling behavior of the system depending on the temperature of the system. However at the intermediate T ($T = 0.3$) with increasing N, α_N decreases below the thermodynamic limit ($\alpha = 0.33$, dashed line in Fig. 7) and, passing through a minimum, it shows an increasing trend for both values of asymmetry parameters. A similar trend was seen for $T = 0.15$ although without the minimum as probably the minimum is located at larger N. As at these two temperatures the local α does not settle to a particular value, it may be concluded that the values of α at the intermediate T are not from the thermodynamic limit of the system.

The presence of two wells separated by a barrier in the DW interaction potential makes the lattice system somewhat different as compared to a usual FPU class of single-well interaction potentials. At the high temperature regime, due to the increased thermal noise from the heat baths the system will be able to transition between the two wells. However, at the low temperature regime the system will be trapped in one of the wells depending on the initial state of the system. In order to assess the temperature dependent dynamic nature of the system, we calculated $\frac{1}{N-1}\sum_{i=1}^{N-1}|\langle x_{i+1} - x_i\rangle|$, an order parameter [29], at various temperatures for two different values of asymmetry parameter k_3 [Fig. 8(a)]. This order parameter essentially reflects the equilibrium average of absolute displacement from the adjacent particle. We find that the value of the order parameter saturates to two distinct regimes at low and high temperatures indicating the temperature dependent disparate nature of the system. The two different types of divergence exponents of thermal conductivity ($\alpha \sim 0.5$ and $\alpha \sim 0.33$) in the low and high T thus correlate with the order parameter of the system. The qualitative nature of the order parameter does not depend on the asymmetry parameter k_3.

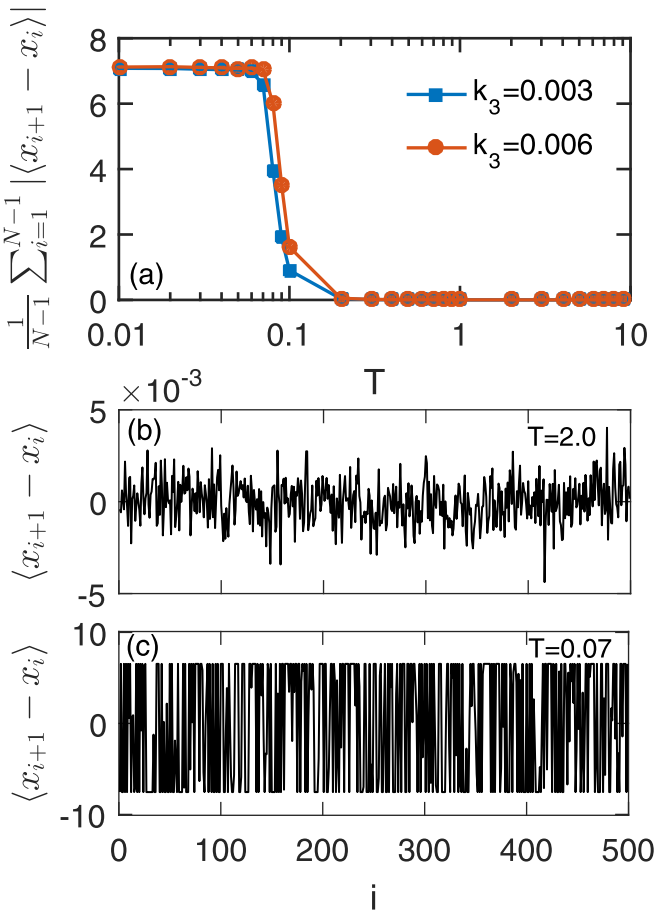

FIG. 8. (a) Temperature dependence of the order parameter for a chain with $N = 500$. The average displacement from the adjacent particle along the chain at $T = 2.0$ (b) and $T = 0.07$ (c).

Further we plotted the ensemble averaged displacement with the adjacent particle, $\langle x_{i+1} - x_i \rangle$, of a chain with $N = 500$ at high [Fig. 8(b)] and low [Fig. 8(c)] temperatures and these two plots suggest the dichotomous dynamical behavior of the lattice with DW potential. Particularly the confinement of the system in the two wells is evident at low T. Whereas at high T the fluctuations are more or less homogeneous. Therefore our estimated temperature dependent divergence characteristics of thermal conductivity is due to the distinct qualitative nature of the system at low and high T.

In the previous studies of the thermal conductivity of nonlinear lattice with DW or FPU-$\alpha\beta$ potential, the values of the coefficients, k_2, k_3, and k_4 in the potential (2) were chosen to be in the range of 1–2 [19,23–25,29]. However in our calculations we have chosen a different set of values for these coefficients and particularly the values ($k_2 = 0.1$, $k_3 = 0.003/0.006$, $k_4 = 0.002$) are much smaller than previously used values. In order to ensure that the contributions from the cubic and quartic terms in the potential are not negligible, we calculated the ensemble average of second, third, and fourth order terms in the potential (Fig. 9) at different temperatures. Our calculations indicate that the contributions from the cubic and the quartic terms are not negligible as compared to the quadratic term. Further the values of these terms show a non-monotonous temperature dependence that is

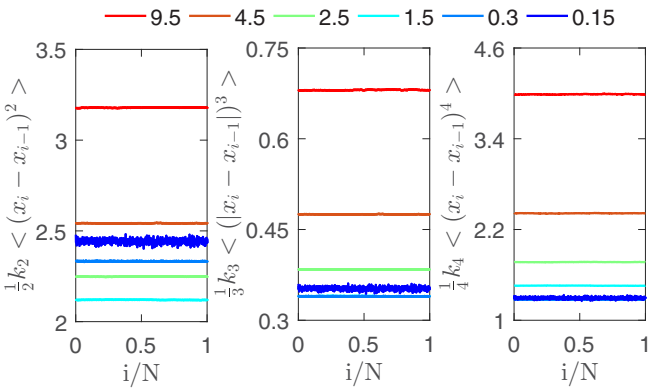

FIG. 9. Absolute average contributions of second, third, and fourth order terms in the potential for a chain with $N = 1000$ and $k_3 = 0.003$. The values of temperature are indicated at the top of the figure. The system behaves similarly with $k_3 = 0.006$ as well.

consistent with the temperature dependent scaling of thermal conductivity. Based on the used values k_2, k_3, and k_4, the absolute values of the coefficients in the DW potential (2) were 0.05, 0.001/0.002, and 0.0005. The progressively decreasing values of these coefficients further justifies the truncation of the polynomial beyond fourth order in Taylor expansion [30].

III. CONCLUSION

Understanding the divergent nature of thermal conductivity in low-dimensional systems has been a longstanding problem. A large number of theoretical and numerical calculations on 1D momentum conserving systems concluded power-law divergence of thermal conductivity with the length of the lattice [1,2]. In this study we used the nonequilibrium simulation method to show that the divergent nature of κ in 1D asymmetric lattice depends on the temperature of the heat baths. In the thermodynamic limit, the system exhibits $\alpha \sim 0.5$ and $\alpha \sim 0.33$ at low and high T, respectively. Therefore our calculations point out two different scaling behaviors of the same system depending on the temperature of the system. At low T our estimated value of α (~ 0.5) becomes the same as given previously by mode coupling theory [8,10,12,13]. Whereas at high T our calculation leads to an α (~ 0.33) as predicted previously by renormalization group analysis [6,11]. Further at the intermediate T, κ appears to saturate against N with a very small value ($\alpha = 0.07$). A similar weak divergence of κ has been reported before in the case of 1D asymmetric momentum conserving lattice [22] and it was characterized as the validity of Fourier's law by the asymmetric system. However later it was determined that the behavior may not be associated with the *true* thermodynamic limit of the system [23,24]. In order to probe the weak divergence of κ in the intermediate T, we calculated local divergence exponent, α_N, and showed that in intermediate T, α_N does not saturate to a fixed value in the length scale of our simulations. Here α_N decreases with N and while passing through a minima it showed a tendency to increase again. Had the system reached its thermodynamic limit, there should not have any further increase of the local α. On the contrary in the low and high temperatures α_N decrease with N and saturate to its respective

thermodynamic limits independent of the extent of asymmetry in the interaction potential. Therefore our calculations indicate that the approach to the thermodynamic limit of α is indeed temperature dependent in the case of the asymmetric interaction potential. We emphasize that our finding of the temperature dependent divergence of thermal conductivity in an asymmetric double well interaction potential may as well be obtained in the case of symmetric double well potential as there is no significant dependence of asymmetry on the divergence behavior.

ACKNOWLEDGMENT

This work is partially supported by Major Research Project scheme of University Grants Commission, India (MRP-MAJOR-CHEM-2013-43860).

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