

# Unraveling the challenges of phase transition and temperature-dependent thermal conductivity in the one-dimensional rotor model

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The one-dimensional rotor model is a classical momentum-conserving system that exhibits normal heat conduction, making it a valuable platform for studying thermal transport. Despite progress in understanding its transport properties, two key issues remain open: (1) whether a phase transition from normal to anomalous heat conduction occurs as temperature decreases and (2) how thermal conductivity  $\kappa$  depends on temperature. Using molecular dynamics simulations and Green-Kubo formalism, we demonstrate that although normal conduction may persist theoretically at any nonzero temperature, the exponentially increasing mean free path at low temperatures renders it practically unobservable, supporting the existence of an effective phase transition. Furthermore, we find that  $\kappa$  exhibits a double-exponential temperature dependence— $\kappa \sim e^{2.54/T}$  at high temperatures and  $\kappa \sim e^{0.49/T}$  at low temperatures—with an intermediate power-law regime  $\kappa \sim T^{-3.2}$  dominated by nonlinearity. To isolate the role of nonlinearity, we study a modified rotor model with suppressed phase jumps, which exhibits  $\kappa \sim T^{-3.6}$ , confirming the influence of interaction nonlinearity. These findings deepen the understanding of temperature-dependent transport in low-dimensional systems.

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## I. INTRODUCTION

Heat conduction in one-dimensional (1D) systems has received broad interest due to its foundational role in nonequilibrium statistical physics and its wide range of practical applications, including, but not limited to, thermal rectification [1–5], heat management and control [6–15], and thermoelectric energy harvesting [16–21]. It has been found that heat conduction in 1D systems often manifests anomalous behavior, deviating from Fourier's law  $j = -\kappa \nabla T$ , where  $j$  is the heat current,  $\kappa$  is the thermal conductivity, and  $\nabla T$  is the temperature gradient. Specifically, the thermal conductivity  $\kappa$  increases with system size  $L$  as  $\kappa \sim L^\alpha$ , where  $0 < \alpha \leq 1$  is the divergent exponent [22–24].

The 1D rotor model, a classical model analogous to quantum spin system, features periodicity and finiteness in its interaction potential, along with the formation of localized rotational modes and phase jumps between potential barriers in its dynamics, making it an extraordinary example of heat transport [25–27]. In 2000, two independent research groups demonstrated that the 1D rotor model conveys normal heat conduction, even though its momentum is conserved [28,29]. Since then, energy transport in the rotor model has attracted extensive attention, leading to several important discoveries, such as the key role of conserved quantities in energy transport [30–32], Gaussian diffusion of momentum

[33], coupled transport and nonequilibrium phase transitions [34,35], thermal rectification [36–38], negative differential thermal resistance [39,40], and subdiffusive energy transport in the long-range rotor model [41,42].

Notwithstanding these advances, to the best of our knowledge, two open questions regarding energy transport in the 1D rotor model remain: (1) Is there a phase transition from normal to anomalous heat conduction as the temperature decreases? If so, what is the critical temperature  $T_c$ ? (2) What is the temperature dependence of the heat conductivity  $\kappa$ ?

The first problem was initially raised by Gendelman and Savin in their original paper on heat conduction in the 1D rotor model, where they suggested that the phase transition temperature  $T_c$  lies within [0.2, 0.3], considering the formation of the localized rotational modes [28]. This argument quickly attracted attention. Based on large-scale equilibrium and nonequilibrium molecular dynamics simulation (MDS), Yang and Hu, in their commentary, argued that the 1D rotor model presents normal heat conduction at temperature  $T = 0.2$ , stating that  $T = 0.2$  is not the critical temperature [43]. Nevertheless, they acknowledged the possibility of the phase transition remaining an open question. In their reply, Gendelman and Savin accepted that  $T = 0.2$  is not the critical temperature, but maintained the viewpoint of abnormal heat conduction in low-temperature limit, which is difficult to demonstrate in numerical simulations due to the enormous demands for computational resources [44]. The existence of the phase transition was also supported by a theoretical analysis of heat conduction in the harmonic-pinned 1D rotor model [45]. Interestingly, Gendelman and coworkers later provided a revised perspective, suggesting that the 1D rotor model reveals normal heat conduction at any nonzero temperature, and that the lower the temperature, the larger the system size required to observe normal heat conduction [38,46,47].

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The phase transition problem also gained insights from the nonlinear fluctuating hydrodynamics (NFH) developed by Spohn and coworkers [48–50]. According to NFH, the conserved quantities are essential in determining the heat conduction properties of 1D systems. The phase jumps of rotors between potential barriers break the conservation of stretch (the angle difference between neighbor rotors) leading to normal heat conduction in the 1D rotor model. However, the transition rate becomes negligibly small as temperature  $T \rightarrow 0$ , since the transition rate decreases exponentially as  $\rho \sim e^{-\Delta V/T}$ , where  $\Delta V$  is the height of the potential barrier. Given that, H. Spohn suggested that heat conduction in the 1D rotor model may resemble that in the Fermi-Pasta-Ulam-Tsingou (FPUT) model [30]. In other words, there is a phase transition in the 1D rotor model. Interestingly, within the same NFH framework, Das and Dhar suggested that heat conduction in the 1D rotor model is always normal, provided the temperature is nonzero, as the phase jumps always occur, breaking the stretch conservation [31]. Furthermore, although the phase transition is considered to exist in the classical XXZ spin model, which shares similarities with the 1D rotor model, the authors propose that no such phase transition occurs in the 1D rotor model [32].

Considering the difficulty in calculating the heat conductivity in low-temperature regimes, Li *et al.* turned to study the problem from the perspective of heat conductance [51,52]. They suggested the nonexistence of the phase transition in the 1D rotor model, based on the observation that the saturation temperature of heat conductance decreases smoothly as the lattice size increases. The saturation of heat conductance is merely a finite-size effect.

To address the second problem, i.e., the temperature dependence of heat conductivity, the situation remains unclear, similar to the first problem. Different viewpoints have been proposed in the two original papers [28,29]. The exponential decrease of heat conductivity with temperature,  $\kappa \sim e^{-CT}$  for  $T \rightarrow \infty$ , was suggested in the paper [28], supported by the paper [45]. Although the authors did not claim a specific low-temperature dependence of heat conductivity, it appears that the linear dependence illustrated in the log-linear scale in Fig. 3 also implies an exponential relation, albeit with a different parameter  $C$  [28]. However, in another paper [29], the authors presented a different exponential relation,  $\kappa \sim e^{1.2/T}$ , for temperatures around  $T = 0.25$ , based on the consideration of the probability of phase jumps,  $\rho \sim e^{-\Delta V/T}$ . A similar viewpoint can be found in the paper [31]. Another exponential relation, with the inverse square root of temperature in the exponent, was numerically shown in [46] as  $\kappa \sim e^{4.45/\sqrt{T}}$ . A completely different power-law dependence,  $\kappa \sim T^{-3.2}$  for  $T > 0.3$ , was given in Refs. [51,52]. The authors deduced that the power-law dependence may be closely related to the momentum diffusion of the kicked rotor model, since they share nearly the same exponent. This power-law dependence has also been reported in Ref. [46].

Given this background, the ongoing discussions suggest that a unified conclusion has yet to be established and that perspectives are needed to resolve the above issues. The mean free path (MFP)  $l$ , or equivalently the lifetime  $\tau$ , of long-wavelength modes plays an important role in energy transport

phenomena, as shown in the Peierls formula  $\kappa = (1/3)C_V v l$ , where  $C_V$  is the specific heat capacity at constant volume and  $v$  is the group velocity [53]. However, we note that the MFP has rarely been discussed in detail in the previous work. Another factor that has not been adequately considered is the nonlinearity of the interaction potential. In the present work, we combine the MFP and the nonlinearity to address these two problems. The MFP analysis implies that although heat conduction in the 1D rotor model may be normal at any nonzero temperature, its exponentially increasing MFP restricts macroscopic-scale observability, rendering it effectively abnormal in practice. For the same reason, within the temperature range studied, we find that  $\kappa \sim e^{2.54/T}$  for  $1 \leq T \leq 10$  and  $\kappa \sim e^{0.49}/T$  for  $0.15 \leq T \leq 0.5$ . In the intermediate range of  $0.3 \leq T \leq 3$ , where nonlinearity plays a significant role, we find  $\kappa \sim T^{-3.2}$ .

Recently, several studies have reported normal or near-normal heat conduction in one-dimensional systems with double-well interparticle potentials, which exhibit phase-jumping dynamics similar to those in rotor models. For example, Xiong investigated crossover phenomena and underlying mechanisms for temperature-dependent transport in such systems [54,55]. Roy also reported a transition from anomalous to normal transport in double-well lattices under varying temperature regimes [56]. While these studies have highlighted the importance of jumping dynamics and nonlinearity in thermal transport, the present work advances the understanding by providing a more systematic and quantitative investigation of temperature-dependent conductivity and by uncovering a clearer physical mechanism underlying the phase transition in the rotor model.

The Green-Kubo (GK) formula [57,58] is the primary method adopted in our study. The main reason for prioritizing the GK formula over nonequilibrium MDS [22,23] and energy diffusion [59,60] is that these approaches encounter challenges, particularly at low temperatures, in fully capturing the intrinsic characteristics of heat conduction in the 1D rotor model. However, heat conduction at low temperatures is of primary interest to us. Moreover, due to boundary resistance in nonequilibrium MDS, the calculated heat conductivity  $\kappa$ , based on the Fourier law, exhibits large fluctuations, as shown in Refs. [31,43]. Therefore, the heat conductivities computed via nonequilibrium MDS were merely used to compare with those obtained through the GK formula to ensure the reliability of our data.

## II. MODEL AND METHODS

The Hamiltonian of the 1D rotor model is given by

$$H = \sum_n \frac{1}{2} \dot{\theta}_n^2 + V(\theta_{n+1} - \theta_n), \quad (1)$$

where  $\theta_n$  is the angular variable of the  $n$ th rotor and  $\dot{\theta}_n = d\theta_n/dt$  denotes its time derivative. The interaction potential between the rotors is given by  $V = 1 - \cos(\theta_{n+1} - \theta_n)$ , which is periodic and bounded. In this model, both the moment of inertia and the lattice constant are set to 1; thus, all the relevant variables are dimensionless. Additionally, the number  $N$  of rotors is equal to the system length  $L$  under periodic boundary

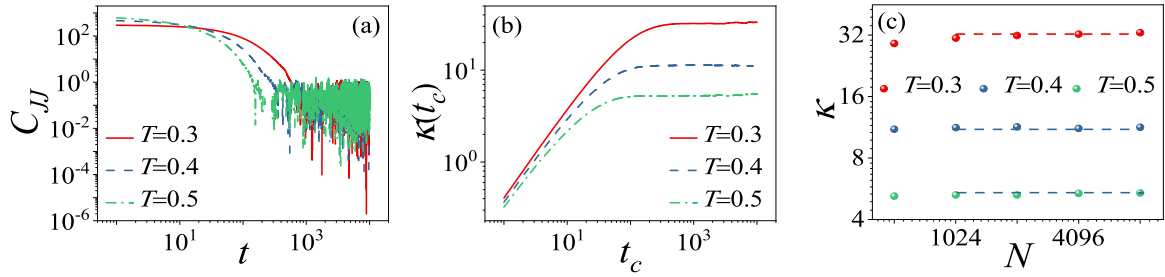


FIG. 1. Comparison of thermal conductivity from equilibrium and nonequilibrium MDS at  $T = 0.3, 0.4$ , and  $0.5$ . Panel (a) shows the heat current correlation  $C_{JJ}(t)$  and panel (b) presents the corresponding thermal conductivity  $\kappa(t_c)$  calculated using GK formula, where  $t_c$  is the truncation time. The final thermal conductivity for equilibrium MDS is extracted within the saturation range. In the equilibrium MDS, rotors of  $N = 8192$  are used. Panel (c) shows the thermal conductivity results from nonequilibrium MDS for different system sizes  $N$ , with dashed lines indicating the corresponding equilibrium MDS results, demonstrating consistency across temperatures.

condition. As a typical example of nonlinear dynamics, it has been demonstrated that the model has two integrable limits: the harmonic limit at low temperatures and the free rotor limit at high temperatures [25,26]. In our study, the leap-frog algorithm with a step size of 0.01, ensuring that the relative error in energy density remains within  $10^{-5}$ , is employed to simulate the dynamic evolution of the system according to its Hamiltonian canonical equations of motion.

Usually, thermal conductivity can be derived either via equilibrium MDS or via nonequilibrium MDS. In the former case, thermal conductivity is calculated using the GK formula  $\kappa = \lim_{t_c \rightarrow \infty} \lim_{L \rightarrow \infty} 1/k_B T^2 L \int_0^{t_c} C(t) dt$ , where  $k_B$  is the Boltzmann constant, defined as 1,  $t_c$  is the truncation time, and  $C(t) = \langle J(0)J(t) \rangle$  is the heat current correlation, with  $J = \sum_n \dot{\theta}_n \partial H(\theta_{n+1} - \theta_n) / \partial \theta_n$  being the total current, and  $\langle \cdot \rangle$  denotes the ensemble average. To suppress the fluctuations of  $C_{JJ}(t)$ , averaging over initial conditions can also be employed. In the present work, 25 or 50 initial conditions are used for averaging, depending on the temperature.

Although the GK formula has not been rigorously proven for one-dimensional nonlinear systems such as the rotor model [45], it remains a widely accepted tool for estimating thermal conductivity in such contexts. In our simulations, particular care was taken to ensure the convergence of the heat current autocorrelation function, including the use of large system sizes, and ensemble averaging over multiple initial conditions. Furthermore, we cross-validated the results with those from nonequilibrium simulations, which consistently yielded compatible values. These steps help mitigate the limitations of the GK approach, such as the finite-size effect [61], especially in the low-temperature regime.

In nonequilibrium MDS, two heat baths at different temperatures are attached to the two ends of the system to simulate heat transport, respectively. After the nonequilibrium steady state is reached, thermal conductivity can be calculated via Fourier's law as  $\kappa = jN/T_H - T_L$ , where  $j = (1/N) \sum_n \dot{\theta}_n \partial H(\theta_{n+1} - \theta_n) / \partial \theta_n$  is the average heat current, and  $T_H$  and  $T_L$  denote the temperatures of the high- and low-temperature heat baths, respectively. In the present work, the Langevin heat bath is used to drive the system to a nonequilibrium steady state, and 24 atoms are placed in each heat bath to suppress boundary resistance. We set  $T_H = T(1 + 0.1)$  and  $T_L = T(1 - 0.1)$  to maintain a temperature difference of 20% relative to the average temperature  $T$ . Thermal conductivities

in this work are primarily derived using the first approach, with the second employed to confirm the results obtained from the first.

### III. RESULTS AND DISCUSSION

To ensure reproducibility, all raw data underlying this study are provided in Ref. [62]. Before proceeding to the formal discussion, we first verify our results to ensure their reliability by comparing the thermal conductivity  $\kappa$  from equilibrium and nonequilibrium MDS. The corresponding results are shown in Fig. 1. The heat current correlation  $C_{JJ}$  for a system size  $N = 8192$  is shown in Fig. 1(a) for temperature  $T = 0.3, 0.4$ , and  $0.5$  in a double-logarithmic scale. As expected, all of them decrease rapidly, demonstrating the convergence of thermal conductivity, which is confirmed by the integrals of GK formula as shown in Fig. 1(b). The thermal conductivities  $\kappa$  for system sizes  $N = 512, 1024, 2048, 4096$ , and  $8192$ , calculated using nonequilibrium MDS at average temperatures  $T = 0.3, 0.4$ , and  $0.5$ , are shown as points in Fig. 1(c). The convergence of thermal conductivity is also well confirmed. For comparison, the thermal conductivity at the corresponding temperature  $T$  from Fig. 1(b) is also presented as a dashed line, which collapses well with the result from nonequilibrium MDS, indicating the accuracy of our data. In particular, for  $T = 0.3$ , our thermal conductivity  $\kappa = 32.34$ , which is consistent with the value of 31.8 reported in Ref. [28], considering statistical errors and differences in simulation setups. These confirmations support the reliability of our simulation framework. We will now proceed with the discussion based on the results from the equilibrium MDS.

Let us first discuss the problem of the existence of the phase transition. Considering that the inconsistency focuses on the temperature of  $T \leq 0.2$ , we will study the change in the relaxation behavior of heat current correlation  $C_{JJ}(t)$  with decreasing temperature from  $T = 0.2$ . To exclude the finite-size effect, for each considered temperature  $T = 0.2, 0.15$ , and  $0.1$ ,  $C_{JJ}(t)$  for three system sizes of  $N = 8192, 16384$ , and  $32768$  is calculated. The system size scaled  $C_{JJ}(t)$  and their integrals are shown in Fig. 2. We observe that for all the considered temperatures, the scaled  $C_{JJ}(t)$  collapse very well onto each other, suggesting that the finite-size effect has almost negligible influence. A similar influence can also be found in the purely quartic lattice system [63]. For the scaled

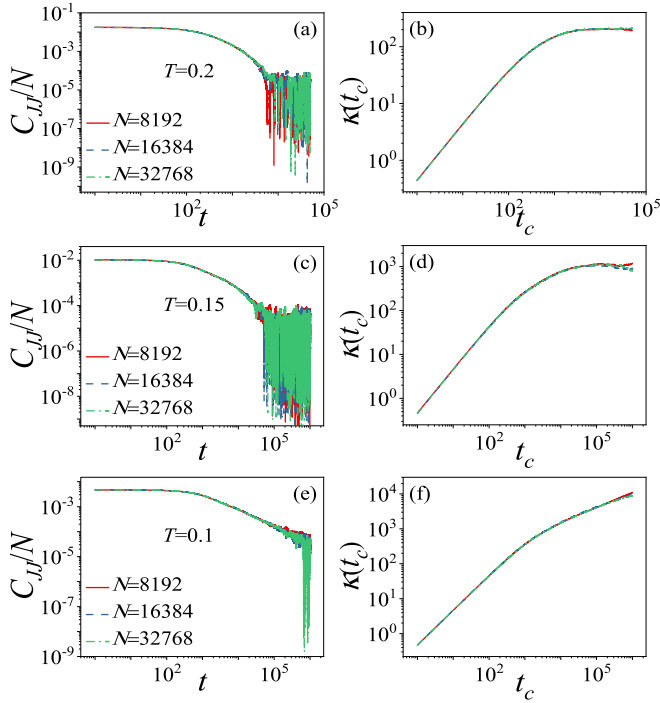


FIG. 2. Thermal transport behavior for  $T \leq 0.2$ . Panels (a), (c), and (e) show the heat current correlations  $C_{JJ}$  scaled by system size  $N$ , while panels (b), (d), and (f) present the corresponding thermal conductivities calculated using the GK formula. For each temperature, system sizes of  $N = 8192$ ,  $16384$ , and  $32768$  are used to exclude the finite-size effects.

heat current correlation at  $T = 0.2$  and  $0.15$  [see Figs. 2(a) and 2(c)], we observe that before the rapid decrease, both endure a long period of almost no decay. Moreover, the lower the temperature, the longer the period, as seen from the comparison of the results for  $T = 0.2$  and  $0.15$ . These phenomena are also reflected in the integral of  $C_{JJ}(t)$ , i.e., the thermal conductivity  $\kappa$  [see Figs. 2(b) and 2(d)]. We see that  $\kappa$  undergoes a linear increase with the integral time before starting to converge. For  $T = 0.2$ , steady convergence occurs at around  $10^4$  time units, while for  $T = 0.15$ , it occurs at around  $10^5$ , which is 10 times longer than that for  $T = 0.2$ . These results demonstrate the intrinsic difficulty of numerically observing normal heat conduction in the 1D rotor model at low temperatures, and it becomes impossible as  $T \rightarrow 0$ . This is likely the reason for the contradictions regarding the existence of the phase transition, which is readily demonstrated at  $T = 0.1$ . As shown in Fig. 2(f), no signs of convergence appear even at the maximal time of  $10^6$ . We conjecture that convergence may occur at around  $10^8$ , but it becomes computationally infeasible to verify this numerically within practical timescales.

It is important to emphasize that, although our numerical results demonstrate signatures of normal heat conduction even at  $T = 0.15$ , the timescale required to observe convergence increases dramatically. At  $T = 0.1$ , convergence becomes practically unobservable within any reasonable simulation time or system size. This is attributed to the exponential growth of the MFP as temperature decreases (see below). Therefore, we suggest that the 1D rotor model exhibits an effective phase transition, not in the strict thermodynamic

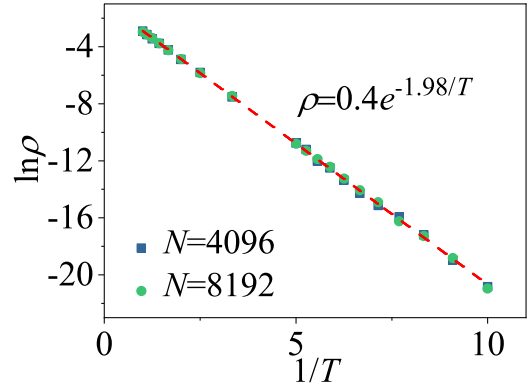


FIG. 3. Phase jumping rate  $\rho$  as a function of temperature  $T$ , in agreement with thermodynamic predictions.

sense with a well-defined critical temperature, but rather from a practical perspective. In this sense, the concept of a phase transition remains valid, but the critical temperature loses its conventional meaning, as it depends on how one defines observability. This interpretation is consistent with the observed exponential behavior of both the MFP and the mode lifetimes, and it explains why different studies have arrived at apparently conflicting conclusions depending on simulation settings and system size.

We note that a prior study [36] proposed a transition point at  $T = A/5$  ( $A$  is the amplitude of rotor potential) based on a qualitative change in the distribution of inter-rotor forces, and used this to motivate the design of a thermal rectifier. While we suggest that this may not yield a quantitatively sharp critical point, the underlying mechanism they describe—namely, the anomalous heat transport at low temperatures—is consistent with our finding that the MFP increases exponentially as  $T \rightarrow 0$ , making normal transport practically unobservable. Thus, our results support the same physical picture and offer additional evidence for the practical effectiveness of the rotor model in nonlinear thermal device design.

We now proceed to investigate the MFP. As stated in the paper [29], phase jumps act as random kicks to the energy carriers, leading to the scattering of heat current. According to thermodynamics, the jumping rate  $\rho$  for a single rotor satisfies  $\rho \sim e^{-\Delta V/T}$ , with  $\Delta V$  being the height of the potential barriers ( $\Delta V = 2$  in our model). Numerically, the jumping rate can be calculated from its definition  $\rho \equiv \lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} M/Nt$  in the equilibrium state at temperature  $T$ , where  $M$  is the number of transitions during time  $t$  and  $N$  is the total number of rotors in the system. The results of  $\rho$  for different temperatures are shown in Fig. 3 for  $N = 4096$  and  $8192$ . One can see that the two results agree very well at all the considered temperatures. After fitting, we find that  $\rho = 0.4e^{-1.98/T}$ . The exponent  $1.98$  can be viewed as being equivalent to the height of the potential barriers. Once the jumping rate  $\rho$  is obtained, the MFP  $l$  of energy carriers can be roughly evaluated through the following argument. The MFP  $l$  should be proportional to the number  $N$  of rotors required to ensure that a rotor undergoes a phase jump within a unit time at a given temperature  $T$ . Based on this consideration, the required number  $N$  of rotors is determined to be  $N = 2.5e^{1.98/T}$ . This also means that the MFP  $l$  increases exponentially with the decrease in

temperature as  $l \sim e^{1.98/T}$ . Take temperature  $T = 0.1$  as an example. Inserting  $T = 0.1$  into the expression for  $l$ , we obtain  $l \sim 10^8$ , which represents approximately 1 cm in practice. This implies that normal heat conduction is unlikely to be observed at the macroscale for  $T = 0.1$ , which is close to room temperature in reality [64]. Although our method may lead to an overestimation of the MFP  $l$ , the key insight is the exponential trend of  $l$ , which severely hampers the observability of normal heat conduction at macroscopic scales as  $T \rightarrow 0$ . This is why we suggest that the heat conduction in the 1D rotor model is abnormal at low temperatures in effect.

In the following, we further verify our arguments in terms of the lifetime of long-wavelength modes, as these modes play a key role in energy transport phenomena [22,23,65]. According to single-mode relaxation time approximation theory [66], the lifetime  $\tau$  of a mode is given by  $\tau = 1/2\Gamma$ , where  $\Gamma$  is the scattering rate, which can be extracted from the full width at half maximum (FWHM) of the power spectrum of the mode. More precisely, the power spectrum  $P(\omega)$  of a mode  $Q_k = Ae^{i\omega_0 t}e^{-\Gamma t}$  ( $A$  and  $\omega_0$  are the amplitude and angular frequency, respectively, and  $i^2 = -1$  is the imaginary unit) is the square of the module of its Fourier transform, namely,  $P(\omega) = |\int_0^\infty Q_k e^{-i\omega t} dt|^2 = A^2/[(\omega - \omega_0)^2 + \Gamma^2]$ , which is a Lorentzian function centered at angular frequency  $\omega_0$ , with FWHM exactly equal to  $2\Gamma$ . It should be noted that in numerical calculations,  $P(\omega)$  is not a perfect Lorentzian function but rather a more complex multipeak structure due to thermal fluctuations. To implement this method, the system must first be thermalized to a given temperature. Then, the spatial Fourier transform is applied to the coordinate, yielding  $Q_k(t) = \frac{1}{\sqrt{N}} \sum_{n=1}^N \theta_n(t) e^{-i(2\pi k/N)n}$ , where  $k$  is the integer denotes the  $k$ th mode. For the momentum, the corresponding transform is  $P_k(t) = \frac{1}{\sqrt{N}} \sum_{n=1}^N \dot{\theta}_n(t) e^{-i(2\pi k/N)n}$ . After recording the time series of  $Q_k$  or  $P_k$ , the power spectrum can finally be obtained by performing the time Fourier transform on these quantities.

Considering our limited computing resources, we will restrict ourselves to the long-wavelength modes of  $k = 5, 6, 7, 8, 9$ , and  $10$ . Depending on the parity of  $k$ , we classify the modes into two categories: odd and even modes, since they follow distinct selection rules [67,68] and exert different effects on the early stages of energy equipartition process [69,70]. In our calculations, the two-sided spectrum is applied, and the lifetime  $\tau$  is averaged from both sides. Additionally, depending on the mode and the temperature, 10–25 initial conditions are also used to compute the average. Generally, the lower the mode  $k$  and temperature, the more initial conditions are needed. Furthermore, the sampling frequency should satisfy the sampling theorem, and the resolution of the time Fourier transform should also be adjusted according to the mode  $k$  and temperature to ensure the accuracy of the results. However, meeting the latter condition perfectly can be challenging. As an illustration (see Fig. 4), for mode 5 at temperature  $T = 0.1$ , even with the highest achievable resolution of  $7.6 \times 10^{-9}$ , the resulting lifetime does not have reasonable accuracy.

As an example, the two-sided power spectrum and the Lorentzian function fitting (red dot-dashed line) for modes 5 and 6 at temperature  $T = 0.2$  are shown in Figs. 4(a) and

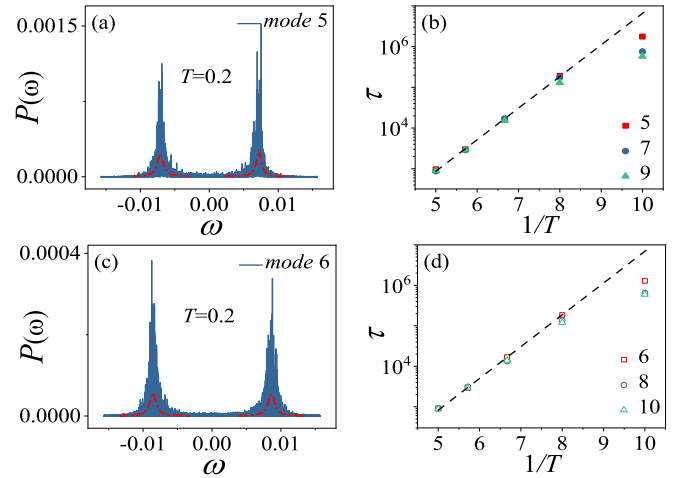


FIG. 4. Lifetime  $\tau$  behavior for long-wavelength modes within  $T \leq 0.2$ . Two typical two-sided power spectra  $P(\omega)$  for modes 5 and 6 are shown in panels (a) and (c), with the red dot-dashed line representing the Lorentzian fitting function. The lifetime  $\tau$  is extracted from the FWHM. Panels (b) and (d) show  $\tau$  as a function of  $1/T$  for odd modes (5, 7, 9) and even modes (6, 8, 10), respectively, revealing an exponential increase. System size  $N = 4096$  is used.

4(c), respectively. The results of lifetime  $\tau$  with respect to the inverse temperature  $1/T$  for odd modes and even modes are presented in Figs. 4(b) and 4(d), respectively. Excluding the results for  $1/T = 10$ , an excellent linear relation between lifetime  $\tau$  and  $1/T$  can be observed in the log-linear scale for both types of modes, implying that  $\tau \sim e^{C_k/T}$ , with  $C_k$  being the mode-dependent fitting parameter. This suggests that the lifetime increases exponentially with decreasing temperature, supporting the existence of the phase transition as revealed by the MFP  $l$ . For the same reason, the phase transition temperature is no longer important, as it depends on how one defines it.

It is worth noting that although Ref. [45] considers a harmonic-pinned version of the 1D rotor model, their analysis predicts ballistic heat transport at low temperatures due to the energy current becoming proportional to the temperature difference. This behavior is qualitatively consistent with our findings for the unpinned rotor model, where the exponentially increasing MFP leads to effectively unobservable normal conduction behavior. This agreement across different model setups reinforces the interpretation of a low-temperature regime dominated by quasi-ballistic dynamics for the 1D rotor model.

Let us revisit the results for  $1/T = 10$ , taking mode 10 as an example. Following the previous linear dependence, the lifetime of mode 10 at  $T = 0.1$  is approximately  $3 \times 10^6$ , and the corresponding scattering rate  $\Gamma$  is  $1.6 \times 10^{-7}$ . Converting the scattering rate into frequency units, it is approximately  $2.5 \times 10^{-8}$ . To achieve accurate results, the resolution must be at least one-tenth of  $2.5 \times 10^{-8}$ , which is 3 times higher than what we can currently achieve. Moreover, this applies to other low-frequency modes as well. For these reasons, we exclude the results for  $T = 0.1$  and restrict ourselves to mode 5, which is the lowest mode we can resolve.

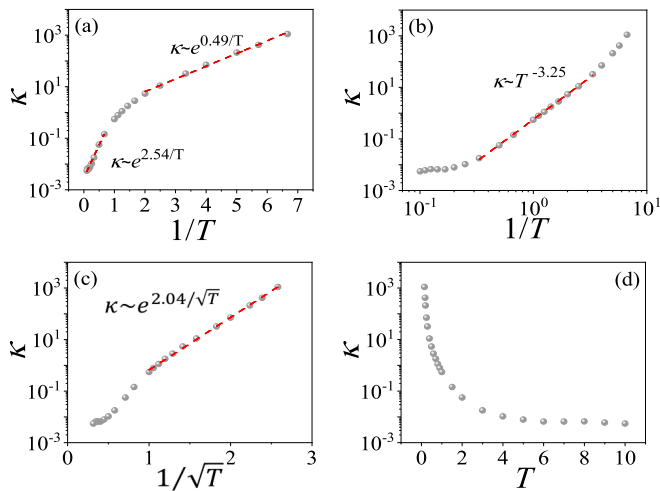


FIG. 5. The temperature dependence of thermal conductivity  $\kappa$  within  $0.15 \leq T \leq 10$ . All the results are derived from the equilibrium MDS with using the GK formula. The red dashed lines in panels (a)–(c) are the fitting lines.

After addressing the first problem, we now turn to the second one, namely, the temperature dependence of thermal conductivity. We will explore this problem over the temperature range  $0.15 \leq T \leq 10$ .

According to our literature review, the existing viewpoints on the second problem can be categorized into two main types: the exponential dependence and the power-law dependence [46,51,52]. Furthermore, the exponential dependence can be divided into three subcategories:  $e^{\delta/T}$  [29,31],  $e^{\gamma/\sqrt{T}}$  [46], and  $e^{-CT}$  [28,45], where  $\delta$ ,  $\gamma$ , and  $C$  are positive parameters. We believe that the contradictions likely arise from the excessive attention paid to phase jumps while neglecting the nonlinearity of the interaction potential. We suggest that the temperature dependence of thermal conductivity is the result of the combined effect of phase jumps and nonlinearity. The temperature ranges for these two effects may differ or overlap in some specific intervals. Some insights can be gained from the following reasoning. Nonlinearity does not play a significant role as  $T \rightarrow 0$ , since the system approaches the harmonic limit in this case. On the other hand, as  $T \rightarrow \infty$ , the system turns into free rotational rotors, and the nonlinearity does not manifest itself either. This argument is consistent with the fact that the 1D rotor model has two integrable limits as  $T \rightarrow 0$  and  $T \rightarrow \infty$ . Therefore, the effect of nonlinearity becomes evident at some intermediate temperature, which must be determined through numerical calculation. The thermal conductivity likely follows the power-law dependence on temperature [46,51,52]. Such nonlinearity-induced behavior has also been observed in the  $\phi^4$  model [71–73], the disordered  $\phi^4$  model [74], the generalized nonlinear Klein-Gordon model [73,75], and the FPUT model [76,77]. Outside this intermediate temperature range, phase jumps dominate energy transport. The thermal conductivity will show an exponential increase with temperature, as  $e^{\delta/T}$ , similar to that of MFP. Next, we will verify these arguments.

In Fig. 5, we show the dependence of thermal conductivity on the temperature for the above four cases. Please note the differences in the coordinate scales and the interpretation

of the horizontal axis. In Fig. 5(a), the log-linear scale is used to present the data. Interestingly, a double-exponential dependence is found. Furthermore, we find that the thermal conductivity in the high-temperature regime decreases much faster than in the low-temperature regime. After performing the fitting, we find that for the low-temperature regime of  $0.15 \leq T \leq 0.5$ , the thermal conductivity follows  $\kappa \sim e^{0.49/T}$ , while for the high-temperature regime of  $1 \leq T \leq 10$ ,  $\kappa \sim e^{2.54/T}$ . We note that our exponent value of 0.49 is significantly different from the value of 1.2 reported in Ref. [29]. This is probably related to the differences in the simulation setups. Additionally, our fitting regime spans a much broader temperature range than that in Ref. [29]. The crossover regime of the double-exponential relation ( $0.5 \leq T \leq 1$ ) is suggested to be the regime where nonlinearity plays a significant role. This is confirmed in Fig. 5(b), where an excellent power-law dependence of thermal conductivity on temperature,  $\kappa \sim T^{-3.25}$ , is identified for  $0.3 \leq T \leq 3$ . Note that this power-law dependence is also reported in Refs. [46,51,52]. The crossover region,  $0.5 \leq T \leq 1$ , is located precisely within the power-law regime. Moreover, we find substantial overlapping regimes between the power-law and the exponential dependence in both the high- and low-temperature regimes. This may be another reason for the contradictions in the temperature dependence of thermal conductivity.

The exponential dependence  $\kappa \sim e^{4.45/\sqrt{T}}$  for temperature  $T \leq 0.5$  was first reported in Ref. [46]. Out of curiosity, we also plot the thermal conductivity  $\kappa$  with respect to  $1/\sqrt{T}$  in Fig. 5(c) in a log-linear scale. Interestingly, we find that our data also show a similar relation but with a different exponent, as  $\kappa \sim e^{2.04/\sqrt{T}}$  for  $T \leq 1$ . A complete theoretical explanation for this behavior remains an open question and requires further investigation. However, we suggest that an exponential dependence of the form  $e^{\delta/T}$  is more physically reasonable, given the proportionality between thermal conductivity  $\kappa$  and the MFP  $l$ .

We also show the relation between the thermal conductivity  $\kappa$  and temperature  $T$  in a log-linear scale in Fig. 5(d). No signs of linearity are observed across the entire temperature range we investigated. Therefore, we conclude that the relation  $e^{-CT}$  is unlikely to apply in this case.

Thus far, we have illustrated the temperature dependence of thermal conductivity as a consequence of the combined effect of phase jumps and nonlinearity and have identified an unexpected double-exponential relation. Why does this occur? What happens to the long-wavelength modes? To answer these questions, we extended our study on the lifetime of the long-wavelength modes over a broader temperature range of  $0.1 \leq T \leq 1$ , and something interesting is found. Moreover, why does the power-law dependence arise as a result of nonlinear interactions? We will study this problem later.

The lifetime of odd modes and even modes is shown in a log-linear scale in Figs. 6(a) and 6(b), respectively. It can be seen that none of the considered modes sustain the single-exponential dependence shown in Fig. 4. Instead, we find that all modes reach their minimum lifetime at  $T = 0.3$  and subsequently increase as the temperature rises. It should be emphasized that the increase in the lifetime at  $T \geq 0.3$  is unrelated to the thermal conductivity. If it were, one would

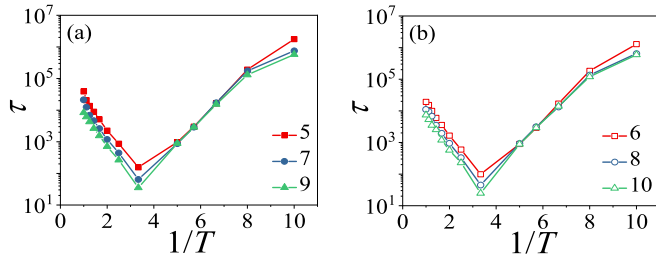


FIG. 6. The lifetime  $\tau$  of odd modes (5, 7, 9) and even modes (6, 8, 10) in a wider temperature range of  $0.1 \leq T \leq 1$ .

expect the thermal conductivity to increase with temperature at  $T \geq 0.3$ , contrary to the observed decrease. In fact, the increase in the lifetime at  $T \geq 0.3$  implies that the concept of long-wavelength modes is no longer applicable. This is indicative of localization, namely localized rotational modes, induced by the frequent phase jumps [27–29]. These localized modes strongly scatter the heat current, leading to a rapid decrease in thermal conductivity in the high-temperature regime.

Now, let us address the problem of the power-law dependence of thermal conductivity. As is well known, the breakdown of stretch conservation due to phase jumps ensures that the 1D rotor model displays normal heat conduction [30–32]. The effect of nonlinearity, however, should manifest in its influence on the temperature dependence of thermal conductivity. To investigate this influence, it is essential to maintain normal heat conduction without altering the nonlinearity while simultaneously eliminating phase jumps. To achieve this, our strategy is to introduce an on-site harmonic potential  $(1/2)\Omega\theta_n^2$  that restricts the motion of the rotors to a single potential well. Another possible approach is to add a hard-sphere potential at the maximum of the interaction potential, as proposed in Ref. [32]. However, this alternative modifies the nonlinearity of the potential, which fails to meet the requirements. Therefore, the on-site harmonic potential is a more suitable choice. To prevent phase jumps, the on-site harmonic potential,  $(1/2)\Omega\theta_n^2$ , must intersect with the interaction potential at its first maximum point, yielding  $\Omega = 4/\pi^2$ . It is worth noting that the incorporation of the on-site harmonic potential is not entirely rigorous, as it alters the system's dispersion relation. Fortunately, since the coefficient of the on-site harmonic potential is relatively small, this influence is expected not to be strong, and we can still derive meaningful insights.

The heat current correlation  $C_{JJ}(t)$  and its integral  $\kappa(t_c)$  for  $T = 0.4, 0.6$ , and  $0.8$  are presented in Figs. 7(a) and 7(b) for this modified model. The rapid decay of  $C_{JJ}(t)$  and the convergence of  $\kappa(t_c)$  are clearly distinguishable, which is consistent with the understanding that momentum nonconserving systems exhibit normal heat conduction [22–24]. The temperature dependence of thermal conductivity for this modified model is shown in Fig. 7(c) over the range  $0.2 \leq T \leq 1$ , plotted on a log-log scale. A clear linear relationship is observed, indicating a power-law dependence of thermal conductivity on temperature. After fitting, we find  $\kappa \sim T^{-3.6}$ . The exponent is slightly larger than that of the original system, likely attributable to the incorporation of the weak on-site harmonic potential. This result provides strong evidence supporting our argument that the power-law dependence arises from the system nonlinearity. These findings support the argument that the temperature-dependent behavior of thermal conductivity in the 1D rotor model results from a combination of phase jump and system nonlinearity.

#### IV. CONCLUSION

To summarize, we have studied heat conduction in the 1D rotor model in detail and addressed two key issues: the existence of the phase transition and the temperature dependence of thermal conductivity. Theoretically, the 1D rotor model may support normal heat conduction at any nonzero temperature. However, practical considerations suggest anomalous heat conduction in the low-temperature regime, because the exponential growth of the mean free path as temperature decreases precludes observation of normal conduction at macroscopic scales as  $T \rightarrow 0$ , including at temperatures conventionally considered “room temperature.” Consequently, the phase transition temperature loses practical relevance, as its value is definition-dependent.

Regarding the second issue, we find that it arises from the combined effects of phase jumps and nonlinearity, revealing an unexpected double-exponential relationship between the thermal conductivity and temperature. At low and high temperatures, heat conduction is primarily governed by phase jumps, while by nonlinearity at intermediate temperatures. Specifically, we find that  $\kappa \sim e^{0.49/T}$  for  $0.15 \leq T \leq 0.5$  as a consequence of the exponential increase of mean free path and  $\kappa \sim e^{2.54/T}$  for  $1 \leq T \leq 10$  due to the frequent phase jumping and the formation of localized rotational modes.

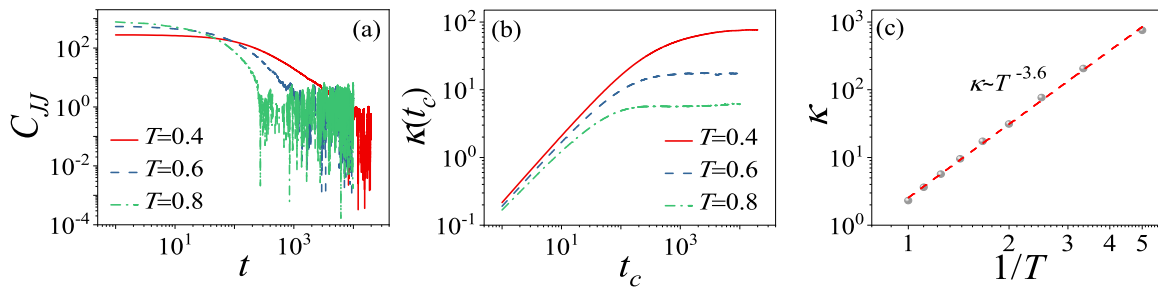


FIG. 7. The temperature dependence of thermal conductivity for the modified rotor model. Panel (a) shows the heat current correlation  $C_{JJ}$  at  $T = 0.4, 0.6, 0.8$  and panel (b) presents the corresponding thermal conductivity  $\kappa(t_c)$  with respect to the truncation time  $t_c$ . Panel (c) is the temperature dependence result of thermal conductivity  $\kappa$ ; a power-law relation indicated by the red dashed line can be seen.

In the intermediate temperature  $0.3 \leq T \leq 3$ , nonlinearity dominates, resulting in a power-law dependence of thermal conductivity,  $\kappa \sim T^{-3.2}$ . The overlap between these two temperature-dependent mechanisms likely contributes to the observed contradictions regarding the second problem.

Our arguments are further supported by the power-law temperature dependence of thermal conductivity  $\kappa \sim T^{-3.6}$  in a modified model with an added on-site harmonic potential, where the phase jumps are forbidden but nonlinearity maintained. The present work advances our understanding of heat conduction in the 1D rotor model and provides insights into the design of rotor-based thermal rectification devices [36–38].

Heat transport in the 1D long-range interacting rotor model has also drawn significant attention [41,42]. According to Ref. [41], a phase diagram of this model was proposed, identifying three regimes—adiabatic, normal heat conduction, and anomalous heat conduction—with respect to temperature and the long-range interaction exponent. However, the system

sizes considered in Ref. [41] were relatively small (up to 200). Therefore, further investigations involving larger system sizes are necessary, and this work is currently underway.

Similar challenges arise in the study of heat transport in models with both internal anharmonic and external harmonic interactions [78–82]. Resolving these issues necessitates further research, and our work may provide a heuristic framework for understanding heat transport in such models.

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## DATA AVAILABILITY

The data that support the findings of this article are openly available in [62].

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