Thermal Conduction in one dimensional $\Phi^4$ chains with colliding particles

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Abstract

Studying thermal conduction in low-dimensional non-integrable systems is necessary for understanding the microscopic origin of macroscopic irreversible behavior and Fourier’s law of heat conduction. Two distinct types of low-dimensional thermal conduction models have been proposed in the literature: ones that display normal thermal conduction (like the $\Phi^4$ chain) and others that show anomalous thermal conduction (like the Fermi-Pasta-Ulam chain). However, in both these models, nothing prevents two nearby particles from crossing each other. In this manuscript, we introduce a modification in the Hamiltonian of the traditional $\Phi^4$ chain (henceforth called $\Phi^{4C}$ model) through soft-sphere potential that prevents two particles from crossing. The proposed model is then subjected to thermal conduction by keeping its two ends at different temperatures using Nosé-Hoover thermostats. Equations of motion, derived from the Hamiltonian, are solved using 4th order Runge-Kutta method for 1 billion time-steps, where each time-step is of 0.0005 time units. Averages have been computed using the last 750 million time-steps. Our results indicate that the boundary effects due to contact with the thermostats is minimized in the $\Phi^{4C}$ model as compared to the traditional $\Phi^4$ chain, ensuring a smoother temperature distribution across the chain. Further, the rate of convergence of heat flux is much faster in the $\Phi^{4C}$ chain vis-à-vis the traditional $\Phi^4$ chain. However, the absolute value of heat flux is much smaller in the $\Phi^{4C}$ chain. These results suggest that collision plays an important role in quickly ensuring that a steady-state is reached and diminishing the magnitude of heat flux. Interestingly enough, collision does not significantly alter the diffusive properties of the chain, irrespective of the temperature gradient within the chain.

I. INTRODUCTION

Recent advance in science and technology has enabled the researchers to develop new-age materials such as graphene, carbon nanotubes (CNTs), nanowires, etc. In many of these materials, the motion of the particles (atoms) are severely restricted in one or more dimensions, making them examples of low-dimensional systems. Because of their interesting thermal transport properties, low-dimensional systems have generated significant interest.
amongst the researchers. Of specific importance is to identify the link between the macro-
scopic Fourier’s law of heat conduction with its low-dimensional counterpart. For a one
dimensional system, Fourier’s law may be stated as:

\[ J = -\kappa \frac{\partial T}{\partial x}, \]  

(1)
i.e. the heat current, \( J \), is proportional to the temperature gradient, \( \partial T/\partial x \), with the
constant of proportionality given by the thermal conductivity of the system, \( \kappa \). This macro-
scopic statement of Fourier’s law is independent of the system size and length. But, situation
becomes complicated when dealing with atomistic scale low-dimensional systems. For ex-
ample, CNTs exhibit length (as well as temperature) dependent thermal conductivity [1].
Similarly, graphene has an exceptionally high thermal conductivity [2].

In a bid to explain these anomalous deviations away from normal thermal transport
properties, simplified one-dimensional models have been studied extensively. Two of the
most studied pedagogical models are the Fermi-Pasta-Ulam (FPU) chain [3] and the \( \Phi^4 \)
chain [4]. While the FPU chain exhibits anomalous thermal conduction similar to CNTs
with \( \kappa \) following a power-law with system size, \( \kappa \sim L^\alpha \) with \( \alpha \neq 0 \), \( \Phi^4 \) chains obey Fourier’s
law [3]. The generalized Hamiltonian, \( H \), governing the two chains comprising of \( N \) particles
can be expressed as:

\[
H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V_H(\Delta x_{i-1,i}) + V_A(\Delta x_{i-1,i}) + U(x_i) \right],
\]  

(2)
where \( p_i \) is the momentum of the \( i^{th} \) particle having a mass of \( m \), \( V_H \) is the harmonic part of
the potential that depends on the distance between the two nearby particles \( \Delta x_{i-1,i} \), \( V_A \) is the
anharmonic part of the potential that also depends on \( \Delta x_{i-1,i} \) and \( U(x_i) \) is the anharmonic
tethering part of potential. FPU chain is obtained when \( V_A(\Delta x_{i-1,i}) = \frac{1}{4}c_1\Delta x^4_{i-1,i} \) and
\( U(x_i) = 0 \), while the \( \Phi^4 \) chain is obtained when \( V_A = 0 \) and \( U(x_i) = \frac{1}{4}c x^4_i \).

The difference in the nature of the Hamiltonian results in FPU chain being momentum
conserving and \( \Phi^4 \) chain being momentum non-conserving. Across several scientific works,
it has been argued in the literature that momentum conservation is a key reason for the
FPU chain to display anomalous thermal conduction [5]. The argument, however, does not
hold true for all one-dimensional modes as has been identified by Prosen and Campbell [6].
Over the years, several momentum non-conserving models have been proposed that show
normal thermal transport properties. For example, working with a chain of coupled rotators, Giardina et. al. [7] have shown that the system obeys Fourier’s law. Similarly Xiong et. al. [8] have shown through non-equilibrium molecular dynamics that their one-dimensional chain with asymmetric interparticle interactions has a convergent thermal conductivity in thermodynamic limit.

Another possible origin of anomalous thermal transport in momentum conserving one-dimensional chains has been attributed to the slow diffusion of energy carried by the long-wavelength modes [9]. These long-wavelength modes act as undamped energy transport channels, and result in long-distance as well as time correlations in the system. As a result, such momentum conserving systems possess anomalous thermal transport. Further, it has been suggested that in one-dimensional systems having tethering potential, the energy transported by the long-wavelength modes gets diffused quickly due to the tethering potential. Particularly for the $\Phi^4$ chain, it has been argued that the localized modes having frequency greater than the linear phonon regime are responsible for normal thermal conduction. However, explanation of ballistic thermal conduction in the momentum non-conserving $\Phi^4$ chain, under weakly non-linear tethering potential, still remains elusive [10].

In the traditional models of FPU and $\Phi^4$ chains, two nearby particles may cross each other. This is in contrast with realistic systems, where any two particles experience large repulsive forces when they come near each other. The presence of such repulsive forces may have a significant bearing on the thermal conductivity properties owing to their ability to create new phonon modes. Keeping this in mind, in this manuscript, we generalize the traditional $\Phi^4$ chain so that no two individual particles can cross each other. This is achieved by addition of a soft-sphere type potential to the Hamiltonian associated with $\Phi^4$ chain. The resulting Hamiltonian is solved numerically to answer the following questions – (i) how does the thermal conductivity and heat flux change when particles are not allowed to cross each other, (ii) does enabling collision has any bearing on the temperature gradient being created across the chain, and (iii) does collision alter the density profile within the chain and the diffusive characteristics of the chain.

The manuscript is organized as follows: the next section details the model proposed in this manuscript that prevents two particles from crossing over along with a brief description of the traditional $\Phi^4$ chain, subsequently we highlight the numerical simulation strategy adopted in this study and the results obtained from our simulations. Lastly, concluding
remarks are presented that provides direction for future research.

II. Φ⁴ AND Φ⁴C ONE DIMENSIONAL CHAINS

Consider $N$ particles, each of mass $m$, lying on a one-dimensional line. Let the equilibrium distance between any two particles be $l_{eq}$. As in equation 2, let $V_H(\Delta x_{i,j})$ and $V_A(\Delta x_{i,j})$ be the harmonic and anharmonic inter-particle interactions between two particles $i$ and $j$. These interactions solely depend on the relative displacement of the two particles from their equilibrium positions, $\Delta x_{i,j} = x_i - x_j - (j - i)l_{eq}$. Further, let each particle interact only with its nearest neighbor, i.e. $V(\Delta x_{i,j}) \rightarrow V(\Delta x_{i-1,i})$. In presence of an on-site tethering potential, $U(x_i)$, the Hamiltonian is given by:

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \sum_{i=1}^{N-1} \frac{k}{2} (x_i - x_{i-1} - l_{eq})^2 + V_A(\Delta x_{i-1,i}) + U(x_i) \right]$$  \hspace{1cm} (3)

Choosing $k = 1.0$, the traditional Φ⁴ chain is obtained from equation 3 by substituting $V_A(.) = 0$ and $U(x_i) = c\frac{(x_i-x_{i,0})^4}{4}$. Thus, the Hamiltonian of Φ⁴ chain, with $c = 0.1$, is given by:

$$H_{\Phi^4} = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \sum_{i=1}^{N-1} \frac{1}{2} (x_i - x_{i-1} - l_{eq})^2 \right]$$  
$$+ \sum_{i=1}^{N} \left[ 0.1 \left( x_i - x_{i,0} \right)^4 \right]$$  \hspace{1cm} (4)

The reason for choosing $c = 0.1$ in equation 4 is to ensure that the anharmonic energy contribution is a fraction of harmonic energy for the majority of simulation time. In the limit of large anharmonic contributions ($c = 1$), thermal transport characteristics of $\phi^4$ chain have been extensively studied by Hu et. al [5], and Aoki and Kusnezov [11] using deterministic thermostats. Hu et. al argued that as the momentum conservation breaks down due to the tethering potential, thermal conduction follows Fourier’s Law where $J \sim \frac{1}{N}$ and dissipation of momentum decays exponentially in time. Using large scale simulations, it was found that the thermal conductivity depends on temperature according to: $\kappa = 2.724/T^{1.382}$ [12]. Patra and Bhattacharya [13] employed a Φ⁴ chain to study thermal rectification and differential thermal conduction. Although researchers have extended the Φ⁴ model to more than one dimensions [12], we focus only on one-dimensional chains in the present study. However, the existing Φ⁴ model does not constrain two particles from crossing each other. In the present work, we modify $H_{\Phi^4}$ so that two particles are prevented from crossing each other.
The proposed $\Phi^4C$ Hamiltonian contains an extra soft sphere collision term $V_C(.) = -a \frac{(x_i - x_{i-1})^6}{(x_i - x_{i-1})^6}$ which ensures that two particles, upon coming very close to each other, experience a large repulsive force. The choice of the constant $a$ is governed by two factors: (i) the effective radius of the particles, $r$, so that when the distance between the two particles is less than $2r$, a large repulsive force is experienced by the particles, and (ii) the contribution of $V_C \to 0$ when the distance between the two particles is greater than $2r$. In the present work, we choose $a = 5 \times 10^{-10}$ corresponding to an effective radius of $r = 0.025$. The resulting Hamiltonian is:

$$H_{\Phi^4C} = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} \right] + \sum_{i=1}^{N-1} \left[ \frac{1}{2} (x_i - x_{i-1} - l_{eq})^2 \right]$$

$$- N \sum_{i=1}^{N-1} \left[ 5 \times 10^{-10} \frac{(x_i - x_{i-1})^6}{(x_i - x_{i-1})^6} \right]$$

$$+ \sum_{i=1}^{N} \left[ \frac{0.1}{4} (x_i - x_{i,0})^4 \right]$$

Figure 1 depicts the soft-sphere potential and its corresponding force vis-à-vis the harmonic potential and harmonic force. Beyond $2r$, the interparticle potential and force is dominated by the harmonic potential and the corresponding force, respectively.
III. SIMULATION METHODOLOGY

We now describe the simulation methodology adopted in the study. The particles of both $\Phi^4$ and $\Phi^{4C}$ chains are initialized at their equilibrium positions such that $l_{eq} = 1$. Therefore, the initial position of $i^{th}$ particle is $x_{i,o} = i - 1$. So, in a chain comprising of $N$ particles, the initial coordinates range from 0, 1, \ldots, $N - 1$. Initial velocities of the particles are randomly sampled from a uniform distribution between $\pm 0.5$. Fixed-fixed boundary conditions have been implemented in the chains by means of fictitious fixed particles present at the coordinates $-1$ and $N$. The first (last) boundary particle interacts with only the first (last) particle of the chain through $V_H(.) + V_A(.)$ whose mathematical forms are given in equations 4 and 5. A pictorial representation of the chain is depicted in figure 2.

We create a thermal gradient in the chains by controlling the temperature of the first and the last particles. While the first particle is kept in contact with a hot heat reservoir (at temperature $T_H$), the last particle is kept in contact with a cold heat reservoir (at temperature $T_C$). Amongst the different deterministic thermostats\cite{14, 17}, we choose Nosé-Hoover thermostat \cite{18, 20} for temperature control due to its simplicity and wide adoption. The Nosé-Hoover thermostat’s mass for both the hot and the cold thermostats are taken as unity. Particles present in between the first and the last particles are governed by the standard Hamiltonian evolution equations. Thus, the resulting equations of motions for all
the particles are given by:

\[ \dot{q}_i = \frac{\partial H}{\partial p_i} \]
\[ \dot{p}_i = -\frac{\partial H}{\partial q_i} - \delta_1 \zeta_H p_i - \delta_N \zeta_C p_N \]
\[ \zeta_H = \frac{p_i}{T_H} - 1 \]
\[ \zeta_C = \frac{p_i}{T_C} - 1 \]

where:

\[ \delta_1 = 1\{i = 1\} \]
\[ \delta_1 = 0\{i \neq 1\} \]
\[ \delta_N = 1\{i = N\} \]
\[ \delta_N = 0\{i \neq N\} \]

These equations of motion are solved using fourth order Runge-Kutta method with incremental time step equalling \( h = 0.0005 \). Each simulation run comprises of two parts: (i) first 250 million steady-state runs: equations of motion are solved for 250 million time-steps under the prescribed boundary conditions so that chains reach steady state conditions, and (ii) last 750 million output runs: in order to compute all time averages equations of motion are solved for a further 750 million time-steps. To understand the effect of chain length, simulations are run with different values of \( N \): 16, 32, 64, 128, 256, 384 and 512. For each case, three different temperature values are imposed on the boundary particles: \((T_H, T_C) = (1.1, 0.9); (0.55, 0.45)\) and \((0.11, 0.09)\) such that the mean temperatures, \( T_M = 0.5(T_H + T_C) \), are 1.0, 0.50 and 0.10, respectively.

A. Heat Flux Computation:

Let us begin with a hypothetical case where a chain comprising of \( N \to \infty \) particles is brought away from equilibrium through a thermal gradient. In such a case, the chain becomes a continuous entity, and the different thermodynamic quantities may be defined on a spatial point \( x \). With local thermodynamic equilibrium conditions prevailing within the system, it is possible to define an instantaneous local temperature field \( T(x, t) \) that varies slowly in \( x \) and time, \( t \). In a similar way, the local heat current density \( J(x, t) \) may be defined. For the chains under consideration, where \( N \) is finite, we make an assumption that the temperature gradient is small enough so that the chain is near-equilibrium and local thermodynamic equilibrium hypothesis holds true. In such a scenario, we can now
define locally both temperature and heat currents for a particle. From amongst the different definitions of temperature [21, 22], we restrict ourselves to kinetic temperature, which can locally be expressed as:

\[ k_B T_i = m v_i^2, \]  

(7)

where, \( k_B \) is the Boltzmann constant and taken as unity for the remainder of this study, and \( T_i \) is the kinetic temperature of the \( i^{th} \) particle. Local heat current may be obtained by taking the time derivative of the local energy density associated with the \( i^{th} \) particle [23]:

\[ \dot{\epsilon}_i = \frac{\partial \epsilon_i}{\partial t} + \left[ j_{i,i-1} - j_{i+1,i} \right], \]  

(9)

which can be written as

\[ \dot{\epsilon}_i = \frac{\partial \epsilon_i}{\partial t} + \left[ j_{i,i-1} - j_{i+1,i} \right], \]  

(9)

where, \( j_{i,j} \) is the energy current flowing from particle \( j \) to particle \( i \). When steady state is reached [23], \( \langle \dot{\epsilon}_i \rangle = 0, \langle \frac{\partial \epsilon_i}{\partial t} \rangle = 0 \) along with \( \langle \frac{dV(x_i-1-x_i)}{dt} \rangle = 0 \), so that:

\[ \langle j_{i,i-1} \rangle = \langle \frac{1}{2} (v_i + v_{i-1}) f_{i,i-1} \rangle = \langle v_i f_{i,i-1} \rangle \]  

(10)

This gives \( \langle j_{i,i-1} \rangle = \langle j_{i+1,i} \rangle = \langle j(x,t) \rangle = J \). So, the net heat flux, \( J \), and its time averaged value, \( \langle J \rangle \), may be computed as:

\[ J = \frac{\sum_{i=1}^{N} j_{i,i-1}}{N} \implies \langle J \rangle = \frac{\langle \sum_{i=1}^{N} j_{i,i-1} \rangle}{N} \]  

(11)

Thermal conductivity may now be calculated through:

\[ \kappa = \frac{\langle J \rangle N}{\Delta T} \]  

(12)

For large \( N \), systems with normal thermal conductivity gives finite \( \kappa \), while systems with abnormal thermal conductivity gives:

\[ \kappa \sim N^\alpha, \alpha \neq 0 \]  

(13)

IV. RESULTS & DISCUSSIONS:

A. Verification & Check for Steady State Conditions

Before proceeding further, the simulation code is verified. For this purpose, a \( \Phi^4 \) chain, having \( k = c = 1 \) in equation 4 and \( N = 512 \) particles, has been considered. The simulation
TABLE I. A $\Phi^4$ chain with $k = 1$ and $c = 1$ is subjected to thermal conduction as per the methodology highlighted before. Our simulation results for thermal conductivity ($\kappa$) are compared with those obtained by Aoki and Kusnezov [12]: $\kappa_{th} = 2.724/T^{1.382}$. The difference in the results arise because of different boundary conditions adopted for finding $\kappa_{th}$.

| $T$  | $\langle J \rangle$ | $J \times N$ | $\kappa$ | $\kappa_{th}$ |
|------|---------------------|--------------|----------|--------------|
| 1    | 0.0011              | 0.570        | 2.849    | 2.724        |
| 0.5  | 0.0013              | 0.647        | 6.470    | 7.100        |
| 0.1  | 0.0023              | 1.574        | 57.870   | 65.646       |

methodology remains the same as discussed previously. Three values of $T_M$ have been considered: $T_M = 1.0, 0.5$ and 0.1. The higher temperature, $T_H = T_M + 0.1 \times T_M$, while the lower temperature, $T_C = T_M - 0.1 \times T_M$, so that temperature difference, $\Delta T = 0.2 \times T_M$. Thermal conductivity values, $\kappa$, obtained from the simulation are compared with $\kappa_{th} = 2.724/T^{1.382}$ [12]. The values are compared in table I. Simulation results are comparable with those reported earlier at higher temperatures. At lower temperature, a difference may be observed and can be attributed to the different boundary conditions used for computing $\kappa_{th}$.

We now check if steady state conditions prevail within the simulated chains. The check is based on the argument that $\langle j_{1,2} \rangle = \ldots = \langle j_{i,i-1} \rangle = \langle j_{i+1,i} \rangle = \ldots = \langle j_{N-1,N} \rangle$. In steady state conditions, the net heat current, $J$, must equal local heat current flowing between any two adjacent particles. A significant deviation of local heat current between any two adjacent particle pair indicates that the system has not yet attained steady state. The check is performed for $\Phi^4$ chains with $N = 512$ particles and stiffness parameters as described in the previous section. Results in the format ($J, |J - \min\langle j_{i-1,i} \rangle|, |J - \max\langle j_{i-1,i} \rangle|$) for $T_M = 1.0, 0.5$ and 0.1 are: (0.0221, $4.71 \times 10^{-5}, 5.88 \times 10^{-5}$), (0.0237, $3.383 \times 10^{-5}, 2.366 \times 10^{-5}$), (0.009955, $1.4206 \times 10^{-5}, 7.7032 \times 10^{-6}$), respectively. The small deviation of local heat currents from the total heat current indicates that the chain has steady state conditions after 750 million time steps, and meaningful time averages may be computed.
FIG. 3. Scaled temperature profile of $\Phi^4$ and $\Phi^{4C}$ chains with $N = 512$ subjected to three different $T_M$. Scaling is done so that $T_H = 1.1$ and $T_C = 0.9$. $T_i$ values of the remaining particles are interpolated. The green straight line indicates a perfectly linear plot. As can be seen from the figure, deviation from a linear profile decreases for $\Phi^4$ chain as $T_M$ increases. For $\Phi^{4C}$ chains, the deviation from linearity is comparatively lesser. Boundary jumps in temperature are more predominant for $\Phi^4$ chains than in $\Phi^{4C}$ chains.

B. Temperature Profile

Under an imposed temperature gradient, assuming local thermodynamic equilibrium, each particle of a chain has a well defined kinetic temperature. Since three different $T_M$ values have been considered, for each particle $i$, a scaled kinetic temperature, $T_{S,i}$, is defined:

$$T_{S,i} = 1.0 + 0.2 \times \frac{T_i - T_M}{T_H - T_C}$$

so that the temperature of a particle always varies between 1.1 and 0.9 and a meaningful comparison can be made. The scaled temperature profile of $\Phi^4$ and $\Phi^{4C}$ chains with $N = 512$ is shown in figure 3. A typical $\Phi^4$ chain exhibits boundary jumps in temperature profile which becomes more prominent with decreasing $T_M$. Introduction of soft-sphere collisions drastically reduce the boundary temperature jumps in the $\Phi^{4C}$ chain. A stark contrast can be seen for the two chains especially at lower values of $T_M$. It must be noted that the exact reason for boundary jumps in $\Phi^4$ chains is still open to research.

Researchers have argued that in between the temperature jumps, the temperature profile
TABLE II. A comparison of deviation from linearity, $d_L$, for $N = 512$ particles and three values of $T_M$. As is evident, the deviation from linearity is minimum for $\Phi^4C$ chain.

| $T_M$ | $\Phi^4$ | $\Phi^4C$ |
|-------|----------|-----------|
| 1     | 0.279    | 0.2568    |
| 0.5   | 0.603    | 0.1585    |
| 0.1   | 1.175    | 0.4876    |

of a $\Phi^4$ chain varies linearly. Neglecting the temperature jumps, we now calculate the deviation of the profiles from a linear behavior (the green straight line of figure 3), using the following distance measure:

$$d_L = \sum_{i=1}^{N} \sqrt{(T_{S,i} - Y_i)^2}$$

Table II shows the results of $d_L$. The results indicate that the deviation from linearity decreases when soft-sphere collisions are introduced in the chain. The reduction in boundary jumps and deviation from linearity suggests that the $\Phi^4C$ chain allows for quicker thermalization and mimics macroscopic behavior better than the standard $\Phi^4$ chain at lower temperatures.

C. Heat Flux and Thermal Conductivity

Figure 4 shows thermal conductivity, $\kappa$, calculated using equation 12, for both $\Phi^4$ and $\Phi^4C$ chains with varying $N$ and $T_M$. Thermal conductivity of $\Phi^4$ chains conform with the existing literature [25] – with increasing $T_M$, $\kappa$ decreases. At low $T_M$, harmonic interparticle potential dominates the dynamics, and consequently, thermal conduction is near ballistic (see the solid blue line of figure 4). In such scenarios, where anharmonic effects are small, the different modes of vibrations (phonons) do not interact significantly, and the temporal evolution of energy of the lower modes occurs relatively unimpeded. As $T_M$ increases, the particles get displaced further away from their equilibrium positions, and the anharmonic tethering potential starts to dominate. Phonon-phonon interactions increase, as a result, and energy of lower modes gets channelled to other modes, causing a severe reduction in thermal conductivity.
FIG. 4. Variation of thermal conductivity, $\kappa$, with $N$ and $T_M$ for $\Phi^4$ and $\Phi^{4C}$ chains. While in the $\Phi^4$ chain, $\kappa$ increases with decreasing temperature owing to harmonic effects being predominant, the behavior of $\Phi^{4C}$ chain is not straightforward. It first decreases with temperature and then suddenly increases.

The case of $\Phi^{4C}$ chains is peculiar. At very low $T_M$, one obtains relatively high thermal conductivity (see blue dashed line in figure 4). This may be attributed to the dominating effect of harmonic potential over the soft-sphere and tethering potentials. However, there is a sudden trend reversal, as is evident from the red and black dashed lines corresponding to $T_M = 0.5$ and 1.0, respectively – $\kappa$ for $T_M = 1.0$ is more than that of $T_M = 0.5$. Thermal conductivity further increases as $T_M$ is increased from 1.0 to 2.0. This trend reversal – higher thermal conductivity at high temperatures – is typically absent in most one dimensional chains, and signify the importance of not allowing the particles to cross each other. The exact reasoning behind such trend reversal requires further research, and at this moment we can only offer a conjecture – at higher temperatures, more particles collide, and as a result, energy transfer between two particles increase, causing increased thermal conductivity. It is evident from figure 4 that thermal conductivity converges much quickly with $N$ for $\Phi^{4C}$ chains vis-à-vis $\Phi^4$ chain, so only a fraction of $\Phi^{4C}$ particles are necessary to study the limiting behavior.
V. CONCLUSIONS

This manuscript generalizes the $\Phi^4$ model such that no two adjacent particles cross each other. In simpler terms, the $\Phi^4$ particles can now “collide” and repel each other. This is achieved by adding an anharmonic soft-sphere potential to the standard $\Phi^4$ Hamiltonian. The effect of not allowing the particles to cross each other is investigated through molecular dynamics. Specifically, we focus on temperature profile and thermal transport properties of the chain.

It is observed that the addition of soft-sphere potential significantly alters the temperature profile while satisfying Fourier’s law without significantly altering the diffusion characteristics. The boundary jumps present in $\Phi^4$ chains become negligible in $\Phi^{4C}$ chains, with the difference being more pronounced at low temperatures. The results suggest that the $\Phi^{4C}$ model may be used to study multiscaling behavior with ease at lower temperatures. Being closer to a realistic system, where two particles cannot cross each other, an exhaustive study is in order to understand the behavior of $\Phi^{4C}$ model in depth.

Perhaps, the most interesting results arise for thermal conductivity. Like $\Phi^4$ chain, at very low temperatures, one observes large thermal conductivity for $\Phi^{4C}$ chain as well. However, unlike $\Phi^4$ chain, thermal conductivity does not always increase with decreasing temperature. We suspect that heat flux due to the interplay between soft-sphere and harmonic potentials determines the magnitude of thermal conductivity – with increasing temperature there is a marginal rise in thermal conductivity – possibly because of increased heat flux due to more frequent “collisions” between the particles at higher temperature. Again, an in-depth study is required to ascertain the veracity of our explanation. One can split the contributions of heat flux due to the different potentials along with monitoring the frequency of collisions to understand the interplay. Alternatively, one can look at the Fourier space, and continuously monitor the modal energies to identify if there is more interaction between the phonons (phonon-phonon interaction) resulting in peculiar behavior of thermal conductivity. As of now, the problem remains wide open to research community.

Lastly, we would like to highlight that the numerical solution to the equations of motion relies upon Taylor series expansion. With the inclusion of soft-sphere potential, the nonlinear behavior starts to dominate when two particles come very close, and this requires a very small time step for solution. It is preferable to use adaptive time integration methods for
this problem.

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