Crossover between different universality classes: Scaling for thermal transport in one dimension

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Abstract – For thermal transport in one-dimensional (1D) systems, recent studies have suggested that employing different theoretical models and different numerical simulations under different system’s parameter regimes might lead to different universality classes of the scaling exponents. In order to well understand the universality class(es), here we perform a direct dynamics simulation for two archetype 1D oscillator systems with quite different phonon dispersions under various system’s parameters and find that there is a crossover between the different universality classes. We show that by varying anharmonicity and temperatures, the space-time scaling exponents for the systems with different dispersions can be feasibly tuned in different ways. The underlying picture is suggested to be understood by phonons performing various kinds of continuous-time random walks (in most cases, be the Lévy walks but not always), probably induced by the peculiar phonon dispersions along with nonlinearity. The results and suggested mechanisms may provide insights into controlling the transport of heat in some 1D materials.

Transport in one dimension has, for a long time, been realized to be anomalous in most cases [1,2], with signatures of a universal power-law scaling of transport coefficients, among which the heat transport has been extensively investigated in the recent decades, both by various theoretical techniques, such as the renormalization group [3], mode coupling [4,5] or cascade [6–8], nonlinear fluctuating hydrodynamics [9–11], and Lévy walks [12–15]; and also by computer simulations [16–26]. For all studied cases two main scaling exponents have been given the most focus, i.e., $\alpha$ describing the divergence of heat conductivity with space size $L$ as $L^\alpha$ and $\gamma$ characterizing the space($x$)-time($t$) scaling of heat spreading density $\rho(x,t)$ as $t^{-\frac{1}{\gamma}}\rho(t^{-\frac{1}{\gamma}},x,t)$. Unfortunately, however, depending on the focused system’s different parameter regimes, different theoretical models have been employed, and different predictions have been suggested. Thus, the universality classes of both scaling exponents and their relationship [27] remain controversial: i) for $\alpha$, two classes, $\alpha = 1/3$ [3,9,14–16,19] and $\alpha = 1/2$ [4,5,9], have been reported; however, the universality has been doubted [25,26] and a Fibonacci sequence of $\alpha$ values converging on $\alpha^* = (3 - \sqrt{5})/2$ ($\simeq 0.382$) [6–8] has been suggested; ii) for $\gamma$, two universality classes, $\gamma = 5/3$ [9–11,13–15,20–23] and $\gamma = 3/2$ [9–11,22,23], have been recently predicted.

The discussion of the latter scaling exponent $\gamma$ is currently very hot [9–15,20–23,28,29] because it involves more detailed space and time information [30], thus it can present a very detailed prediction for heat transport. It is also relevant to the dynamical exponents in general transport processes far away from equilibrium, such as that described by the famous Kardar-Parisi-Zhang (KPZ) class [31]. Recently, a new class of dynamical exponent $5/3$ [32] and a novel Fibonacci family of dynamical universality classes [33] beyond the KPZ class, quite similar to the universality of $\alpha$ and $\gamma$ [6–8], have been proposed.

Nevertheless, simulations to precisely identify the dynamical exponents, especially the exponent $\gamma$ for heat transport, from direct dynamics, are actually hard to carry out, causing quite few reliable numerical results [22,23,28,29]. With this question in mind, in

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1There may be a generic relationship between $\alpha$ and $\gamma$; such as $\alpha = 2 - \gamma$ suggested by the Lévy walks theory, obtained from simultaneously combining $\alpha = \mu - 1$ and $\mu = 3 - \gamma$, where $\mu$ is the time scaling exponent of the mean squared displacement of energy fluctuations spreading $\sigma^2(t)$: $\sigma^2(t) \sim t^\mu$. However, it should be noted that $\alpha = 2 - \gamma$ has not been fully confirmed yet as the relation between $\alpha$ and $\mu$ is still controversial.
This work, by employing a direct dynamic simulation method [34] we provide a very precise estimate of \( \gamma \) from the new perspective of different phonon dispersions and under various system’s parameter regimes, from which a crossover between the different universality classes of \( \gamma \) can be clearly identified. We argue that different dispersions along with nonlinearity could result in quite different microscopic environments surrounding phonons continuous-time random walking (CTRW), which then leads to the different scaling exponents. The results present the very convincing numerical evidences for identifying the universality classes of \( \gamma \) and present also a suggestive picture of the reason why it is so.

More specifically, to illustrate our viewpoint, two archetype oscillator systems with and without usual phonon dispersions, i.e., a Fermi-Pasta-Ulam-\( \beta \) (FPU-\( \beta \)) lattice and its extension to double-well (DW) version, will be employed. To identify the scaling exponent \( \gamma \), the heat, rather than the total energy’s fluctuation relaxation [34] of the systems will be investigated. We assume that the dispersion may have its effect along with the system anharmonicity and temperatures. Thus, we shall study how the scaling depends on these parameters.

Both focused systems are momentum-conserved and with an even symmetric potential, thus appearing to follow the \( \gamma = 3/2 \) universality class predicted by some related theoretical models under appropriate parameter regimes [11,22,23], whose Hamiltonian can be represented by

\[
H = \sum_{k} \frac{p_k^2}{2} + V(q_{k+1} - q_k),
\]

where \( q_k \) is the displacement of the \( k \)-th particle from its equilibrium position, \( p_k \) the momentum, \( V(\xi) = \xi^2/2 + \beta \xi^4/4 \) (-\( \xi^2/2 + \xi^4/4 \)) for the FPU-\( \beta \) (DW) systems. From the Hamiltonian, it is clear that the former bears the usual phonon dispersions under harmonic approximation; however, the latter does not. We expect that such key distinction may affect the universality class(es) of \( \gamma \).

The direct dynamics simulation method [34] adopted here employs the following spatio-temporal function:

\[
\rho(x,t) = \frac{\langle Q_i(t) \rangle}{(\Delta Q_i(t)^2)}
\]

to characterize the heat spreading density, where \( \langle \cdot \rangle \) represents the spatio-temporal average, \( \Delta Q_i(t) = Q_i(t) - \langle Q_i(t) \rangle \); \( Q_i(t) \equiv \sum Q(x,t) \) is the total heat energy density in an equal and appropriate lattice bin (the number of particles in each bin is equal to \( n = L/b \) (\( n \equiv 2 \)) with \( b \) the total bins number), \( E(x,t) \equiv M(x,t) + \langle (E) + (F) \rangle M(x,t) \) [35] is the single-particle’s heat energy at an absolute displacement \( x \) and time \( t \), with \( E(x,t) \) and \( M(x,t) \) the corresponding energy and mass density, \( (E) \), \( (M) \) and \( (F) \) (\( \equiv 0 \)) the spatio-temporal average of \( E(x,t) \), \( M(x,t) \) and the internal pressure, respectively.

From this definition, the key point here is concerning the particles heat energy, rather than the usually considered total energy fluctuations [35], which has been verified to be more directly related to heat conduction [36]. In addition,

\[
\rho(x,t) \simeq \frac{1}{t^{1/\gamma}} \rho \left( \frac{x}{t^{1/\gamma}}, t \right),
\]

identifies the scaling exponent \( \gamma \) (see footnote \(^3\)), which just gives the dynamical exponent for the particular heat transport without performing complicated theoretical calculations.

We first consider the FPU-\( \beta \) system. Figure 1 depicts the rescaled \( \rho(x,t) \) for two \( \beta \) values, where the temperature \( T = 0.5 \) is considered\(^4\). In both cases the formula (1) is beautifully satisfied suggesting that their profiles can be well captured by the Lévy walks types; however, the scaling is obviously different. For the frequently considered \( \beta = 1 \) case, the best fitting gives \( \gamma = 1.519 \) (see fig. 1(b)), very close to the \( \gamma = 3/2 \) universality class [10,11,22,23]; however, for \( \beta = 0.02 \), with so slight nonlinearity, the best fitting suggests \( \gamma = 0.996 \) (see fig. 1(a)), which coincides well with the U-like Lévy walks propagator in the ballistic regime [12,37], thus suggesting that the ballistic Lévy walks theory might be appropriate for describing ballistic heat transport. It is also interesting to note that this \( U \)-shaped distribution has also been found useful in the statistical description of blinking quantum dots [38].

We thus check pictures for other \( \beta \) values and summarize them in fig. 2, from which, regardless of \( L \) and as \( \beta \) increases, \( \gamma \) first remains constant at about \( \gamma \approx 1 \) (\( \beta \leq 0.02 \)), then it increases continuously and nonmonotonously. In particular, for \( \beta \) close and up to 1, most of \( \gamma \) concentrate between \( 3/2 \) and \( 5/3 \), then both previous expectations of the \( \gamma = 3/2 \) [9–11,22,23] and \( \gamma = 5/3 \) [13–15,20,21,24] classes are understandable, because most of them are focused on the \( \beta = 1 \) case (under

\(^3\)The scaling of the two side sound modes are also predicted by the related theories, here we only limit our focus to the central heat mode scaling.

\(^4\)This temperature has been verified to be quite accessible by our simulations for FPU-\( \beta \) systems.

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\[ x, t \]

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\[ L \]

---

\[ T \]

---

\[ \rho \]

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\[ M(x,t) \]

---

\[ (E), (M) \]

---

\[ (F) \]

---

\[ \gamma \]

---

\[ \beta \]

---

\[ \rho(x,t) \]

---

\[ \Delta Q_i(t) \]

---

\[ \langle Q_i(t) \rangle \]

---

\[ \sum Q(x,t) \]

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\[ E(x,t) \]

---

\[ M(x,t) \]

---

\[ (E) + (F) \]

---

\[ \rho \left( \frac{x}{t^{1/\gamma}}, t \right) \]

---

\[ t^{1/\gamma} \]

---

\[ \frac{1}{t^{1/\gamma}} \rho \left( \frac{x}{t^{1/\gamma}}, t \right) \]

---

\[ \gamma = 1.519 \]

---

\[ \gamma = 0.996 \]

---

\[ \beta = 1 \]

---

\[ \beta = 0.02 \]

---

\[ L \]

---

\[ \rho \]

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\[ M \]

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\[ (F) \]
appropriate temperatures). Obviously, to more precisely characterize \( \gamma \) in this range, longer space size simulations are still required\(^5\). But, anyway, based on the focused space range here, one can clearly identify a crossover from ballistic (\( \gamma = 1 \)) to superdiffusive (\( \gamma > 1 \)) transport at about \( \beta_c \simeq 0.01–0.02 \), suggesting that a finite \( \beta \) phase transition would probably take place. Perhaps, more surprising is the continuous variation of \( \gamma \) (\( 1 \leq \gamma < 1.7 \)), which clearly suggests that there is a crossover between the different universality classes of \( \gamma \).

Next we refer to the DW case. Figure 3(a)–(c) plot the rescaled \( \rho(x,t) \) and panel (d) presents \( \gamma(T) \) (see footnote \(^6\)). From (a)–(c) a perfect coincidence with Lévy walks scaling following formula (1) (but with different \( \gamma \)) can be clearly identified. In addition to this similarity to figs. 1 and 2, it is worth noting that around \( T = 0.1 \), in fig. 3(b) the two side sound modes seem completely disappeared, causing \( \rho(x,t) \) to be very close to the Gaussian profile (\( \gamma = 2 \)). So it is reasonable to see normal heat conduction (\( \alpha = 0 \)) found previously just near this temperature [39]. However, it should be emphasized that the appearance of a diffusive mode shown here seems to indicate that the two sound modes could be completely absent in some 1D Hamiltonian systems under appropriate anharmonicity or temperature [32] from the perspective of hydrodynamics, which may be attributed to the no-bear usual phonon dynamics [40].

By further carefully examining \( \gamma(T) \) (see fig. 3(d)), we show, as expected that, a crossover from superdiffusive (\( 1 < \gamma < 2 \)) to normal transport (\( \gamma = 2 \)) at about \( T_c \simeq 0.1 \) is likely to take place, though longer space size simulations remain required to confirm the transition. Surprisingly, these results also indicate a continuous variation of \( \gamma \) (\( 1.4 < \gamma < 2 \)), thus further supporting that the universality classes of \( \gamma \) may be changed when the system’s dispersion becomes so unusual.

Finally let us discuss why here we see a crossover between different universality classes\(^7\). As all the observed densities \( \rho(x,t) \) show good coincidence with Lévy walks profiles, then a natural picture in mind is that phonons, as main heat carriers, might perform various kinds of CTRW to support the different scaling exponents, probably induced by many complicated environments. We thus argue that such surroundings of phonons may mainly result from the very peculiar phonon dispersions along with nonlinearity. Then, under appropriate anharmonicity and temperatures, many distinct nonlinear excitations, such as solitary waves [41], discrete breathers (DBs) [42] and soft modes [43] will be excited in various kinds of systems with quite different dispersions. Such excitations will interact with phonons, eventually leading to the different \( \gamma \). With this picture we now turn to analyzing the power spectrum of thermal fluctuations, which covers both phonons and their environments information and may provide a suggestive understanding of the observed crossover.

Figure 4 depicts the typical spectrum \( P(\omega) \), defined by 
\[
P(\omega) = \lim_{t \to \infty} \frac{1}{T} \int_0^T v(t) \exp(-i\omega t) dt
\]
calculated and by a frequency \( \omega \) analysis of the equilibrium velocity \( v(t) \) along the chains (for the calculation details, see the appendix of the review [44]). As expected, \( P(\omega) \) shows strong \( \beta \)- and \( T \)-dependence, similarly to \( \gamma \). We here address two points. First, in view of the whole spectrum, as \( \beta \) increases, FPU-\( \beta \) system’s \( P(\omega) \) walks towards the direction of high frequencies, suggesting that phonons tend to

\(^5\)Our preliminary results showed a variation of \( \gamma \) with the increase of \( \beta \), quite similar to the Fibonacci family of universality classes as suggested by [6–8,33]. In fact, the results of fig. 2 in this work also have indicated some hints.

\(^6\)The lowest temperature considered here is \( T = 0.02 \), up to which we have confirmed that the final results are not sensitive to the initial states assigned to just one of the potential wells; or between the two wells alternately, or randomly.

\(^7\)The crossover means that there may be a particular universality classes existing under certain system parameter regimes, just as predicted by some related theoretical models; however, in view of the different phonon dispersions for different systems, the crossover between different universality classes should appear.
become “harder” (see fig. 4(a), (b)). Further careful examination of the excitations indeed supports the emerging of both solitary waves [41] and DBs [42] (not shown); rather, in the DW systems, phonons seem to become “softer”, especially around $T \approx 0.2$ (see fig. 4(e)–(f)), indicating that here the soft modes [43] appear. These tendencies can be readily captured from the indicated peaks in the high frequencies regime.

We refer the second point to the lowest-frequency components (see fig. 5). Phonons with the lowest frequency, usually called long-wavelength (goldstone) modes, are generally believed to be very weakly damped due to the conserved feature of momentum [45]. Because of their weak damping, the lowest-frequency modes can greatly affect heat transport. From fig. 5 the damping of phonons first originates from high frequencies and then quickly walks towards the low ones, also showing strong $\beta(T)$-dependence. In particular, in the DW case, the strongest and fastest damping seems to appear around $T_c \approx 0.1$ (see fig. 5(d)), which may explain why a transport close to normal could be found.

For the FPU-\(\beta\) chains, up to $\beta_c \approx 0.01$–0.02, a fast damping can be observed (see fig. 5(a), (b)); however, we are unable to identify $\beta_c$ just from the damping. Fortunately, $\beta_c$ seems related to the strong stochasticity threshold addressed in [46]. For the particular $\beta = 1$ case, ref. [46] suggested an energy-density threshold about $\langle E \rangle_c \approx 0.1$. Then viewing that in our case $\langle E \rangle \approx 1.0$ (since $T = 0.5$), a straightforward analysis of $\langle E \rangle_c \sim \beta_c^{3/2}$ infers $\beta_c \approx 0.01$, which is consistent with the results of fig. 2.

Given the above macroscopic and microscopic evidences, it would be suggestive to propose such an understanding of the different universality classes: different

nonlinear spectrum dynamics can result in quite distinct heat transport behaviors described by phonons performing various kinds of CTRW, eventually leading to the different scaling exponents. We emphasize that here this picture attributes the main mechanism to the phonons dispersions along with nonlinearity, which seems not contradicted by the above direct dynamics simulations.

In summary, by employing two representative oscillator systems bearing (and not) usual phonon dispersions, we have demonstrated with precise and convincing numerical evidences that there is a crossover between different universality classes of the space-time scaling exponent $\gamma$ for heat transport in various kinds of 1D systems with different phonon dispersions. With the difference of phonons dispersions in mind and by varying the anharmonicity and temperature, we have showed that $\gamma$ can be feasibly tuned from $\gamma = 1$ to $\gamma = 2$ (for the two focused systems), indicating that the corresponding transport can be controlled from ballistic, superdiffusive ($1 < \gamma < 2$), to normal. We have also suggested an understanding for the crossover by assuming phonons performing various kinds of CTRW induced by the peculiar dispersions along with nonlinearity, which seems to be supported by the analysis of both systems phonon spectrum. These findings and the suggested picture thus imply some potential applications. For example, in virtue of the DW systems, one may be able to vary the phonons spectrum by tuning system temperatures, and finally manipulate heat. Such an idea would be realized by the variation of the trapping frequencies in the recent focused ion chains [47], where a structural phase transition very similar to the DW systems has been found [48].

As we have understood this crossover, then apart from those applications, further careful theoretical examinations, especially the numerical ones, are expected to be stimulating. In fact, the quite efficient direct dynamics simulation method [34] adopted here has special

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Fig. 4: (Color online) $P(\omega)$ of the thermal fluctuations ($L = 2000$): ((a), (b)) FPU-\(\beta\) chains; ((c), (f)) DW chains. The dotted lines indicate $\omega_p$ in a high-frequency regime.

Fig. 5: (Color online) Log-log plot of fig. 4, where the dotted lines indicate $\omega_D$ below which phonons are weakly damped.
advantages for identifying the scaling of transport, because it is applicable to any other physical quantities diffusion in a large variety of complicated systems with any phonon dispersion under various anharmonicity and temperatures; however, many of them are not accessible by the existing theories. Thus, we expect to extend this method to other kinds of systems and higher dimensions (it is straightforward). For example, a quick application to two-dimensional systems will be studied.

Another aspect of further works may be devoted to the underlying picture. It has been well proposed [12–15] that anomalous heat transport in 1D systems can be understood by phonons performing Lévy walks. Though all of the above simulations seem in good agreement with the Lévy walks description, in our opinion, the walks may not always be of the Lévy type as the phonon dispersions could be more complicated. In fact, our quite recent simulations of a FPU-β model chain with both nearest-neighbor (NN) and next-nearest-neighbor (NNN) couplings having a phonon dispersion of a high-order form [25] (the Hamiltonian is \( H = \sum_k \beta_k p_k^4/2 + V(q_{k+1} - q_k) + rV(q_{k+2} - q_k) \) with \( r \) the ratio of the NNN to NN couplings and the potential \( V(\xi) = \xi^2/2 + \beta \xi^4/4 \); note that here the dispersion depends on the ratio \( r \)), indeed support a more complicated density shape which has not been covered yet by the existing progress of the Lévy walks theory [12] (see fig. 6, the central ranges imply some localizations, which may be due to the effects of the peculiar dispersions along with nonlinearity enabling us to excite the intraband DBs [25]; note that here the Lévy walks scaling might not be satisfied, so we are unable to show the exact scaling exponent \( \gamma \)). That is why we attribute the mechanism to generic CTRW but it is not limited to Lévy walks. We also note that further efforts to understand the picture may have to provide the random walks mechanism with a “hydrodynamic” foundation [12]. However, regardless of the picture, fig. 6 again supports the fact that different universality classes will be observed in different 1D nonlinear systems with quite different phonon dispersions.

![Graph showing the density \( \rho(x,t) \) for the FPU-β chain with both NN and NNN couplings, \( L_{\text{effective}} = 2000 \), \( \beta = 0.2 \), \( T = 0.5 \), and the ratio \( r = 0.25 \).](image)

**References**

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