In solid phases, phonons are collective, elementary vibrations in harmonic lattices and as such play a prominent role for plenty physical transport phenomena [1–4], of which the conduction of heat is the most well known. In harmonic lattices these phonons constitute nondecaying, stable propagating waves obeying a dispersion relation for angular frequency ω and the corresponding wavenumber k. This in turn implies that these phonons possess strictly infinite mean free paths (MFPs). Consequently, heat transport in harmonic lattices is ballistic [5, 6] and thus no temperature gradient (inherent with the validity of Fourier’s law) can be sustained.

Generally, however, everyday solid materials are far from being perfect harmonic lattices. Therefore, the phonon concept bears no solid basis away from its underlying (effective) harmonic approximation. As pointed out by Peierls long ago [2, 3], such anharmonicity is essential for Umklapp scattering — an indispensable process for a finite, size-independent thermal conductivity κ in three dimensional (3D) materials. Phenomenologically [3, 4], the thermal conductivity is approximated in terms of a wavenumber-dependent phonon MFP l_k; i.e. \( γ = (1/3) \sum_k C_k v_k l_k \). Here, \( C_k \) is the specific heat of the phonon mode and \( v_k \) its phonon group velocity.

Thus, we encounter a dilemma in the sense that the rigorous existence of a phonon excitation in a nonlinear lattice is self-contradictory to the very existence of a finite MFP. Particularly, this concept of a nonlinear or anharmonic phonon may cause considerable unease when dealing with strong nonlinear interaction forces and/or high temperatures where thermal excitations no longer predominantly dwell the harmonic well regions of corresponding interaction potentials. The state of the art overcoming this dilemma involves the so termed renormalized phonon picture [7–12]. In essence, this approach uses an effective harmonic approximation of the nonlinear interaction forces via a temperature-renormalized phonon dispersion.

The objective of finite MFPs and corresponding relaxation times is, however, not within the scope of renormalized phonon theory. One possibility addressing the missing link consists in combining approximate Boltzmann transport theory for heat transport with a single mode relaxation time approximation [13, 14]. In fact, while this phenomenological scheme is commonly adopted nowadays, its regime of validity has never been justified from first principles [15, 16]. This open challenge notably calls for its resolution. Particularly, this is the case for heat transport in low dimensional nonlinear lattices where the corresponding thermal conductivity may even diverge with increasing length [17–19]. For consistency this then implies that anharmonic phonons in these 1D systems must as well exhibit a divergent scaling for its low k phonon MFPs.

With this letter we put forward an experiment-inspired theoretical picture for the role of propagating anharmonic
phonons \((a-ph)\) when ubiquitous strong nonlinear interaction forces are ruling the lattice dynamics. Our main objective is to significantly advance an \(a-ph\) concept that simultaneously solves the following challenges: (i) the concept inherently allows for an \textit{a priori} visualization of the physical existence of \(a-ph\)’s together with their MFPs, (ii) the concept is manifest nonperturbative in the strength of nonlinearities and, additionally, (iii) is neither restricted to low temperature nor to low frequencies.

**Triggering anharmonic phonons.** To elucidate whether a phonon picture still holds in a strongly nonlinear lattice we use a “tuning fork experiment” as sketched with Fig. 1(a). Here, a tuning fork operating at small driving strength and at a fixed frequency \(\omega\) is placed in front of a crystalline, nonlinear lattice slab held at a temperature \(T\). This driving source will generate sound that propagates along the slab. For a phonon picture to hold up it is then required, — at least in good approximation — that the propagating disturbance physically causes a collective, plane wave-like response. Moreover, for the MFP to exist the spatially dependent wave amplitude necessarily must undergo attenuation with increasing spatial spread. Preferably, this so decaying amplitude of the propagating plane wave exhibits a unique scale only. If so, this renders the searched MFP for \(a-ph\)’s in a nonlinear lattice. The \(a-ph\) still holds up, however, for cases with the attenuation occurring non-exponentially; i.e., when exhibiting multiple spatial scales.

Importantly, this so devised experiment can conveniently be modeled in theory by means of classical molecular dynamics (MD). Additionally, the driving force is set sufficiently small so that the response occurs solely within its linear regime; i.e., yielding the output signal at exactly the same (driving) frequency only [20].

To realize this thought experiment, we start with the lattice being held at thermal equilibrium. We next apply an external weak force \(f_a(t) = f_1 \cos \omega t\), see in Fig. 1(b), to the first particle and measure the resulting response occurring at all the remaining particles. For the \(a-ph\) concept to make sense this collective response must assume the form of a plane wave; i.e., the thermally averaged velocity \(v_n(t)\) of the \(n\)-th particle is required to read for \(n = 1, 2, \cdots\):

\[
\langle v_n(t) \rangle = |A_n| \cos(\omega t + \phi_n) = \text{Re}(|A_n|e^{i(\phi_n + \omega t)}),
\]

(S1)

with the phase obeying

\[
\phi_n = -kn + \phi_0.
\]

(S2)

In the expression, \(\langle \cdot \rangle\) denotes the statistical average under the influence of the driving force. This so parameterized excited motion defines an effective phonon with a frequency \(\omega\) that precisely matches the input driving frequency \(\omega\). The coefficient, \(k = -d\phi_n/dn\), plays the role of the wavenumber \(k\). With the amplitude \(|A_n|\) assumed to decay exponentially as

\[
|A_n| \propto e^{-n/\ell},
\]

(S3)

its decay length \(\ell\) provides the searched MFP for this \(a-ph\).

For the sake of simplicity, but without a loss of generality, we next formulate the concept for 1D nonlinear lattices only. The scheme can readily be generalized to higher dimensions and complex materials by applying forces to atoms lying on a chosen lattice plane that trigger either longitudinal or transverse waves which propagate perpendicular to the plane [21]. In terms of phase space variables \((\{x_n\}, \{p_n\})\) the lattice Hamiltonian assumes the dimensionless [22] general form:

\[
H_0 = \sum_{n=1}^{N} \left[ \frac{p_n^2}{2} + V(x_{n+1} - x_n) + U(x_n) \right],
\]

(S4)

where \(V(x_{n+1} - x_n)\) is the inter-particle potential and \(U(x_n)\) denotes a possibly present on-site potential. Following the common approach we employ the periodic boundary conditions \((b.c.)\). The role of finite temperature \(T\) enters by using a canonical ensemble with the unperturbed distribution reading, \(\rho_{eq} = Z^{-1}\exp\left(\beta_\tau H_0\right)\), where \(\beta_\tau = 1/k_B T\) is the inverse temperature and \(Z\) the canonical partition function.

Applying a weak single–frequency signal, \(f_a\), to the first particle of the anharmonic lattice, we can calculate the thermally averaged velocity at each site \(n\) using well-known canonical linear response theory [20, 24], yielding [21]:

\[
\langle v_n(t) \rangle_f = \beta_\tau \int_0^t ds \langle v_n(t-s)v_1(0) \rangle f_a(s),
\]

(S5)

where \(\langle \cdot \rangle\) denotes the canonical ensemble average.

For \(f_a(t) = f_1 \cos \omega t\), the excited motion can equivalently be cast into the form of Eq. (S1), which involves the Fourier transformed susceptibility \(\chi(\omega)\), i.e.,

\[
\langle v_n(t) \rangle_f = f_1 \text{Re}[\chi_n(\omega)e^{i\omega t}]; \quad \text{with}
\]

\[
\chi_n(\omega) = \beta_\tau \int_0^\infty d\tau \langle v_n(\tau)v_1(0) \rangle e^{-i\omega \tau} \equiv |\chi_n(\omega)| e^{i\phi_n}.
\]

(S7)

This appealing result allows one to assign the existence of an \(a-ph\) and its corresponding MFP: (i) an \(a-ph\) exists with a wavenumber \(k(\omega)\) if and only if the linear relationship in (S2) is fulfilled and (ii) possesses a unique MFP \(\ell(\omega)\) when \(|\chi_n(\omega)| \propto \exp((1-n/\ell(\omega)))\). This very form considerably simplifies the numerical efforts as compared by directly studying the excited waves via the MD method; i.e., one finds the whole frequency-resolved phonon properties at once.

It is verified readily that this so introduced \(a-ph\) concept is consistent with the strict harmonic limit where \(V(x)\) is quadratic and \(U(x) = 0\). The phonon band width renders the known result; i.e., standing waves form for \(0 < \omega < 2\) with the wavenumber satisfying \(k(\omega) = 2 \arcsin \frac{\omega}{2}\) due to the periodic \(b.c.\) used. The corresponding MFP consistently is infinite. Outside this common phonon frequency bandwidth \((\omega > 2)\), however, the wavenumber \(k\) expectedly assumes complex values. This renders an exponentially decaying amplitude (or MFP), see in [21].
detecting anharmonic phonons. We apply our concept to three archetype 1D nonlinear lattices of varying complexity covering extended regimes of temperature $T$ and frequencies $\omega$. Of timely interest in the context of anomalous vs. normal heat conduction are the FPU-\(\beta\) lattice, the FPU-\(\alpha\beta\) lattice and the \(\phi^4\) lattice. Numerical details are specified in the supplementary material \[21\].

FPU-\(\beta\) lattice. The prevalentely studied nonlinear 1D lattice dynamics in the prior literature is the FPU-\(\beta\) dynamics with $V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$ and $U(x) = 0$ \[25, 26\]. Its lattice dynamics has been demonstrated to exhibit superdiffusive heat transport \[17–19, 27\].

Our results are depicted in Fig. 2 for $\chi_n(\omega)$ vs. lattice sites $n$, using different driving frequencies $\omega \in (0.0096, 2.675)$ at the dimensionless temperature $T = 0.2$. Beyond $\omega = 2.675$ the response decays extremely fast, yielding also a very short phonon MFP. This limits the evaluation of the corresponding wavenumber $k$; practically, it cannot be extracted with good confidence near $k \approx \pi$, cf. Fig. 3.

The findings in Fig. 2 provide twofold relevant information: (i) Firstly, for all frequencies depicted, the phase $\phi_\omega$ perfectly decreases linearly with $n$. This finding corroborates the existence of $a$-$ph$'s with a corresponding wavenumber $k$ given by the slope. We evaluate $k(\omega)$ for different driving frequencies $\omega$, as depicted in Fig. 3(a) and compare our results with predictions taken from the renormalized phonon theory (dashed lines) \[11, 12\], where

$$\omega = 2\alpha(T) \sin \frac{k}{2}.$$  \hspace{1cm} (S8)

Here, $\alpha(T)$ denotes the temperature-dependent renormalization factor that quantifies the strength of nonlinearity. It further yields the speed of sound $v_s = \frac{\partial V}{\partial k}|_{k=0} = \alpha(T)$. For the FPU-\(\beta\) lattice $\alpha(T) = \left(1 + \frac{\int x^4 e^{-(x^2/2)}/\sqrt{\pi} \ dx}{\int x^2 e^{-(x^2/2)}/\sqrt{\pi} \ dx} \right)^{1/2}$ \[11, 12\]; it increases with temperature, starting out at 1. As can be deduced from Fig. 3(a), excellent agreement is obtained for low frequency $a$-$ph$'s. The difference between $a$-$ph$ and renormalized phonon theory occur at large frequencies only, with deviation slightly increasing with increasing temperature. Put differently, the effective phonon theory self-consistently applies for weak anharmonic forces and long wavelength phonons only.

(ii) Secondly, within the depicted frequency regime the absolute value of the amplitude $|\chi_n|$, Fig. 2(b), nicely decays exponentially with increasing $n$. Therefore, a sensible MFP $\ell$ is obtained for each $a$-$ph$, cf. in Fig. 3(b), where we depict the MFPs at three different ambient temperatures. Moreover, the MFP diverges with the decreasing wavenumber $k$. This is a salient feature known for momentum conserving 1D-systems \[28\]. With increasing $k$ the MFPs rapidly and smoothly decrease. This is in contrast to the harmonic case where an abrupt crossover occurs at the boundary of the phonon band $\omega = 2$.

Interestingly, a power-law divergence $\ell(k) \sim k^{-\mu}$ with $\mu \approx 1.70$ is observed for small $k$ for various temperatures. The numerical result closely matches the prediction of Peierls–Boltzmann theory at weak anharmonic nonlinearity, rendering $\mu = 5/3$ \[16, 29, 30\]. A divergent exponent $\mu > 1$ causes an anomalous divergent heat conductivity $\kappa \sim N^{\beta}$ with $\beta = 1 - 1/\mu$ \[16, 18\]. Therefore, we numerically find $\beta \approx 0.411$. This $\beta$-value is very close to the most recent numerical result reported in Ref. \[31\].

We remark that with our concept of $a$-$ph$ the existence of MFPs (or its corresponding transport relaxation time $\tau_k$) in the FPU-\(\beta\) lattice is here not postulated $a$ priori \[16, 29, 30\] but is confirmed independently via MD simulations.
**FPU-αβ lattice.** The FPU-αβ lattices containing a non-vanishing cubic term $V(x) = \frac{1}{4}x^2 + \frac{1}{4}x^3 + \frac{1}{4}x^4$ and $U(x) = 0$ differ from FPU-β lattices distinctly. The inherent asymmetry of the interaction potential yields a nonvanishing internal pressure which causes thermal expansion [32, 33]. Fig. 4 shows the response function for the FPU-αβ lattice. The perfect linear dependence of the phases $\phi_n$ on $n$ can still be observed. Thus it corroborates the existence of $a$-ph’s in FPU-αβ case with corresponding wavenumbers. The amplitude $|\chi_n|$, however, now deviates from single exponential decay but instead depicts multiple scales. Observing that the amplitude profiles curve downwards, an effective single scale $\ell_{\text{eff}}$ can still be defined if we average over all scales; i.e., $\ell_{\text{eff}}(\omega) := \int_0^\infty \langle |\chi_n(\omega)|/|\chi_1(\omega)| \rangle$. The dispersion relation and the effective MFPs are displayed in Fig. 5.

Although a renormalized phonon theory for FPU-αβ lattices does not exist, we still find that Eq. (88) holds approximately true for the dispersion of our $a$-ph’s, see the dashed lines in Fig. 5. The corresponding sound speed $\alpha(\mathbf{T})$ matches well a recent result in [34].

**ϕ^4-lattice.** Here, the inter-particle potential is $V(x) = \frac{1}{4}x^2$ and an onsite potential $U(x) = \frac{1}{4}x^4$ is present. Also for this nonlinear lattice we identify that the phase follows an excellent linear decay. The MFP for the corresponding $a$-ph exists as well with a unique scale; i.e., $|\chi_n(\omega)|$ nicely decays exponentially, as shown with the supplementary material [21]. Thus, the $a$-ph concept holds up even in the presence of an onsite interaction. The dispersion relation and the related MFP’s are depicted in Fig. 6. Here, the long wavelength phonons exhibit a non-diverging finite MFP. This is due to the breaking of momentum conservation, as induced by the onsite potential. As a consequence, we obtain the validity of Fourier’s law with a normal heat conductivity [35, 36]. The dispersion relation agrees well with renormalized phonon theory [37], namely $\omega = \sqrt{4 \sin^2 \frac{\omega}{2} + \sigma}$ with $\sigma = \sum_{i=1}^N \langle x_i^2 \rangle / \sum_{i=1}^N \langle x_i \rangle^2$.

**Summary and discussion.** The challenge of identifying phonon excitations in strongly nonlinear lattices beyond their corresponding harmonic approximation, termed here anharmonic phonons ($a$-ph’s), has been tackled via a theoretically imposed “tuning fork experiment”. Doing so enables one to account for the role of temperature, large frequencies and nonlinearity far beyond a perturbation scheme. This experiment-inspired phonon concept has been successfully tested over extended parameter regimes of frequency and temperature for three archetype one-dimensional nonlinear lattices. We like to stress that a temperature dependent phonon MFP is typically not accessible in prior theories without reference to additional assumptions [13–16]. The put forward concept of the MFP holds up with a single, exponentially decaying scale for both, the FPU-β lattice, exhibiting anomalous heat conductivity, and the $\phi^4$ lattice, exhibiting normal heat conductivity. The case of the nonlinear FPU-αβ lattice turned out more intriguing in that the MFP no longer exhibits a single scale but decays with multiple scales.

A hallmark of our scheme is that the existence of the $a$-ph’s and their MFP’s is not postulated a priori, but instead is physically corroborated by following the propagation of waves within a thought experiment. The outcome then either validates, or in cases also invalidates the existence of $a$-ph with a finite MFP. This being so, our scheme distinctly differs from the recently proposed, inspiring anharmonic perturbation phonon quasiparticle scheme, see in Refs. [38, 39], being equally applicable and most useful when weak anharmonicity is present. A characteristic feature within our scheme is that here we directly search for the the existence of an $a$-ph MFP. This MFP relates to a phonon transport relaxation time which does generally not equal the phonon relaxation time [40]. The transport relaxation time is affected by Umklapp scattering only, while the latter is affected via both, Umklapp scattering and Normal scattering [2, 40]. This $a$-ph concept allows to characterize as well infinite MFPs and multiple spatial decay scales; all being features that crucially impact anomalous thermal transport away from normal in low-dimensional systems.

Therefore, the proposed $a$-ph concept may as well find its use for efficient design of novel materials exhibiting optimal heat transport characteristics, such as phononic metamaterials [41–43].

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Supplementary Material for “Anomalous Heat Diffusion”

In this supplementary material we detail our theoretical and numerical analysis and provide additional insight in our study.

EXCITED WAVES IN HARMONIC LATTICES

We first calculate the excited waves in harmonic lattices with Hamiltonian reading

$$H_0 = \sum_{n=1}^{N} \left[ \frac{1}{2M} p_n^2 + \frac{K_0}{2} (x_{n+1} - x_n)^2 \right].$$  \hspace{1cm} (S1)

Periodic boundary conditions are adopted so that $x_{0/1} = x_{N/N+1}$ and $p_{0/1} = p_{N/N+1}$. We naturally expect to recover the known dispersion relation

$$k(\omega) = 2\sqrt{\frac{M}{K_0}} \arcsin \frac{\omega}{2}$$ \hspace{1cm} (S2)

and infinite MFPs for those phonons with frequencies obeying $0 < \omega < 2\sqrt{\frac{K_0}{M}}$.

With a periodic driving force $f_d = f_1 \cos \omega t$ switched in the infinite past and applied to the first particle in a 1D-chain, the equations of motion (EOMs) can be put into a compact matrix form, reading

$$M\ddot{x} = -\Phi x + F(t).$$ \hspace{1cm} (S3)

Here, $\Phi$ is the force matrix with elements $\Phi_{i,j} = 2K_0 \delta_{i,j-1} - K_0 \delta_{i,j+1}$ and $F = f \cos(\omega t) = \{f_1, 0, \cdots, 0\}^T \cos(\omega t)$. Its solution is additive due to $F(t)$ entering a linear equation of motion. Thus, the excitations of $F(t)$ can be obtained by Fourier transformation, reading

$$\langle x(t) \rangle_f \mid F(t) = \int_{-\infty}^{\infty} G(\omega') \tilde{F}(\omega') e^{i\omega't} d\omega',$$ \hspace{1cm} (S4)

where $\tilde{\cdot}$ denotes a Fourier transform and $G$ is the phonon Green’s function

$$G(\omega) = (\Phi - \omega^2 M)^{-1}.$$ \hspace{1cm} (S5)

For a driving $f_d = f_1 \cos \omega t$, we have $\tilde{F}(\omega') = \frac{1}{2} f_1 [\delta(\omega - \omega') + \delta(\omega + \omega')]$. Therefore, in a scalar form the excited motion reads

$$\langle x_n(t) \rangle_f = \frac{1}{2} \left[ G_{n,1}(\omega) f_1 e^{i\omega t} + G_{n,1}(-\omega) f_1 e^{-i\omega t} \right] = f_1 \text{Re} G_{n,1}(\omega)e^{i\omega t},$$ \hspace{1cm} (S6)

and consequently

$$\langle v_n(t) \rangle_f = f_1 \text{Re}i\omega G_{n,1}(\omega)e^{i\omega t}.$$ \hspace{1cm} (S7)

The inversion of the phonon Green’s function can be analytically obtained. Its first column reads

$$G_{n,1} = -\frac{\cos \left( \frac{N}{2} - n + 1 \right) z}{2K \sin \frac{N}{2} z \sin z}.$$ \hspace{1cm} (S8)

The second column is obtained by cyclically shifting the first column by one element. The third column is obtained by cyclically shifting the first column by two elements, and so on. In the expression the part $e^{\pm iz}$ are the two roots of the quadratic equation $-K_0 + (2K_0 - M\omega^2)x - K_0x^2 = 0$. Therefore, $z$ satisfies

$$\cos z = \frac{2K_0 - M\omega^2}{2K_0} = 1 - \frac{M\omega^2}{2K_0},$$ \hspace{1cm} (S9)

which can be verified by substitution.
For $0 < \omega < 2 \sqrt{K_0/M}$, $z$ is a real number. According to (S7) and (S8), the velocity of excited wave varies with $n$ as

$$\langle v_n(t) \rangle_f \sim \cos \left[ \frac{N}{2} - n + 1 \right] \sin \omega t. \quad (S10)$$

It represents a standing wave formed by two plane waves with the same wavenumber $k = z$ satisfying

$$\omega = 2 \sqrt{\frac{K_0}{M}} \sin \frac{k}{2}, \quad (S11)$$

which just yields the intrinsic dispersion relation for the pristine harmonic lattice.

For a driving frequency outside of the phonon band, i.e., for $\omega > 2 \sqrt{K_0/M}$, $z$ becomes a pure imaginary number since $\cos z < -1$. If we set $\omega = \sqrt{K_0/M} (2 + \delta \omega)$ with $\delta \omega > 0$, we can get $z = \pi + i \delta z$ with $\delta z$ satisfying

$$\frac{2 + \delta \omega}{2} = \sin \left( \frac{\pi}{2} + \frac{i \delta z}{2} \right) = \cos i \delta z = \cosh \delta z. \quad (S12)$$

Then,

$$R_n = i \omega G_{n, 1} \approx (-)^n \frac{i \omega}{2K_0} \frac{e^{-(n-1)\delta z}}{\sinh \delta z} = \frac{i \omega}{2K_0} \frac{e^{\delta z}}{\sinh \delta z} e^{i \pi n - \delta zn}, \quad (S13)$$

which represents, as expected, an evanescent wave. Its amplitude decays exponentially with increasing $n$. The phase of the oscillations alters between $\pi$ and $-\pi$.

**EXCITED WAVES IN ANHARMONIC LATTICES**

In this section, we derive Eq. (6) for the excited waves in anharmonic lattices. We take a general anharmonic lattice with Hamiltonian $H_0$ composed of inter-particle interactions and possibly also onsite interactions. Then, in thermal equilibrium characterized by the temperature $T$, the probability for the phase space coordinates obeys with the inverse temperature $\beta_T = 1/(k_T T)$ the canonical phase space density, reading

$$\rho_{eq} = \frac{1}{Z} e^{-\beta_T H_0} \quad \text{with} \quad Z = \int e^{-\beta_T H_0} d\Gamma, \quad (S14)$$

where $d\Gamma = dx_1 \cdots dp_1 \cdots$.

With a driving force $f_i(t)$ applied to the $i$'th particle, the system Hamiltonian changes to $H_{tot} = H_0 + H_f = H_0 - f_i(t)x_i$. The evolution of the phase space density $P(x; v; t)$ is then governed by the Liouville equation:

$$\frac{\partial \rho_{tot}(t)}{\partial t} = {\mathcal L}_{tot} \rho_{tot} = \{H_{tot}, \rho_{tot}\}, \quad (S15)$$

where $\{A, B\}$ denotes the Poisson bracket

$$\{A, B\} = \sum_j \left( \frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} \right). \quad (S16)$$

Moreover, for convenience, we introduce $L_0 = \{H_0, \cdot\}$ and $L_f = \{H_f, \cdot\}$ and thus $L_{tot} = L_0 + L_f$.

Following canonical linear response theory, we deal with an initial condition given by: $\rho_{tot}(t = -\infty) = \rho_{eq}$. By writing

$$\rho_{tot}(t) = \rho_{eq} + \rho(t), \quad (S17)$$

we obtain the linear response solution to the first order of $f_i$, reading:

$$\rho(t) = \int_{-\infty}^{t} d\tau e^{L_0(-\tau)} L_f(\tau) \rho_{eq} = \beta_T \int_{0}^{\infty} d\tau e^{\beta_T \tau} v_i \rho_{eq} f_i(t - \tau). \quad (S18)$$

If we next consider the response of the particles’ velocities to the external force as we did in the harmonic case, we obtain

$$\langle v_n(t) \rangle_f = \int \int \int \rho_{tot}(t) d\Gamma = \beta_T \int_0^{\infty} f_d(t - \tau) d\tau \int \int \rho_{eq} e^{\beta_T \tau} v_i f_i(t - \tau) = \beta_T \int_0^{\infty} d\tau \langle v_n(\tau) v_i(0) \rangle f_i(t - \tau), \quad (S19)$$
where \( \langle ... \rangle_f \) denotes the averaged over \( \rho(t) \); it thus represents the excited motion and \( \langle ... \rangle \) denotes the canonical thermal equilibrium average with density \( \rho_{eq} \).

Upon setting \( i = 1 \) in (S19), we obtain Eq. (6) in the main article.

In order to generalize our method to three dimensional cases, we must apply a periodic driving force at the same frequency to each particles in a plane. Mores specifically, if we want to study the wave propagation along the direction \( \mathbf{k} = h \mathbf{b}_1 + k \mathbf{b}_2 + l \mathbf{b}_3 \) where \( \mathbf{b}_1, \mathbf{b}_2 \) and \( \mathbf{b}_3 \) are the primitive vectors in the reciprocal lattice, we first choose a plane with Miller indices \( (hkl) \), denoted as \( \alpha \), being orthogonal to the direction \( \mathbf{k} \). Then, we apply forces to all particles in the plane. To trigger longitudinal waves, we apply out-of-plane forces that are perpendicular to the plane. To trigger transverse waves, we apply in-plane forces. Therefore, (S19) is generalized to read

\[
\langle v^d_N(t) \rangle_f = \beta_T \sum_{i \in \alpha} \int_0^\infty d\tau \ \langle v^d_{N}(\tau)v^d_{n}(0) \rangle f^d_i(t-\tau), \tag{S20}
\]

where \( d = \perp \) or \( \parallel \) which specifies whether the direction of the force and velocity is out-of-plane or in-plane. We now identically set \( f^d_i(t) = f^d_{\parallel}(t)/N_\alpha \) (\( N_\alpha \) is the number of particles in that plane) for all \( i \in \alpha \), then (S20) can be simplified to read

\[
\langle v^d_N(t) \rangle_f = \beta_T \int_0^\infty d\tau \ \langle v^d_{\parallel}(\tau)v^d_{n}(0) \rangle f^d_{\parallel}(t-\tau) \tag{S21}
\]

where \( v^d_{\parallel} = (1/N_\alpha) \sum_{i \in \alpha} v^d_i \) denotes the average velocity for all particles in the plane \( \alpha \). We can further take an average for all particles in the same lattice plane, denoted as \( \beta \), which has the same Miller index (so that it is parallel to \( \alpha \)) but contains the \( n \)-th particle. Therefore, we obtain for the average velocity for that very plane the result

\[
\langle v^d_{\beta}(t) \rangle_f = \beta_T \int_0^\infty d\tau \ \langle v^d_{\beta}(\tau)v^d_{n}(0) \rangle f^d_{\parallel}(t-\tau). \tag{S22}
\]

From this result we can infer whether an anharmonic phonon with a wavevector pointed towards the same direction of \( \mathbf{k} \) exists or not, by following the same reasoning used for one dimensional lattices.

Note that the derivation is independent of the form of the Hamiltonian. So the method is equally applicable to study wave transport in inhomogeneous lattices, such as junctions formed by different materials.

**NUMERICAL DETAILS**

For our numerics we use throughout a fourth order symplectic eSABA\textsubscript{2} algorithm to integrate the Hamiltonian equations of motion. The time step has always been chosen as \( h = 0.02 \) and the length has been set at \( N = 2048 \), using periodic boundary conditions, for all models studied. At the beginning of each simulation, a total time \( t = 2 \times 10^6 \) is used to thermally equilibrate the system. After that, the time-homogeneous equilibrium velocity correlation \( \langle v_n(t)v_1(0) \rangle \) is calculated by using the time average which replaces, using ergodicity for the nonlinear lattice, the corresponding ensemble average. An average over \( 3.2 \times 10^9 \) steps is used. The correlation \( \langle v_n(t)v_1(0) \rangle \) is calculated for each \( n = 1, 2, \cdots, N \) and \( t = 0, h, 2h, \cdots, t_{\max} \). Afterwards, \( \chi_n(\omega) \) is obtained by taking a Fourier transform according to Eq. (7).

The upper time limit \( t_{\max} \) is properly chosen such that the excited waves along the periodic ring of size \( N \) do not overlap with each other for \( t \in (0, t_{\max}) \). Namely, \( t_{\max} < N/2v_s \) where \( v_s \) is the largest group velocity of the phonons studied, i.e., the corresponding sound velocity. On the other hand, \( t_{\max} \) is the frequency resolution. The larger \( t_{\max} \) is, the smaller is the frequency resolution. Specifically, \( t_{\max} = 655.36 \) has been used for all three models.

A few samples of the velocity correlation \( \langle v_n(t)v_1(0) \rangle \) are depicted in Fig. 7(a) for the FPU-\( \beta \) lattice at a temperature \( T = 0.2 \). \( \chi_n(\omega) \) is then calculated via Fourier transformation according to Eq. (7). For the other models, we also observe similar oscillation behavior for the velocity-velocity correlation function. In Figs. 7(b)–7(d) we present a few samples for \( \chi_n(\omega) \) as a function of \( n \) for the FPU-\( \beta \) lattice, the FPU-\( \alpha \) lattice and the \( \phi^4 \) lattice, respectively.

For the FPU-\( \alpha, \beta \) lattice, the spatial decay of the amplitude of \( \chi_n \) exhibits multiple scales rather than being single-exponential-like. Therefore, a strict MFP cannot be defined and an effective MFP can be introduced as

\[
\ell_{\text{eff}} = \frac{1}{|\chi_1(\omega)|} \int_{n=1}^{n=\infty} |\chi_n(\omega)|dn. \tag{S23}
\]

Naturally, \( n = \infty \) cannot be achieved within MD simulations. The maximal \( n \) which can be achieved is limited by \( t_{\max} \) as \( n_{\max} = v_s t_{\max} \). For our chosen \( t_{\max} \) value this corresponds to approximately \( n \sim 700 \).
FIG. 7: (a) velocity-velocity correlation function \( \langle v_n(t)v_1(0) \rangle \) for the FPU-\( \beta \) lattice. (b)-(d) \( \chi_n(\omega) \) as a function of lattice site \( n \) for a specific driving frequency \( \omega \) for the FPU-\( \beta \) lattice, the FPU-\( \alpha \beta \) lattice and the \( \phi^4 \) lattice, respectively. The temperature is \( T = 0.2 \) in all cases. The insets in (b)-(d) show the principal values of the arguments \( \text{Arg}[\chi_n] \in [-\pi, \pi) \). The principal value jumps discontinuously by \( 2\pi \) when \( -\pi \) is reached. To obtain a continuous varying phase \( \phi_n \), as depicted in the upper panels, we shift the arguments by \( 2\pi \) after each such jump.

For those frequencies satisfying \( |\chi_n=700(\omega)| \ll |\chi_n=1(\omega)| \) we find that

\[
\ell_{\text{eff}}^{\text{approx}} = \frac{1}{|\chi_1(\omega)|} \int_{n=1}^{n=700} |\chi_n(\omega)| \, dn
\]  

presents a very good approximation for Eq. (S23). For \( |\chi_n=700(\omega)| \) and \( |\chi_n=1(\omega)| \) being of the same magnitude implies that we fail to evaluate the \( \ell_{\text{eff}} \) with trustworthy accuracy. Consequently, we have limited ourselves to driving frequencies for which we find \( |\chi_n=700(\omega)|/|\chi_n=1(\omega)| < 0.1 \). We then plot \( \ell_{\text{eff}}^{\text{approx}} \) as the approximation for \( \ell_{\text{eff}} \), see Fig. 5 in the main article.