

Energy Carriers in the Fermi-Pasta-Ulam β Lattice: Solitons or Phonons?

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We investigate anomalous energy transport processes in the Fermi-Pasta-Ulam β lattice, in particular, the maximum sound velocity of the relevant weakly damped energy carriers. That velocity is numerically resolved by measuring the propagating fronts of the correlation functions of energy-momentum fluctuations at different times. We use fixed boundary conditions and stochastic heat baths. The numerical results are compared with the theoretical predictions of the sound velocities for solitons and effective (renormalized) phonons, respectively. Excellent agreement has been found for the prediction of effective long wavelength phonons, giving strong evidence that the energy carriers should be effective phonons rather than solitons.

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Energy transport in low dimensional systems has attracted enduring interest [1–4]. One striking finding is the phenomenon of anomalous transport [5–7], which has recently been experimentally verified for carbon nanotubes [8]. Most theoretical efforts [2,9,10] follow the pioneering work of Peierls and focus on the low temperature region, where weakly interacting phonons are considered to be the responsible energy carriers. A microscopic transport theory beyond the low temperature regime is still lacking, which leaves the explanation for most existing numerical and experimental results unsatisfactory. One central question concerns the type of energy carriers whose properties determine the underlying transport behavior at higher temperatures. As temperature or nonlinearity is increased, collective motions other than phonons could also be excited. It is thus necessary to identify the specific energy carriers for these low dimensional systems.

The Fermi-Pasta-Ulam β (FPU- β) lattice is a classic example showing the effect of anomalous transport, and therefore a perfect test bed for developing a correct theoretical understanding and description. Anomalous transport manifests through an increase of the heat conductivity with the system size. This in turn implies that the responsible energy carriers are anomalously weakly damped. Because of nonlinearity, solitons [11,12] and interacting phonons [13–17] are candidates for these carriers. Supersonic solitons have been considered as major energy carriers which are responsible for the anomalous transport behavior [18–20]. The reason is the numerical observation of ultrasonic energy transfer. The sound velocity c_s of energy transfer was measured by following the spreading of an initial energy pulse, using both nonequilibrium [18,21] and equilibrium [19] methods. The temperature-dependent sound velocity c_s is compared with a prediction derived from soliton theory [12] and good agreement has

been found in Ref. [18]. However, strong finite size effects of the soliton velocities were not clarified in Ref. [12]. The same data for c_s in Ref. [18] are also in good agreement with the predicted velocity for effective phonons [16]. The uncertainty of the computed data in Ref. [18] is too large to distinguish between the two predictions. To identify the true energy carriers, a more accurate numerical determination of c_s is needed.

In the present Letter, we apply the equilibrium approach recently developed by Zhao [19] to study the energy transport properties in the FPU- β lattice. We apply fixed boundary conditions and Langevin heat baths. As demonstrated in Ref. [19], the sound velocities c_s can be measured with very high precision. We show that the numerical results are in very good agreement with the prediction for effective phonons and the agreement is not limited to the FPU- β lattice. The soliton predictions show clear deviations and can be ruled out.

We consider the dimensionless Hamiltonian for the FPU- β lattice

$$H = \sum_i \left[\frac{p_i^2}{2} + \frac{1}{2}(q_i - q_{i-1})^2 + \frac{1}{4}(q_i - q_{i-1})^4 \right], \quad (1)$$

where p_i denotes the momentum and q_i denotes the displacement from equilibrium position for the i th atom with $i = 0, \pm 1, \pm 2, \dots, \pm N/2$. The local energy density is defined as $H_i = p_i^2/2 + (q_i - q_{i-1})^2/2 + (q_i - q_{i-1})^4/4$. We use fixed boundary conditions $q_{-N/2-1} = q_{N/2+1} = 0$. The two next-to-end atoms with $i = \pm N/2$ are coupled to Langevin heat baths with $\ddot{q}_i = -\partial H/\partial q_i + \xi_i - \lambda \dot{q}_i$ with white noise $\langle \xi_i \rangle = 0$ and $\langle \xi_i(t) \xi_i(0) \rangle = 2\lambda k_B T \delta(t)$ where $\langle \cdot \rangle$ denotes ensemble averages. T is the temperature, k_B the Boltzmann constant, and λ denotes the coupling strength between system and heat bath. The normalized correlation functions of energy and momentum fluctua-

tions are defined as [19]

$$\begin{aligned} C_E(i, t) &= \frac{\langle \Delta H_i(t) \Delta H_0(0) \rangle}{\langle \Delta H_0(0) \Delta H_0(0) \rangle}, \\ C_P(i, t) &= \frac{\langle p_i(t) p_0(0) \rangle}{\langle p_0(0) p_0(0) \rangle}, \end{aligned} \quad (2)$$

where $\Delta H_i(t) \equiv H_i(t) - \langle H_i \rangle$. Note that $C_{E/P}(i, t=0) = \delta_{i,0}$. Therefore, the correlation functions $C_{E/P}(i, t)$ describe the spatiotemporal spreading of the initial energy-momentum fluctuations [19].

In Fig. 1, we depict the spatial distributions of the correlation functions $C_{E/P}(i, t)$ at $t = 60$ for different temperatures. The values $T = 0.02, 0.5$, and 5 correspond to low, intermediate, and high temperature regimes, according to the scaling behavior of the aspect ratio $\epsilon = \langle (q_i - q_{i-1})^4 \rangle / \langle (q_i - q_{i-1})^2 \rangle$. This ratio scales as $\epsilon \propto T$ and $\epsilon \propto T^{1/2}$ in the low and high temperature regime. As can be seen from Fig. 1, both distributions possess symmetric propagating fronts with identical speeds. These propagating fronts are induced by the fastest traveling energy carriers [18,19]. With increasing temperature the propagation velocity increases, which is caused entirely by the presence of nonlinear terms in the equations of motion. The fluctuations of $C_P(i, t)$ are much smaller than those of $C_E(i, t)$. Therefore, we will determine the sound velocity c_s by measuring the peak positions of the propagating fronts for $C_P(i, t)$, as in Ref. [19].

Let us briefly introduce the predictions of sound velocity for solitons and effective phonons. According to [11,12], the soliton profile with $z \sim q_i - q_{i-1}$ is given by

$$Q_s(z) = \sqrt{2(c_s^2 - 1)} \operatorname{sech}\left(2z\sqrt{(c_s^2 - 1)/c_s^2}\right). \quad (3)$$

It follows that the energy of a soliton is proportional to $c_s^3 \sqrt{c_s^2 - 1}$, where we assume $c_s > 0$ without loss of generality. Using a Boltzmann distribution for energies of excitations, we conclude that the temperature T introduces

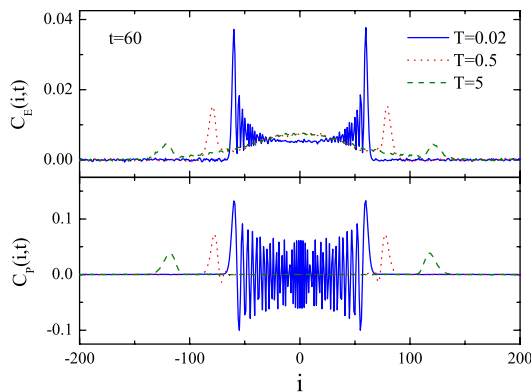


FIG. 1 (color online). Spatial distributions of $C_E(i, t)$ (upper panel) and $C_P(i, t)$ (lower panel) at $t = 60$ for $T = 0.02, 0.5$, and 5 for the FPU- β lattice with $N = 500$.

an energy scale such that larger soliton energies are exponentially suppressed. At the same time smaller energies imply smaller sound velocities. Therefore a Boltzmann distributed gas of solitons will typically show maximum sound velocities which correspond to solitons with an energy of the order of the temperature T . Thus [18]

$$c_s^3 \sqrt{c_s^2 - 1} = \eta T. \quad (4)$$

The constant η is a free fit parameter. Note that $c_s \rightarrow 1$ as $T \rightarrow 0$ and $c_s \approx \eta^{1/4} T^{1/4}$ as $T \gg 1$.

For the effective phonons, the sound velocity is defined as the maximum group velocity of the renormalized phonons. Here, renormalization implies a mean field treatment of nonlinear terms in the equations of motion. As a result eigenfrequencies of phonons are renormalized, and will increase with increasing temperature. Therefore, renormalized phonons will also yield sound velocities which increase with increasing temperature, becoming supersonic as compared to the case of $T \rightarrow 0$. In particular, $c_s = \partial \hat{\omega}_k / \partial k|_{k=0}$ where $\hat{\omega}_k = 2\sqrt{\alpha} \operatorname{sinc} k/2$ with $0 \leq k < 2\pi$ and $\alpha = 1 + \langle \sum_i (q_i - q_{i-1})^4 \rangle / \langle \sum_i (q_i - q_{i-1})^2 \rangle$ [16]. It follows [16]

$$c_s = \left(1 + \frac{\int_0^\infty x^4 e^{-(x^2/2+x^4/4)/T} dx}{\int_0^\infty x^2 e^{-(x^2/2+x^4/4)/T} dx} \right)^{1/2}. \quad (5)$$

For $T \rightarrow 0$ we find $c_s \rightarrow 1$, and in the high temperature region $c_s \approx \sqrt{\int_0^\infty x^4 e^{-x^4/4T} dx / \int_0^\infty x^2 e^{-x^4/4T} dx} \approx 1.22 T^{1/4}$. Both predictions (solitons and phonons) yield three similar results for the sound velocity: (i) $c_s \geq 1$; (ii) $c_s(T \rightarrow 0) \rightarrow 1$; (iii) in the high temperature regime, the sound velocities exhibit the same scaling with temperature as $c_s \propto T^{1/4}$.

In Fig. 2, we plot the sound velocity c_s as the function of temperature T for the FPU- β lattice. The computational

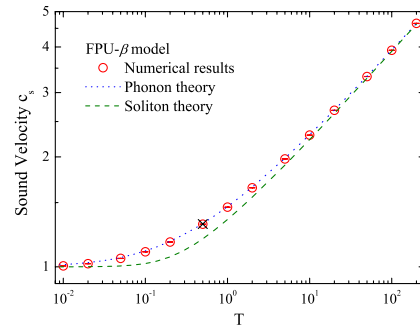


FIG. 2 (color online). Sound velocity c_s as the function of temperature T for the FPU- β lattice with $N = 1000$. The circles are the numerical results. Error bars have been plotted, but they are much smaller than the symbol size. The dotted line is the analytic prediction for effective phonons from Eq. (5) and the dashed line is the analytic prediction for solitons from Eq. (4) with $\eta = 2.215$. The numerical result obtained for $T = 0.5$ in Ref. [19] is plotted with a cross symbol.

errors are extremely small and c_s is measured very accurately. The numerical results are compared with the predictions for solitons from Eq. (4), and for effective phonons from Eq. (5). Excellent agreement has been observed for the effective phonon result in the entire temperature region being explored. The soliton curve corresponds to $\eta = 2.215$, which reproduces the correct high temperature result. However, the deviation from the prediction for solitons of Eq. (4) is quite distinct in the intermediate regime where $0.05 \leq T \leq 2$. We note that variations and optimizations of η do not improve this discrepancy. The cross symbol in Fig. 2 represents the sound velocity $c_s = 1.31$ measured at $T = 0.5$ in Ref. [19]. This result is actually coinciding both with our numerical data and with the effective phonon results. This finding provides strong evidence that the effective phonons, rather than the solitons, should be the energy carriers responsible for anomalous transport in the FPU- β lattice. It also shows that the type of heat bath (Nose-Hoover [19] or Langevin) is not relevant.

To visualize the energy transport processes, in Fig. 3 we plot the spatiotemporal evolutions of local energy densities $H_i(t)/T$ and the relative displacement $q_i(t) - q_{i-1}(t)$ for the harmonic lattice and the FPU- β lattice, respectively. The systems are thermalized at a given temperature and then the heat bath is removed. The evolution functions are recorded at thermal equilibrium and results for a suitable time window are displayed. The spatiotemporal patterns for both FPU- β lattice and harmonic lattice are qualitatively similar. Since solitons are definitely excluded for the harmonic lattice, there appears to be no signature for soliton transport in the FPU- β lattice as well. The qualitative behavior of the spatiotemporal evolutions does not change for larger time windows.

In the high temperature limit, the FPU- β model can be reduced to an H_n model with $n = 4$ assuming the following Hamiltonian: $H_n = \sum_i [p_i^2/2 + |q_i - q_{i-1}|^n/n]$. To

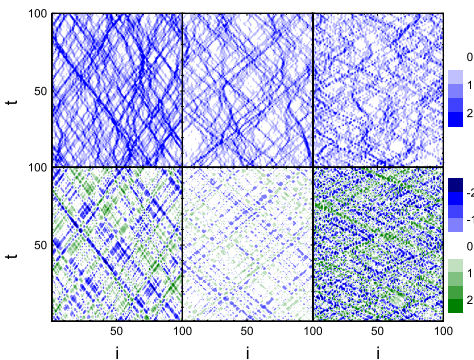


FIG. 3 (color online). Spatiotemporal evolution of energy densities $H_i(t)/T$ (upper panels) and relative displacements $q_i(t) - q_{i-1}(t)$ (lower panels) at thermal equilibrium. The left, middle, and right columns correspond to the harmonic lattice at $T = 1$, and the FPU- β lattice at $T = 1$ and $T = 20$, respectively. The lattice size $N = 100$ and periodic boundary conditions are applied.

demonstrate the power and consistency of the effective phonon formulation, we consider three different cases with $n = 3, 4$, and 5 . Following the same procedure as for FPU- β lattice, the sound velocities of effective phonons can be expressed with a compact formula

$$c_s = [\Gamma((n+1)/n)/\Gamma(3/n)]^{1/2} (nT)^{1/2-1/n}. \quad (6)$$

These predictions are plotted in Fig. 4 and compared with numerical results. We again find quantitative agreement for all three models.

Let us turn to the correlation functions. In Fig. 1, the distribution functions of $C_{E/P}(i, t)$ show many peaks between the two propagating fronts at $T = 0.02$. These peaks are typical for coherent phonon propagation in harmonic lattices. For $T = 0.5$ and 5 , there are no visible additional peaks for both distributions and a big hump emerges in the interior region for $C_E(i, t)$. The disappearance of the intermediate peaks can be therefore attributed to relaxation processes. Indeed, the distribution functions $C_{E/P}(i, t)$ for $T = 0.5$ at various spreading times $t = 10, 30, 50$, and 70 in Fig. 5 show that the short time behavior at $T = 0.5$ is similar to that for $T = 0.02$. The phonon modes relax faster at higher temperatures, while on the other hand, the long wavelength phonon modes possess very long correlation times even at very high temperatures. According to Ref. [19], the correlation function of energy fluctuations $C_E(i, t)$ is nothing but the energy density probability distribution function (PDF). Therefore we can study the energy diffusion process by measuring the mean square displacement (MSD) as $\langle r^2(t) \rangle = \sum_i i^2 C_E(i, t)$. For PDFs shown in Fig. 5, the MSD is dominated by the area around the propagating fronts and can be approximated as $\langle r^2(t) \rangle \propto t^{2-\nu}$ where the exponent ν characterizes the diminishing of the peak area with time as a consequence of slow but unavoidable dephasing of even long wavelength phonons. According to [19] the exponent $0 < \nu < 1$, and therefore the diffusion process is superdiffusive as $\langle r^2(t) \rangle \propto t^\sigma$ with $\sigma = 2 - \nu$. It is interesting to analyze the connec-

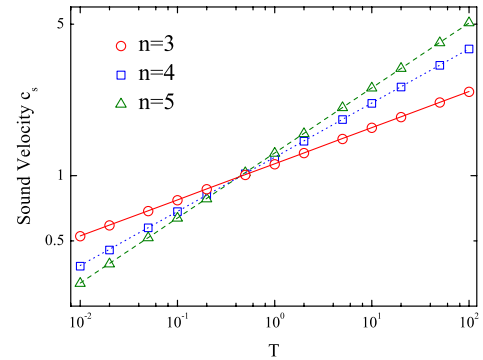


FIG. 4 (color online). Sound velocity c_s vs T for the H_n models with $n = 3, 4$, and 5 . The symbols correspond to the numerical results at $N = 1000$, whereas the lines are the predictions for effective phonons from Eq. (6).

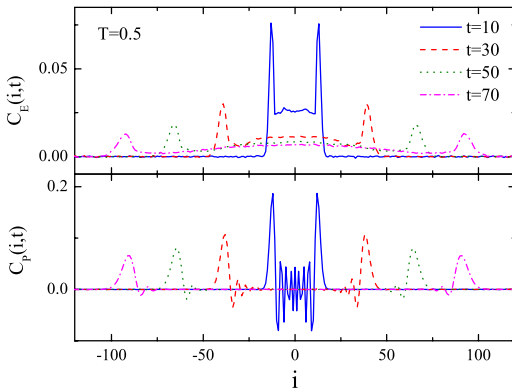


FIG. 5 (color online). Spatial distributions of the correlation functions of $C_E(i, t)$ (upper panel) and $C_P(i, t)$ (lower panel) at $T = 0.5$ for various values of time $t = 10, 30, 50,$ and 70 , for the FPU- β lattice with size $N = 500$.

tion between superdiffusion and anomalous heat conduction for the FPU- β lattice. Recall that the heat flux of phonons is $J_k = v_k E_k$ [2] where k denotes the wave number. The correlation function of the total heat flux ($J = \sum_k J_k$) can be approximately obtained as $\langle J(t)J(0) \rangle \approx \langle c_s^2 E_0(t)E_0(0) \rangle \propto t^{-\nu}$ since the only long time correlation is due to the energy carried by the long wavelength phonon modes. Applying the Green-Kubo formula for heat conductivity [2], we obtain $\kappa \propto \int_0^{N/c_s} \langle J(t)J(0) \rangle dt \propto N^\gamma$ where $\gamma = 1 - \nu$. Without knowing the exact value of γ and σ , we obtain that the superdiffusion and anomalous heat conduction are connected via the exponent relation $\gamma = \sigma - 1$ [19,22]. This relation enables us to derive the nonequilibrium transport properties from the equilibrium properties. The validity is ensured by the fact that a local equilibrium is achieved for FPU- β lattice [2]. In fact, our very rough estimation for $\nu = 0.70 \pm 0.05$ yields $\gamma = 0.30 \pm 0.05$ which is not far away from the calculation of nonequilibrium molecular dynamics [2].

In conclusion, we have investigated the energy transport processes for the FPU- β lattice using an equilibrium approach. To identify the energy carriers, we accurately measure the sound velocity of the energy carriers by following the correlated spreading of the initial energy-momentum fluctuations. The sound velocities are found to be in excellent agreement with theoretical predictions for effective phonons. This predicability has been further confirmed for a series of H_n models. On the other hand, no signature of soliton transport has been detected by visualizing the spatiotemporal evolutions of local energy densities and relative displacements. Therefore our numerical results clearly reveal that the energy carriers are long wavelength phonons for the FPU- β lattice. Our work

thus supports the mechanism of phonon mismatch [23–25] for the thermal rectification effect in coupled nanotubes [26].

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