Numerical extraction of sound velocities of energy transfer based on solitons in Fermi-Pasta-Ulam chains

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(Received 25 March 2018; published 21 September 2018)

According to the Boltzmann distribution assumption of solitons, in thermal equilibrium, there is the most probable soliton whose average kinetic energy per site equals the thermal energy $k_B T$. Based on the momentum excitation method, the soliton can be numerically excited in the static Fermi-Pasta-Ulam (FPU) chains. By associating the excited soliton with the corresponding most probable soliton, the temperature dependence of the velocity of solitons in thermal equilibrium can be numerically evaluated. The results agree very well with the temperature dependence of the sound velocity of energy transfer. This confirms that solitons are promising candidates for energy carriers in FPU chains. Moreover, the validity of the Boltzmann distribution assumption of solitons in FPU chains is also confirmed. This work sheds light on how to numerically (even experimentally) investigate solitons in thermal equilibrium.

DOI: 10.1103/PhysRevE.98.032215

I. INTRODUCTION

In the Fermi-Pasta-Ulam (FPU) β chains, the divergence of thermal conductivity with the length of the chain was numerically discovered [1]. This indicates that although Fourier's law of heat conduction is obeyed ubiquitously in the three-dimensional bulk materials, it can break down in the low-dimensional momentum-conserving nonlinear lattices. The so-called anomalous energy transport has been experimentally observed in various low-dimensional lattices in recent years [2–5].

In the past two decades, numerous works have been devoted to elucidating the underlying mechanism leading to anomalous energy transport (see, e.g., the review articles [6–8]). It has been proved that anomalous energy transport is closely related to anomalous energy diffusion [9]. Whether in the case of nonequilibrium diffusion or equilibrium diffusion, in the low-dimensional momentum-conserving nonlinear lattices that exhibit anomalous energy diffusion, two characteristic side peaks will appear in the spatiotemporal correlation function for some conserved quantities. These two characteristic side peaks are symmetric about the origin and can be predicted on the basis of nonlinear fluctuating hydrodynamics (NFH) [10–14] or the Lévy walk assumption of the energy carriers [15–22]. The side peaks correspond to the sound modes in NFH. They move outward at a constant supersonic velocity. This characteristic velocity is referred to as the sound velocity of energy transfer and has been conventionally used to identify the energy carriers [23–30].

Because both the phonon theory [27] and the soliton theory [26] can predict perfectly the sound velocity of energy transfer in FPU chains, the debate about whether the energy carriers are solitons [23–26,31–35] or effective phonons (renormalized phonons) [27–30,36,37] is not resolved yet. Nevertheless, the supersonic solitons have been numerically observed in a wide variety of lattices [24,34,35,38–51] and, intriguingly, have been experimentally demonstrated in crystalline solids (the corresponding solitons were referred to as strain solitons or acoustic solitons) [52–59]. The connection between the supersonic solitons and the supersonic characteristic side peaks has naturally attracted widespread interest [23–26].

However, only in the Toda chain, the characteristic side peaks have been hitherto confirmed to be contributions from solitons [23,24]. In the FPU chain, there is not enough evidence to distinguish whether the characteristic side peaks originate from solitons or effective phonons. Although the excellent agreement between the average velocity of solitons and the sound velocity of energy transfer has been provided in our previous work [26], the results are only achieved based on the approximate analytical soliton solutions and the Boltzmann distribution assumption of solitons. Direct numerical simulations are required to prove the analytical results. The validity of the Boltzmann distribution assumption also needs to be verified through numerical simulations. However, in thermal equilibrium, solitons cannot be detected directly in FPU chains because they are masked by thermal fluctuations. Solitons are hitherto always numerically studied in the static nonlinear chains based on the method of momentum excitation [24,34,35,47–49]. Therefore, it seems impossible

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to numerically evaluate the temperature dependence of the velocity of solitons in FPU chains.

In this work, one method is proposed to numerically evaluate the temperature dependence of the velocity of solitons in FPU chains. According to the Boltzmann distribution assumption of solitons [26], we find that in thermal equilibrium the soliton whose average kinetic energy per site ϵ_k equals the thermal energy $k_B T$ contributes the most to the local kinetic energy (i.e., the kinetic energy of a single particle) of the chains. We refer to this soliton as the most probable soliton. Because there is the characteristic peak in the autocorrelations of the local kinetic energy [23], we argue that the most probable soliton mainly determines the sound velocity of energy transfer. We numerically excite the soliton in the static FPU β chains, quartic chains, and FPU $\alpha\beta$ chains based on the momentum excitation method. The excited soliton is associated with the most probable soliton. The velocity and the average kinetic energy per site ϵ_k of the soliton are numerically evaluated. Consequently, the temperature dependence of the velocity of solitons can be obtained directly by letting $T = \epsilon_k / k_B$. Strikingly to us, the results agree very well with the temperature dependence of the sound velocity of energy transfer. The slightly discrepancies are attributed to the fact that the shape of the soliton is not the precisely sech shape which is used to evaluate ϵ_k. The numerical results prove that solitons are promising candidates for energy carriers in FPU chains. The results also indicate the validity of the Boltzmann distribution assumption of solitons. The activation energy of a soliton with the prescribed velocity is just the average kinetic energy per site of this soliton. This is consistent with the evidence that there is a threshold for the average kinetic energy of a soliton with the prescribed velocity [60]. Thus, the results presented in this work pave the way for numerically (even experimentally) investigating solitons in thermal equilibrium. We hope this work will stimulate additional experimental and theoretical efforts to investigate solitons in thermal equilibrium.

The rest of the paper is organized as follows. In Sec. II A the models of the studied FPU chains are presented. The method is also given in Sec. II A to associate the average kinetic energy of a soliton with the thermal energy $k_B T$. The numerical details are presented in Sec. II B. The numerical results are presented in Sec. III. Finally, a summary and discussion are presented in Sec. IV.

II. MODEL AND NUMERICAL DETAILS

A. Model and methods

In this work, the FPU β chains, the quartic chains, and the FPU $\alpha\beta$ chains are investigated. Their dimensionless Hamiltonians can be uniformly expressed as

$$H = \sum_{j=1}^{N} \left(\frac{\dot{u}_j^2}{2} + V(\phi_j) \right), \tag{1}$$

where N is the number of particles, $\phi_j = u_j - u_{j-1}$ denotes the relative displacement (strain) between the adjacent particles, u_j is the displacement of the jth particle from its equilibrium position, and the overdot denotes the time derivative. The potential can be expressed as

$$V(\phi_j) = \frac{k}{2}\phi_j^2 + \frac{\alpha}{3}\phi_j^3 + \frac{1}{4}\phi_j^4. \tag{2}$$

In this work, we choose $k = 1$ and $\alpha = 0$ for the FPU β chains, $k = \alpha = 0$ for the quartic chains, and $k = \alpha = 1$ for the FPU $\alpha\beta$ chains.

The equation of motion corresponding to the Hamiltonian (1) is

$$\ddot{u}_j = V'(\phi_{j+1}) - V'(\phi_j), \tag{3}$$

where the prime denotes the derivative of the function with respect to its argument. This equation of motion (3) permits the bell-shaped soliton solutions of ϕ_j (corresponding to the kink-shaped soliton solutions of u_j) [38–46,49], which can be formally expressed as

$$\phi_j(t) = \phi(j - ct) \equiv \phi(z), \tag{4}$$

where c is its velocity and z is the moving coordinate. The bell-shaped soliton solutions can be approximately expressed as [26]

$$\phi(z) = A\,\mathrm{sech}(qz), \tag{5}$$

with

$$A = \frac{-2\alpha \pm \sqrt{4\alpha^2 + 2(c^2 - k)\pi^2}}{\pi}. \tag{6}$$

If $A > 0$, the relative displacement $\phi(z) > 0$ and thus the distance between the adjacent particles is stretched relative to the equilibrium distance. The corresponding solitons are called rarefaction (dilatational) solitons. Otherwise, the solitons are called compressional solitons. In Eq. (5), q can be treated as the wave vector [45] and $\lambda = 2\pi/q$ is the corresponding wavelength.

In a thermal equilibrium state at temperature T, the solitons are assumed to satisfy the Boltzmann distribution and the number of solitons with the prescribed velocity c is [26]

$$f(\epsilon_k) = N_0 \exp\left(-\frac{\epsilon_k}{k_B T}\right), \tag{7}$$

where N_0 is a constant relevant to the length of a chain, ϵ_k is the activation energy, and k_B is the Boltzmann constant (which is chosen as $k_B = 1$ in this work). The activation energy ϵ_k is assumed to be equal to the average kinetic energy per site of a soliton with the prescribed velocity c. This is consistent with the evidence that there is a threshold for the average kinetic energy of a soliton with the prescribed velocity [60].

It should be recalled that there is a characteristic peak in the autocorrelations of the local kinetic energy (i.e., the kinetic energy of a single particle). This peak originates from solitons [23]. According to Eq. (7), the contribution of the soliton with velocity c to the local kinetic energy is $\epsilon_k N_0 \exp(-\epsilon_k/k_B T)/N$. Therefore, the soliton with $\epsilon_k = k_B T$ contributes most to the local kinetic energy and thus the characteristic peak in the autocorrelations of the local kinetic energy. The soliton is referred to as the most probable soliton. We argue that the sound velocity of energy transfer is mainly determined by the most probable soliton.

The same as the other kind of nonlinear excitations which are referred to as discrete breathers (intrinsic localized modes) [61], the activation energy of a soliton is expected to be the same in static lattices and in lattices at thermal equilibrium. Therefore, a soliton excited in the static chain can be associated with the most probable soliton in the chain at thermal equilibrium. The temperature can be evaluated from the average kinetic energy per site of the soliton as $T = \epsilon_k/k_B$. The temperature dependences of the velocity of solitons can thus be numerically obtained from solitons excited in the static lattices. Strikingly to us, the results agree very well with the temperature dependences of the sound velocity of energy transfer. This confirms that solitons are promising candidates for energy carriers in FPU chains. In addition, the results also confirm that the Boltzmann distribution assumption of solitons is valid and the corresponding activation energy is just the average kinetic energy per site of the soliton.

B. Numerical details

The momentum excitation method [24,34,35,47–49] is employed to excite solitons directly in the static lattices. We choose the initial conditions as

$$\dot{u}_j = p\,\delta_{j,1}, \quad u_j = 0 \quad \text{for all } j = 1, 2, \ldots, N, \tag{8}$$

where δ denotes the Kronecker delta. This means that the first particle is kicked at $t = 0$ as $\dot{u}_1 = p$. Thereafter, the kick will be transported along the chain in the course of time. To investigate the transport of the kick along the chain, the implicit midpoint algorithm [62] is used to integrate the equations of motion with the free-boundary condition. In our calculation, we find that when $|p|$ is higher than a certain momentum threshold, a supersonic soliton separating from the spreading radiation can be clearly observed in the chain. This is consistent with Ref. [48]. We also find that the fastest soliton is a rarefaction soliton with $\phi_j > 0$ when $p < 0$ but is a compressional soliton with $\phi_j < 0$ when $p > 0$. This can be explained according to Eq. (4). It is obtained that $\dot{u}(z) = -cu'(z)$ for the traveling soliton solution, where $u'(z)$ corresponds to the strain, i.e., the relative displacement $\phi(z)$. Therefore, the right-moving (i.e., $c > 0$) rarefaction solitons can be excited with $p < 0$ and the right-moving compressional solitons can be excited with $p > 0$.

Once the soliton is excited, its velocity can be numerically evaluated directly. Benefiting from the bell shape of the soliton for the relative displacement, the position of the soliton is determined by the peak position of the relative displacements. Eventually, the velocity of the soliton can be numerically evaluated based on the conventional linear least-squares-fitting method [63].

To numerically evaluate the temperature dependence of the velocity of the soliton, the soliton is treated as the most probable soliton. Its average kinetic energy per site can be associated with the temperature by the equation $T = \epsilon_k/k_B$. To calculate the average kinetic energy per site of a soliton ϵ_k, the total kinetic energy E_k and the width of the soliton W should be evaluated first. The width of a soliton is determined as follows. The soliton is assumed to be sech shaped as shown in Eq. (5). Its width is chosen as the wavelength $W = \lambda = 2\pi/q$ [26]. Then the bell-shaped soliton is symmetrically located between $z = -\pi/q$ [$\phi(z) = A\,\mathrm{sech}(\pi)$] and $z = \pi/q$ [$\phi(z) = A\,\mathrm{sech}(\pi)$] in the moving coordinates. The peak position of the soliton is $z = 0$ [$\phi(z) = A$]. Therefore, the width W can be numerically evaluated by counting the number of particles with $\phi_j/\phi_{j_c} \geqslant \mathrm{sech}(\pi)$, where j_c is the particle position corresponding to the soliton peak. For the solitons which can be clearly recognized in our numerical investigations, their widths are always narrower than 30. Therefore, the total kinetic energy of a soliton can be evaluated as $E_k = \sum_{j=j_c-15}^{j_c+15} \dot{u}_j^2/2$. The average kinetic energy per site of it is thus $\epsilon_k = E_k/W$.

In most of our simulations, the number of particles is set as $N = 8000$ and the simulation time is set as 2000. When the soliton is very slow with its velocity approaching 1, the simulation time is set as 10 000 and the number of particles is set as $N = 15\,000$ to clearly recognize it. When the velocity of a soliton is very high, the number of particles is also set as $N = 15\,000$, but the simulation time is kept as 2000 to avoid the scattering by the boundary of the chain. In our simulations, the velocity and ϵ_k are always averaged in the last 1000 time intervals. When multiple solitons are excited simultaneously, the fastest soliton (the most front soliton) is studied. We have also checked the slower solitons. The dependence of the velocity of the slower solitons on the corresponding ϵ_k/k_B agrees also with the temperature dependence of the sound velocity of energy transfer.

III. NUMERICAL RESULTS

A. The FPU β lattice

The FPU β lattices with $k = 1$ and $\alpha = 0$ are investigated in this section. Because of the symmetry of the interaction potential of the FPU β lattices, the initial excitation momentum $\pm|p|$ will excite two kinds of solitons (the compressional soliton with $\phi_j < 0$ and the rarefaction soliton with $\phi_j > 0$) with the same velocity and the same shape in spite of opposite amplitudes. Therefore, only the results of the compressional solitons (corresponding to the positive p) will be shown in this section.

To investigate the solitons with different velocities, we let p increase from 0.1 to 30 in steps of 0.1. When $p \geqslant 0.8$, the compressional solitons can be clearly recognized. As an example, the result of $p = 0.8$ is shown in Fig. 1. At time 10 000, we observe that a compressional soliton separates from a long phonon tail. This is the typical character of the FPU β lattices [34,35].

The velocity of the soliton increases with p. The dependence of the velocity of solitons on the temperature $T = \epsilon_k/k_B$ is shown in Fig. 2. The numerical results are shown with symbols. For comparison, the prediction of NFH for the dependence of the sound velocity of energy transfer on the temperature is also depicted as the solid line. The symbols agree very well with the solid line. This indicates that the sound velocity of energy transfer can be numerically obtained from solitons directly. This reveals two things. First, the solitons are promising candidates for energy carriers in the FPU β chains. Second, the Boltzmann distribution of solitons (7) is valid. The activation energy is just the average kinetic energy per site of the soliton. This is consistent with the evidence that there is a threshold for the average kinetic energy of the soliton with a prescribed velocity [60].

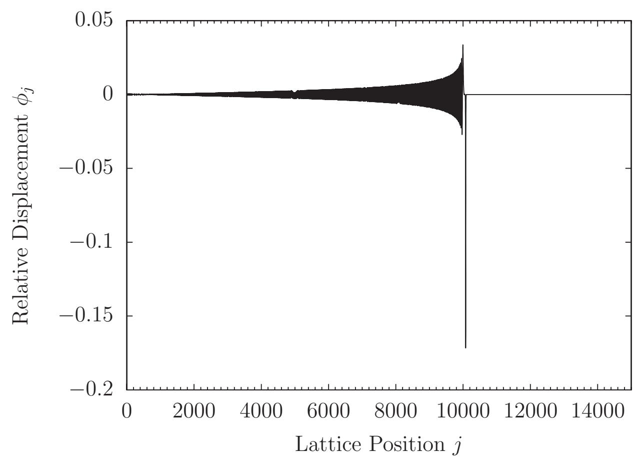

FIG. 1. Snapshot of the compressional soliton in the FPU β chain at time 10 000. The initial excitation momentum is $p = 0.8$.

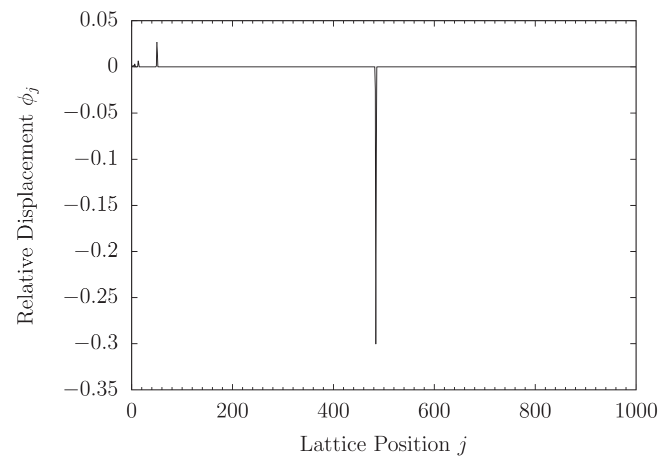

FIG. 3. Snapshot of the solitons in the quartic chain at time 2000. The initial excitation momentum is $p = 0.1$.

In Fig. 2, one can see that there are slight discrepancies between the numerical results and the predictions of NFH. This can be attributed to the fact that the shape of our numerically obtained soliton is slightly narrower than the sech shape [64]. Therefore, for the soliton with a specific velocity (the ordinate), the corresponding precise ϵ_k/k_B (the abscissa) should be slightly larger than our numerical result.

B. Quartic lattice

The quartic lattices with $k = \alpha = 0$ are investigated in this section. As in the FPU β lattices, we only represent the results of the positive p here. We also let p increase from 0.1 to 30 in steps of 0.1. The solitons can be excited when $p = 0.1$. The results are shown in Fig. 3. In contrast to the results of the FPU β lattices, a compressional soliton separates from a tail of several small rarefaction solitons rather than the phonon tail. This is consistent with the fact that phonons are not admissible in a quartic lattice [35,45,65]. We thus expect that even an arbitrarily small p can also excite a soliton in the quartic lattices.

The dependence of the velocity of solitons on ϵ_k/k_B is compared with the temperature dependence of the sound velocity of energy transfer in Fig. 4. Good agreement is achieved again. This proves again that the Boltzmann distribution assumption of solitons is valid and solitons are promising candidates for energy carriers in the quartic chains.

C. The FPU $\alpha\beta$ lattice

The FPU $\alpha\beta$ lattices with $k = \alpha = 1$ are investigated in this section. Contrary to the FPU β lattices and the quartic lattices, the initial excitation momenta $\pm|p|$ will excite the rarefaction soliton and the compressional soliton with the different velocities. For the compressional solitons and the rarefaction solitons, the temperature dependences of the velocities are also different [26].

We let p decrease from -0.1 to -30 in steps of -0.1 to excite the rarefaction solitons and let p increase from 1.1 to 30

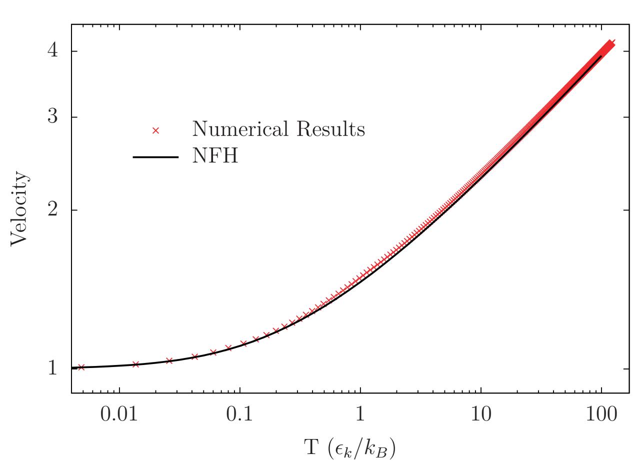

FIG. 2. Velocity of solitons vs ϵ_k/k_B for the one-dimensional FPU β chain. The symbols correspond to the numerical results. The solid line corresponds to the prediction of NFH for the dependence of the sound velocity on the temperature T.

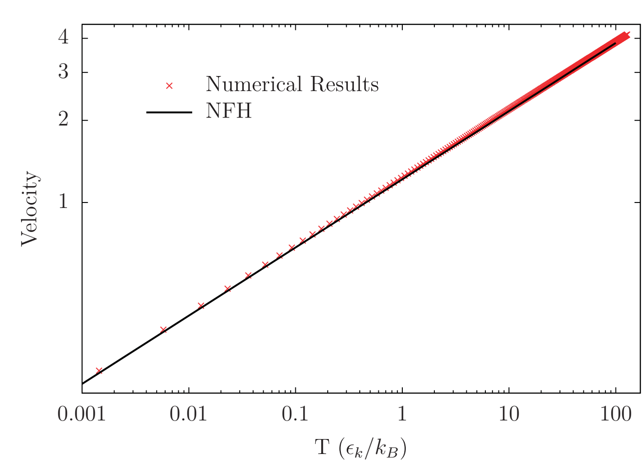

FIG. 4. Velocity of solitons vs ϵ_k/k_B for the one-dimensional quartic chain. The symbols correspond to the numerical results. The solid line corresponds to the prediction of NFH for the dependence of the sound velocity on the temperature T.

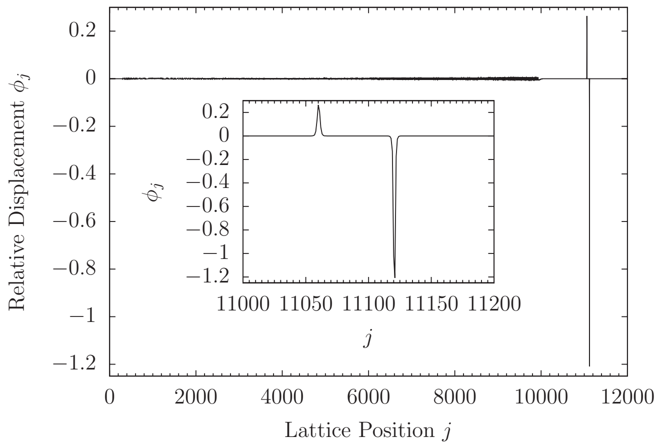

FIG. 5. Snapshot of the solitons in the FPU $\alpha\beta$ chain at time 10 000. The initial excitation momentum is $p = 2.6$. The inset shows a close-up of the solitons.

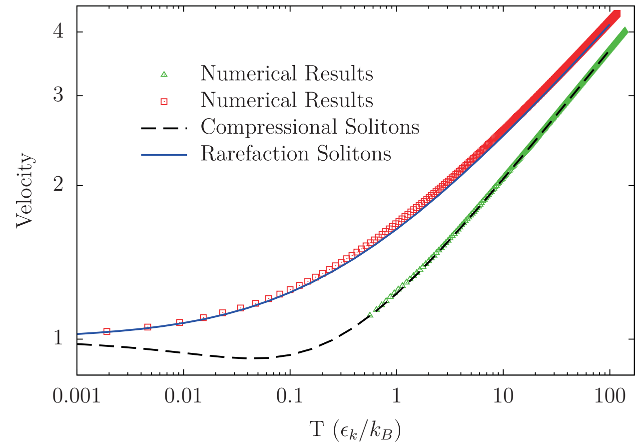

FIG. 6. Velocity of solitons vs ϵ_k/k_B for the one-dimensional FPU $\alpha\beta$ chain. The triangles correspond to the numerical results of the compressional solitons. The squares correspond to the numerical results of the rarefaction solitons. The dashed line and the solid line represent the corresponding analytical results of the dependences of the velocities on the temperature T.

in steps of 0.1 to excite the compressional solitons. The rarefaction solitons can be excited when $p = -0.1$. However, because we can only numerically recognize the compressional soliton with its velocity higher than 1, the compressional solitons can be clearly detected when $p = 2.6$. The results are shown in Fig. 5. According to Eq. (6), when the velocity of a compressional soliton approaches 1, its amplitude approaches $-4/\pi$. In Fig. 5, the amplitude of the compressional soliton is -1.21. It indeed approaches $-4/\pi$.

According to our previous work [26], the sound velocity can be obtained from the velocities of the rarefaction solitons and the compressional solitons. We thus only represent the numerical results of the velocities of these two kinds of solitons in Fig. 6. The numerical results are compared with the corresponding analytical results calculated by using the method of Ref. [26]. Good agreement is obtained. This indicates that the temperature dependence of the velocity of solitons can be numerically obtained. Therefore, this proves again that the Boltzmann distribution assumption of solitons is valid and solitons are promising candidates for energy carriers in the FPU $\alpha\beta$ chains.

IV. CONCLUSION

In summary, in thermal equilibrium, there is a most probable soliton with $\epsilon_k = k_B T$ according to the Boltzmann distribution of the solitons. Based on the momentum excitation method, the solitons can be excited in the static FPU β chains, quartic chains, and FPU $\alpha\beta$ chains. The excited soliton can be associated with the most probable soliton. The average kinetic energy per site of a soliton ϵ_k can thus be associated with the thermal energy $k_B T$. The dependences of the velocity of solitons on ϵ_k/k_B agree very well with the temperature dependences of the velocities of solitons as well as the temperature dependences of the sound velocity of energy transfer. The slight discrepancies are attributed to the fact that the shape of the soliton is not precisely sech shaped. The numerical results prove that solitons are promising candidates for the energy carrier in FPU chains. In addition, the results also prove that the Boltzmann distribution assumption of solitons is valid. The corresponding activation energy is just the average kinetic energy per site of the soliton.

The numerical method presented in this work provides an idea for the numerical investigation of solitons in thermal equilibrium. Because solitons have been experimentally observed in crystalline solids [52–59], we hope this work will stimulate additional theoretical and even experimental efforts to investigate solitons in thermal equilibrium.

ACKNOWLEDGMENTS

Z.-J.D. was supported by the National Natural Science Foundation of China (Grant No. 11574289). Some numerical calculations in this work were performed on the supercomputing system in the Supercomputing Center of USTC.

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