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Citation : Chin. Phys. B, 2025, 34 (**2**): 020501. DOI: 10.1088/1674-1056/ad9ff6
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Excitation threshold of solitons in anharmonic chains

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(Received 11 September 2024; revised manuscript received 3 December 2024; accepted manuscript online 17 December 2024)

This study numerically estimates the momentum threshold required to excite solitons in anharmonic chains. For both Fermi–Pasta–Ulam–Tsingou (FPUT)-$\alpha\beta$ and FPUT-β chains, regardless of whether the interatomic interaction potential is symmetric, the required excitation momentum converges to the momentum of the soliton center (i.e., the peak momentum of the soliton) as the number of initially excited atoms increases. As the amplitude of the soliton approaches zero, the momentum threshold decreases to nearly zero, allowing soliton being excited with infinitesimal initial excitation momentum. These findings enhance the understanding of soliton dynamics and offer insights for optimizing soliton excitation methods, with potential applications in straintronics and nonlinear wave control technologies.

Keywords: solitons, Fermi–Pasta–Ulam–Tsingou chains, excitation threshold

PACS: 05.45.Yv, 63.20.Ry

DOI: 10.1088/1674-1056/ad9ff6 **CSTR:** 32038.14.CPB.ad9ff6

1. Introduction

Solitons (solitary waves) are stable, nonlinear localized wave packets that propagate without changing shape due to a balance between nonlinearity and dispersion.[1,2] Numerous analytical studies have demonstrated the existence of soliton solutions in anharmonic lattices,[3–7] with extensive numerical simulations supporting these findings.[8–39] Importantly, experimental results based on femtosecond/picosecond (terahertz) laser ultrasonics indicate that sufficiently strong pulsed lasers can induce localized strain in anharmonic lattices, leading to the excitation of strain shock waves or even solitons.[40–53] Consequently, solitons are regarded as the energy carriers responsible for anomalous thermal conduction (or thermal diffusion) in anharmonic chains.[16–20,54–59]

However, several numerical studies suggest that to excite shock waves or solitons in anharmonic lattices, the initial excitation momentum must exceed a critical threshold.[11,14,19,34–37] Similarly, experimental observations indicate that the pump laser fluence must exceed a certain threshold to induce strong localized strain in anharmonic lattices, facilitating the excitation of shock waves and solitons.[47–53] This high momentum threshold for soliton excitation raises important questions. For instance, under thermal equilibrium conditions, is it possible to excite solitons in anharmonic lattices solely through thermal fluctuations? Furthermore, is it reasonable to consider solitons as the energy carriers responsible for anomalous thermal conduction and diffusion, particularly at relatively low temperatures?[11] Experimentally, the requirement for high pump laser fluence poses the risk of optical damage to samples, thereby presenting challenges for the application of femtosecond/picosecond laser ultrasonics in the emerging field of "straintronics", which seeks to generate mechanical strain to elicit various functionalities.[60–78]

In theory, the possibility of reducing the initial excitation momentum of solitons in anharmonic chains is critical for understanding their contribution to anomalous thermal conduction and diffusion. Experimentally, the reduction of laser pump fluence required for strain soliton excitation is also crucial for expanding the scope of ultrafast strain applications. Fortunately, recent experimental advances have shown that utilizing multiple laser sources, instead of a single source, can significantly lower the threshold laser pump fluence needed to excite high-amplitude strain shock waves.[53]

Motivated by these findings, we initially excited multiple atoms instead of the conventional single-atom excitation. We numerically investigate the relationship between the initial excitation momentum $p_{\rm ini}$ of solitons and the number of initially excited atoms N_0 in Fermi–Pasta–Ulam–Tsingou (FPUT) chains. Our results reveal that, for both the FPUT-$\alpha\beta$ chain with an asymmetric potential and the FPUT-β chain with a symmetric interaction potential, as N_0 increases, the initial excitation momentum $p_{\rm ini}$ of solitons with a given velocity decreases and eventually reaches a saturation value. Notably, for solitons with any velocity, the corresponding saturation value closely approaches the momentum of the soliton center. Therefore, we propose that the momentum excitation threshold for a soliton with a given velocity corresponds to the momentum of the soliton center, i.e., the peak momentum of the soliton.

Furthermore, our numerical results indicate that as the soliton velocity approaches 1.0, the maximum phase veloc-

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ity of phonons, the momentum excitation threshold converges to zero, along with the momentum of the soliton center. This suggests that an infinitesimal initial excitation momentum is sufficient to excite a soliton, albeit with an infinitesimal amplitude. These findings are crucial for advancing our understanding of soliton dynamics in anharmonic chains and for developing more efficient soliton excitation methods. The insights gained from this research could have significant implications not only for fundamental physics but also for applications in straintronics and other technologies that rely on the precise control of nonlinear wave phenomena.

The rest of this paper is organized as follows. In Subsection 2.1, we present the models of the studied FPUT chains and briefly review the approximate analytical soliton solutions. The numerical details are discussed in Subsection 2.2. The numerical results for the FPUT-$\alpha\beta$ chains and FPUT-β chains are presented in Subsections 3.1 and 3.2, respectively. Finally, the conclusion and further discussions are presented in Section 4.

2. Model and numerical method

2.1. Model and soliton solutions

In this study, we investigate the dimensionless Hamiltonian of an FPUT monoatomic chain with N unitary-mass atoms, given by

$$H=\sum_{j=1}^{N}\left[\frac{p_j^2}{2}+V(u_j-u_{j-1})\right]. \tag{1}$$

Here, the nearest-neighbor interaction potential is described by the expression

$$V(u_j-u_{j-1})\equiv V(\phi_j)=\frac{1}{2}\phi_j^2+\frac{\alpha}{3}\phi_j^3+\frac{1}{4}\phi_j^4, \tag{2}$$

where u_j represents the displacement of the j-th atom from its equilibrium position, and $p_j=\dot{u}_j$ is the corresponding momentum. The term $\phi_j=u_j-u_{j-1}$ denotes the strain, which is the relative displacement between adjacent atoms. In this study, we focus on both the FPUT-$\alpha\beta$ chains, where $\alpha=1$, and the FPUT-β chains, where $\alpha=0$.

The corresponding equation of motion is

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

where the prime denotes the derivative of the potential function with respect to its argument. This equation supports bell-shaped soliton solutions for the strain ϕ_j, which correspond to bell-shaped soliton solutions for the momentum p_j and kink-shaped soliton solutions for the displacement u_j.[3,15,19–29,59]

Using a moving coordinate z, the bell-shaped soliton solutions for ϕ_j can be approximately written as[59]

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

with the amplitude A and wave number q given by

$$A=\frac{-2\alpha\pm\sqrt{4\alpha^2+2(c^2-1)\pi^2}}{\pi}, \tag{5}$$

$$q=\sqrt{\frac{2}{\pi c^2}\left[6\pi(c^2-1)+\alpha(\pi^2-12)A\right]}, \tag{6}$$

where c represents the soliton velocity. The corresponding bell-shaped soliton solution for the momentum is expressed as

$$p_j(t)=\dot{u}_j(t)\equiv\dot{u}(z)=-c\frac{\mathrm{d}u(z)}{\mathrm{d}z}\approx-c\phi(z). \tag{7}$$

Solitons with $A>0$ are classified as rarefactive (or stretched) solitons, indicating that the strain $\phi_j>0$ in the soliton region, meaning the spacing between neighboring atoms exceeds their equilibrium distance. Conversely, solitons with $A<0$ are termed compressive solitons.

According to Eq. (5), in FPUT-β chains, where $\alpha=0$, the rarefactive and compressive solitons with the same velocity exhibit identical shapes, differing only in the sign of their amplitudes. These solitons can be excited by opposite initial excitation momenta. However, in the case of FPUT-$\alpha\beta$ chains, where $\alpha>0$, rarefactive solitons have a lower amplitude compared to compressive solitons of the same velocity, necessitating unequal initial excitation momenta.

2.2. Numerical method

The initial conditions for the simulation are illustrated in Fig. 1. The first N_0 atoms, represented by red beads, are initially excited, while the remaining atoms, represented by blue beads, remain static. The initial excitation is achieved via the momentum excitation method,[13–20] where only the momenta of the first N_0 atoms are set to nonzero values, denoted as p_{ini}. The subsequent evolution of this initial excitation is numerically explored by integrating the equation of motion (3) using the implicit midpoint algorithm,[19,20,79,80] with a free-boundary condition.

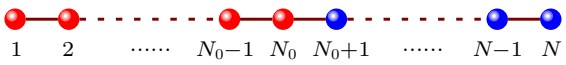


Fig. 1. A schematic representation of the initial conditions for the simulation is provided. The first N_0 red beads represent atoms that are initially excited, while the remaining blue beads represent atoms that are initially static.

The numerical simulations indicate that the initial excitation momentum of a soliton increases monotonically with its velocity. Hence, the bisection algorithm[81] is employed to estimate the initial excitation momentum of a soliton with a specified velocity. The specified velocity is estimated same as in Ref. [19]. The peak point of the soliton, resembling a bell shape, acts as a landmark for finding the soliton. Then the soliton's velocity can be numerically determined using a linear

least-squares-fitting method over the last 1000 simulation time intervals based on its spatial evolution.

In the final 1000 simulation time intervals, the soliton becomes fully separated from the trailing long phonon tail. As time progresses, the soliton center moves through various atomic positions sequentially. However, it is not guaranteed that the soliton center coincides precisely with a specific atomic position at any given instant. Consequently, we define the maximum momentum value of the soliton center, observed during the last 1000 simulation time intervals, as the momentum of the soliton center, i.e., the peak momentum of the soliton.

3. Numerical results

3.1. FPUT-$\alpha\beta$ chains

We investigate the FPUT-$\alpha\beta$ chains ($\alpha = 1$) in this subsection. A carefully chosen negative (positive) initial excitation momentum, $p_{\rm ini}$, can excite rarefactive (compressive) solitons with a specific velocity. It is important to note that the negative or positive sign merely indicates the direction of the momentum. Due to the asymmetry of the interaction potential of the FPUT-$\alpha\beta$ chains and the condition $\alpha > 0$, rarefactive solitons are more easily excited with a lower initial excitation momentum $p_{\rm ini}$ compared to compressive solitons of the same velocity.[14,19] Given that the primary objective of this study is to determine the minimum initial excitation momentum required to excite solitons, we concentrate on exploring the momentum excitation threshold for rarefactive solitons in FPUT-$\alpha\beta$ chains.

The results of solitons with a velocity of $c \approx 1.005$ are presented in Figs. 2 and 3. When a single atom (i.e. $N_0 = 1$) is initially excited, the required initial excitation momentum is $p_{\rm ini} \approx -0.0971$ to excite a momentum pulse propagating at a velocity of $c \approx 1.005$. The evolution of these pulses over time is illustrated in Fig. 2(a), showing ballistic propagation at $c \approx 1.005$. For comparisons, the pulses at different time are horizontally shifted and displayed in Fig. 2(b). The strong overlap of these pulses suggests that the momentum pulse propagates without deformation. Furthermore, the pulse shape at $t = 10^4$ agrees well with the analytical result given by Eq. (7) for $c \approx 1.005$ as shown in Fig. 3. These findings demonstrate that the momentum pulses can indeed be interpreted solitons.

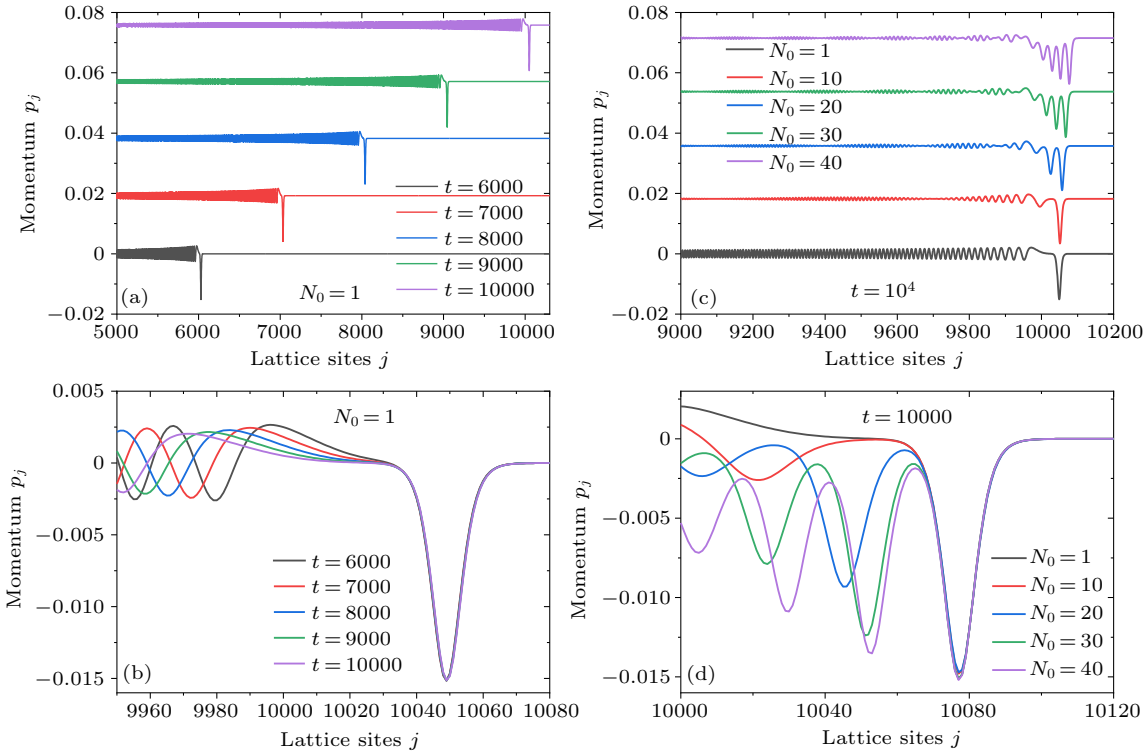


Fig. 2. Solitons with velocity $c \approx 1.005$ in FPUT-$\alpha\beta$ chains. (a) Temporal snapshots of solitons for $N_0 = 1$. The curves are shifted vertically for clarity. The initial excitation momentum is $p_{\rm ini} \approx -0.0971$. (b) The curves from panel (a) are shifted horizontally for comparisons. The solitons demonstrate an excellent overlap. (c) Snapshots of solitons at $t = 10^4$ for different values of N_0. The curves are shifted vertically for clarity. The initial excitation momenta are $p_{\rm ini} \approx -0.0971, -0.0202, -0.0167, -0.0164, -0.0164$ for $N_0 = 1, 10, 20, 30, 40$, respectively. (d) The curves in panel (c) are shifted horizontally. The solitons show an excellent overlap.

Next, we analyze the relationship between the initial excitation momentum and the number of initially excited atoms, N_0. The results of varying N_0 at time $t = 10^4$ are presented in Figs. 2(c) and 2(d). Although a larger N_0 leads to more momentum pulses being excited, the velocity of all the leading momentum pulses in Fig. 2(c) is $c \approx 1.005$. Their shapes

are compared in Fig. 2(d), where the good overlap indicates that the leading momentum pulses with the same velocity are indeed identical solitons. To excite solitons with the specific velocity of $c \approx 1.005$, the initial excitation momentum $p_{\rm ini}$ decreases from -0.097 to -0.0164 as N_0 increases from 1 to 40. Therefore, we conclude that the initial excitation momentum required to excite solitons with a specified velocity decreases as N_0 increases.

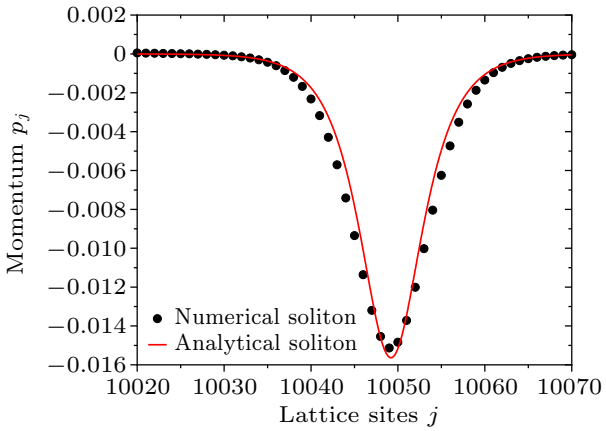


Fig. 3. The numerical soliton with $c \approx 1.005$ at $t = 10^4$ in the FPUT-$\alpha\beta$ chain is compared to the corresponding analytical soliton. The first atom ($N_0 = 1$) is initially excited with an initial momentum of $p_{\rm ini} \approx -0.0971$.

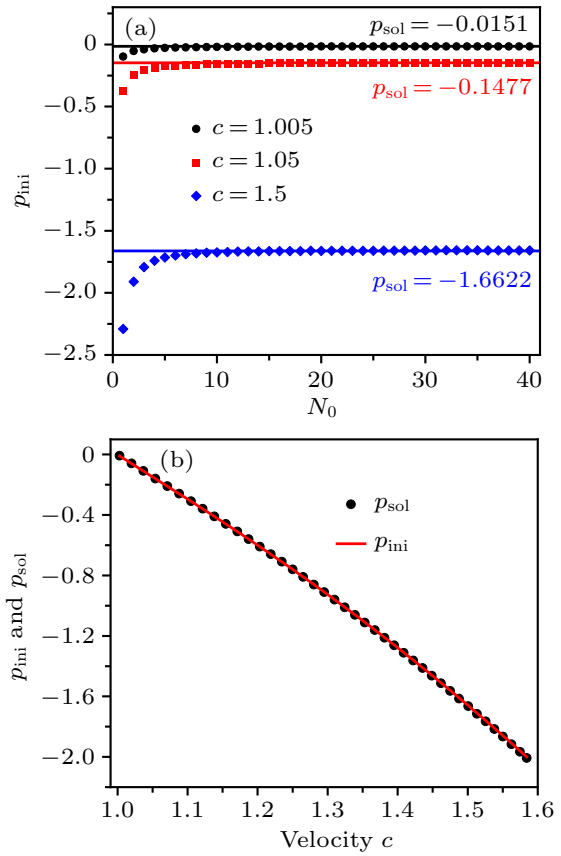


Fig. 4. (a) Initial excitation momentum $p_{\rm ini}$ as a function of N_0 in FPUT-$\alpha\beta$ chains. The symbols represent $p_{\rm ini}$. The horizontal lines indicate the momenta $p_{\rm sol}$ corresponding to the soliton centers. (b) The relationship between $p_{\rm ini}$ and $p_{\rm sol}$ as a function of velocity c, where $N_0 = 40$ is used for simulation. The momenta $p_{\rm ini}$ and $p_{\rm sol}$ approach 0.0 as the velocity c approaches 1.0.

Nevertheless, as depicted in Fig. 4(a), for the three solitons with different velocities, as N_0 increases, the initial excitation momenta $p_{\rm ini}$ converge towards their respective saturation values. Notably, these saturation values closely approach the momentum $p_{\rm sol}$ of the corresponding soliton center (the numerical method for $p_{\rm sol}$ is explained in Subsection 2.2). To further explore the relationship between $p_{\rm ini}$ and $p_{\rm sol}$, we numerically compute these quantities for solitons with various specified velocities. The results, shown in Fig. 4(b), reveal that $p_{\rm ini}$ asymptotically approaches $p_{\rm sol}$ for any soliton, provided that $c < 1.6$. Consequently, we define the momentum of the soliton center as the momentum excitation threshold required to excite this soliton with a specific velocity.

Additionally, both $p_{\rm ini}$ and $p_{\rm sol}$ approach zero as the velocity c approaches 1.0, i.e., the maximum phase velocity of phonons. This observation is consistent with the analytical result given by Eq. (5), which indicates that the amplitude of the rarefactive soliton approaches zero as its velocity approaches 1.0. Consequently, the momentum excitation threshold also approaches zero as the soliton velocity approaches 1.0. This implies that when N_0 is sufficiently large, even an infinitesimal initial excitation momentum can excite a soliton with a velocity arbitrarily close to 1.0.

3.2. FPUT-β lattice

Given that whether the interaction potential is symmetric will cause the thermal diffusion to exhibit different scaling behaviors,[82–84] we investigate whether the momentum excitation threshold will exhibit distinct results in FPUT-β chains. The FPUT-β chain with a symmetric interaction potential, i.e., $\alpha = 0$ in Eq. (2), is investigated in this subsection. Unlike the FPUT-$\alpha\beta$ chain, where asymmetry plays a role, the rarefactive solitons and compressed solitons in the FPUT-β chain, when specified with the same velocity, share the same initial excitation momentum, differing only in the direction of this momentum. Consequently, we concentrate also on exploring the excitation threshold for rarefactive solitons in FPUT-β chains.

The results of solitons with a velocity of $c \approx 1.005$ are presented in Figs. 5 and 6. Similar to the FPUT-$\alpha\beta$ chains, the excited momentum pulses in this case propagate without deformation and coincide with the analytical results of solitons. However, the distinction lies in the fact that, in the FPUT-β chains, solitons with the same velocity require a significantly higher initial excitation momentum: nearly an order of magnitude greater than the needed in the FPUT-$\alpha\beta$ chains. Despite this, the initial excitation momentum required for solitons with a specific velocity still decreases as N_0 increases. As shown in Figs. 5(c) and 5(d), to excite solitons with the desired velocity of $c \approx 1.005$, the initial excitation momentum $p_{\rm ini}$ decreases from -0.7744 to -0.1450 as N_0 increases from 1 to 40.

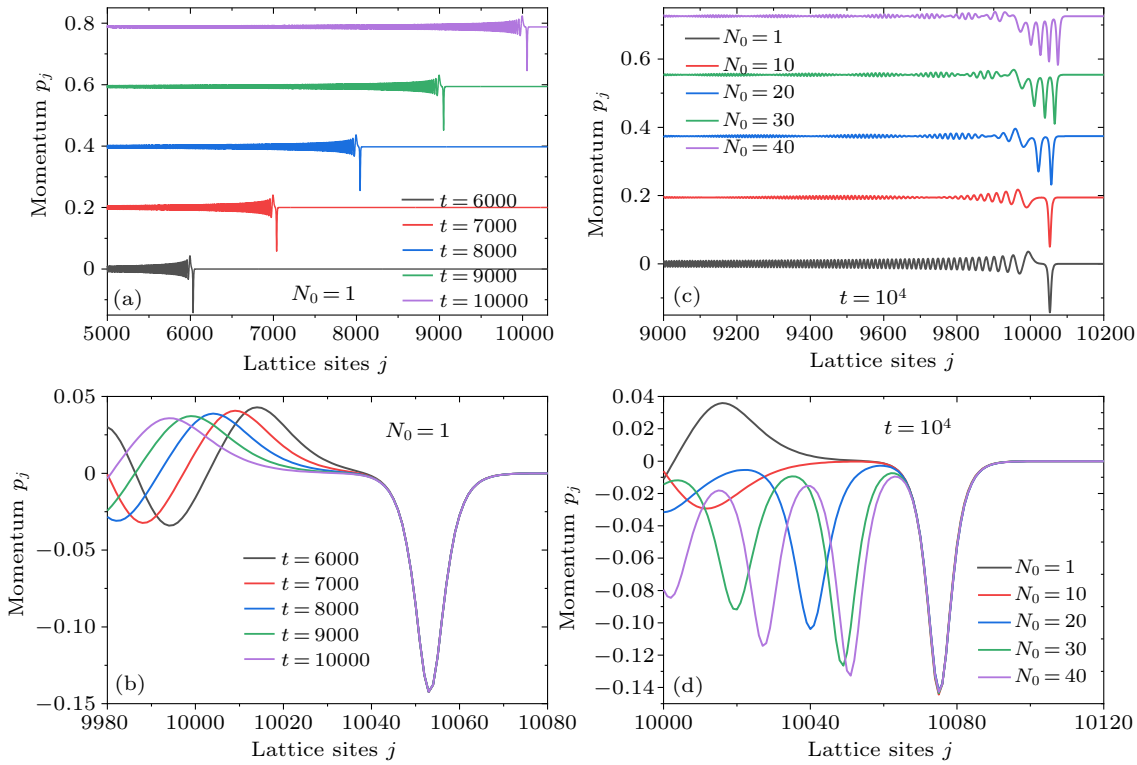


Fig. 5. Solitons with velocity $c \approx 1.005$ in FPUT-β chains. (a) Temporal snapshots of solitons for $N_0 = 1$ at different time. The curves are shifted vertically for clarity. The initial excitation momentum is $p_{\rm ini} \approx -0.7744$. (b) The curves from panel (a) are shifted horizontally for comparisons. The solitons exhibit excellent overlap. (c) Snapshots of solitons at $t = 10^4$ for different values of N_0. The curves are shifted vertically for clarity. The initial excitation momenta are $p_{\rm ini} \approx -0.7744, -0.1758, -0.1552, -0.1489, -0.1450$ for $N_0 = 1, 10, 20, 30, 40$, respectively. (d) The curves from panel (c) are shifted horizontally. The solitons again show excellent overlap.

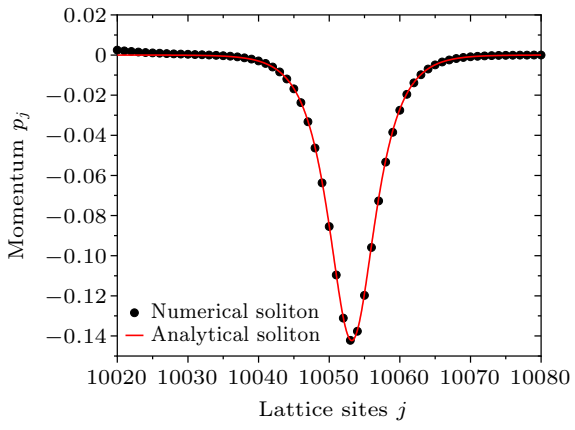


Fig. 6. The numerical soliton with $c \approx 1.005$ at $t = 10^4$ in the FPUT-β chain is compared to the corresponding analytical soliton. The first atom ($N_0 = 1$) is initially excited with $p_{\rm ini} \approx -0.7744$.

As illustrated in Fig. 7(a), similar to the FPUT-$\alpha\beta$ chain, in the FPUT-β chain, the initial excitation momentum $p_{\rm ini}$ also converges towards a saturation value as N_0 increases. These saturation values closely approach the momentum $p_{\rm sol}$ of the corresponding soliton center. As demonstrated in Fig. 7(b), $p_{\rm ini}$ approaches $p_{\rm sol}$ for any soliton, provided that $c < 2.0$. Similarly, both $p_{\rm ini}$ and $p_{\rm sol}$ approach 0.0 as the velocity c approaches 1.0. This is also consistent with the analytical result given by Eq. (5), which indicates that the amplitude of the soliton approaches zero as its velocity approaches 1.0.

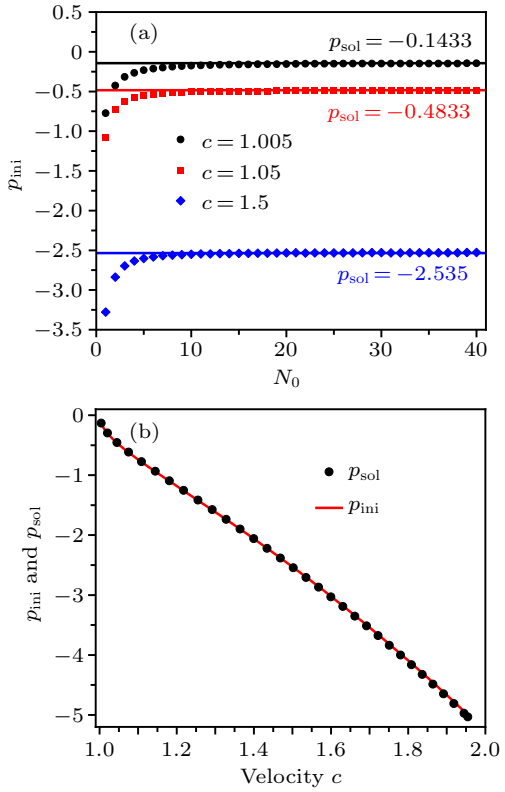


Fig. 7. (a) The initial excitation momentum $p_{\rm ini}$ as a function of N_0 in FPUT-β chains. The symbols represent $p_{\rm ini}$. The horizontal lines denote the momenta $p_{\rm sol}$ corresponding to the centers of solitons. (b) The relationship between $p_{\rm ini}$ and $p_{\rm sol}$ as a function of velocity c, with $N_0 = 40$. The momenta $p_{\rm ini}$ and $p_{\rm sol}$ approach 0.0 as the velocity c approaches 1.0.

In conclusion, similar to the FPUT-$\alpha\beta$ chains, the momentum of the soliton center determines the momentum excitation threshold required to excite a soliton with a specific velocity. This threshold approaches zero as the soliton's velocity approaches 1.0. This result indicates that when N_0 is sufficiently large, an infinitesimally small initial excitation momentum can excite a soliton with a velocity infinitely close to 1.0 in FPUT-β chains.

4. Discussion and conclusion

In summary, the momentum excitation threshold required to excite solitons in anharmonic chains has been numerically estimated. For both the FPUT-$\alpha\beta$ chains with asymmetric interaction potential and the FPUT-β chains with symmetric interaction potential, as the number of initially excited atoms N_0 increases, the initial excitation momentum required to excite a soliton with a specific velocity converges to a saturation value. This saturation value approaches the momentum of the center of the corresponding soliton. Therefore, the momentum of the soliton center (i.e., the peak momentum of the soliton) is regarded as the threshold momentum required to excite this soliton. Moreover, as the soliton's velocity decreases towards the maximum phase velocity of phonons, the corresponding momentum excitation threshold diminishes to nearly zero. In other words, provided that the number of initially excited atoms N_0 is sufficiently large, an infinitesimal initial excitation momentum is adequate to excite a soliton, albeit with an infinitesimal amplitude.

While the excitation thresholds derived in this study cannot be directly compared quantitatively with previous experimental findings,[53] owing to the dependence of strain magnitude on factors such as laser fluence, material reflectivity, laser absorption length, elastic modulus, and thermal expansion coefficient, the experimental results qualitatively align with our conclusions. As demonstrated in Fig. 2 of Ref. [53] the peak strain generated by multiple laser sources is approximately 20 times greater than that produced by a single laser source under identical conditions, enabling the excitation of solitary surface acoustic waves.

Our findings are crucial for advancing the understanding and optimization of shock wave and soliton excitations in two-dimensional materials. Stationary strain solitons[85] (or dislocations[86]) in bilayer graphene have been experimentally observed and widely applied in strain engineering.[87,88] However, the shock waves and solitons predicted numerically in two-dimensional materials[11,12,89–91] remain experimentally unverified, likely due to challenges in realizing the necessary excitation conditions. Our study reveals that replacing the excitation of a single atomic row in the soliton's motion direction with multiple rows can significantly lower the excitation threshold, thereby enhancing the feasibility of experimental realization. This can be achieved through multiple-source picosecond laser ultrasonic techniques[53] or methods similar to those described in Ref. [92], where partial contact between graphene layers allows an impulse applied to one layer to excite the other.

The insights derived from this study may have significant implications not only for fundamental physics but also for practical applications in straintronics and other technologies that depend on the precise manipulation of nonlinear wave phenomena.

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