

Solitons and thermal fluctuations in strongly nonlinear solidsN. Upadhyaya,^{1,*} A. M. Turner,^{2,†} and V. Vitelli^{1,‡}¹*Instituut-Lorentz for Theoretical Physics, Universiteit Leiden, 2300 RA Leiden, The Netherlands*²*Institute for Theoretical Physics, University of Amsterdam, Science Park 904, P.O. Box 94485, 1090 GL Amsterdam, The Netherlands*

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We study a chain of anharmonic springs with tunable power law interactions as a minimal model to explore the propagation of strongly nonlinear solitary wave excitations in a background of thermal fluctuations. By treating the solitary waves as quasiparticles, we derive an effective Langevin equation and obtain their damping rate and thermal diffusion. These analytical findings compare favorably against numerical results from a Langevin dynamic simulation. In our chains composed of two-sided nonlinear springs, we report the existence of an expansion solitary wave (antisoliton) in addition to the compressive solitary waves observed for noncohesive macroscopic particles.

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I. INTRODUCTION

In linear elastic solids, phonons are the basic mechanical excitations responsible for energy propagation. By contrast, an aggregate of macroscopic grains just in contact with their nearest neighbors constitute a novel elastic material where solitary waves or shocks replace phonons as the basic excitations [1–3]. The origin of these strongly nonlinear waves can be traced to the fact that, unlike the case of harmonic springs, the repulsive force between two grains in contact does not depend linearly on the relative compression. So far, little effort has been directed to determine the fate of these strongly nonlinear excitations in a background of thermal fluctuations because temperature is clearly not a parameter relevant to the elastic response of macroscopic grains.

However, granular aggregates at zero pressure are just one example of a broader class of materials that can be prepared in a unique mechanical state called *sonic vacuum* [1]. This term originally coined by Nesterenko in the context of strongly nonlinear granular chains designate a material characterized by a vanishing elastic moduli and linear speed of sound [1,4–8]. Grafted colloidal particles [9] and ultracold atoms in optical lattices [10] are microscopic systems that allow for tunable nonlinear interactions, while being naturally coupled to a source of fluctuation (thermal or quantum). These fluctuations restore rigidity and generate long wavelength phonon modes [11,12]. However, the physics of very high amplitude strain propagation is still predominantly nonlinear and resembles the state of sonic vacuum perturbed by background fluctuations, even if the interaction potentials are typically two sided, unlike granular ones. The nonlinear regime is particularly relevant for some biological systems, where energy transport occurs through localized nonlinear excitations with energy significantly higher than the thermal energy [13,14].

Moreover, systems such as polymer networks and colloidal glasses undergoing an unjamming transition are also charac-

terized by vanishing elastic moduli as the coordination number or packing fraction are lowered towards the critical point [15]. The effect of thermal fluctuations on the *nonlinear* response of materials undergoing an unjamming transition is relatively unexplored, despite the fact that they are obvious examples of a sonic vacuum state at zero temperature [16–18]. Note, that in the case of jamming the linear elastic moduli can be lowered towards zero even if the microscopic interactions are harmonic, simply because there are not enough forces to prevent floppy motions.

In this article, we focus on strongly nonlinear mechanical waves propagating in a background of small thermal fluctuations, a nonequilibrium problem that lies outside the realm of perturbation theory. The starting point of conventional perturbation methods is a linear elastic solid, possibly at finite temperature, perturbed by small anharmonic terms. By contrast, we adopt as a starting point the fully nonlinear state of sonic vacuum whose elementary excitations are long-lived solitary waves [19]. Subsequently we *switch on* temperature as a small perturbation that creates a background of thermal fluctuations.

As a minimal model that is analytically tractable, we study impulse propagation in a one-dimensional lattice of nonlinear springs with a tunable power law interaction. By coupling the lattice to a heat bath, we then study the effects of the thermal fluctuations on the leading solitary wave generated in response to an impulse of energy much higher than the background thermal energy. Our approach in a nutshell is to treat the solitary wave as a quasiparticle and derive an effective Langevin equation that describes its stochastic dynamics. We corroborate our analytical predictions for the damping rate and thermal diffusion of the solitary waves with Langevin dynamic simulations. The sonic vacuum is usually studied with a chain of noncohesive beads that only interact upon compression (one-sided interaction). The system with springs has some of the same properties as the sonic vacuum, since the sonic vacuum is a property of the nonlinear power law interaction (without a harmonic term). In addition to the compressive solitary waves seen in a lattice of macroscopic grains with one-sided repulsive interaction, we report an accompanying antisolitary wave solution for the lattice of nonlinear springs with two-sided interactions.

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II. THE IMPULSE RESPONSE OF NONLINEAR SPRINGS

In Fig. 1, we demonstrate that the compressional solitary wave (SW) excitation discovered by Nesterenko in a chain of noncohesive beads is also seen in a lattice of springs with two-sided interactions. However, unlike the case of a one-sided potential, each compressive SW generated in response to an impulse is accompanied by a corresponding expansion solitary wave (formed by local stretching of springs) of the same magnitude but moving in the opposite direction. This antisolitary wave (ASW) is not sustained by beads interacting with purely repulsive potentials—the beads would merely lose contact.

In Fig. 1, we show the SW-ASW excitations for (a) beads, (b) and (c) particles connected by springs. In Fig. 2, we plot E , the total energy carried by the soliton (after summing over all particles involved) versus P , the total momentum, for the leading SW-ASW. Note that $E = \frac{P^2}{2m_{\text{eff}}}$, where the constant m_{eff} can be viewed as the effective mass of the solitary or antisolitary waves. Inspection of Fig. 2 demonstrates that SW excitations in a lattice of repulsive beads (black circles) have the same effective mass m_{eff} as an SW and an ASW in two-sided springs (red squares).

As shown in Figs. 1(b) and 1(c), the leading SW-ASW generated in response to an impulse imparted to one of the particles towards the right (direction of arrow) is followed by a train of alternating SW-ASW's excitations, of progressively smaller magnitudes. The smaller SW-ASW's are generated as the particle that initially imparted the impulse, recoils with its leftover energy. This process is repeated several times, leading to the generation of the train of smaller excitations. Since the speed of propagation depends upon the amplitude, the SW and ASW that start propagating together initially (appearing bounded), eventually separate and become clearly distinguishable.

III. LANGEVIN EQUATION

The classical energy-momentum relation $E = \frac{P^2}{2m_{\text{eff}}}$ satisfied by the SW motivates the interpretation of the solitary wave as a quasiparticle [1,7,20]. For small perturbations, the SW can still be treated as a quasiparticle provided the effects of the perturbations accrue gradually such that the SW retains its functional form. We now apply this adiabatic approximation to derive an effective Langevin equation for the SW quasiparticle when the lattice of springs is coupled to a heat bath. Recall first, the Langevin equation for a particle of mass m undergoing Brownian motion in one dimension is

$$\frac{dx}{dt} = v, \quad \frac{dE}{dt} = -2\frac{\zeta}{m}K + \sqrt{\frac{2m\beta^2 K}{dt}}N(0,1). \quad (1)$$

Here, E, K are the total and kinetic energies, respectively, and ζ, β are the dissipation and diffusion coefficients related via the fluctuation dissipation theorem $\beta^2 = 2\zeta \frac{k_B T}{m^2}$, where k_B is the Boltzmann constant. $N(0,1)$ is a normal random variable with mean 0 and variance 1, and encapsulates the effects of random fluctuations during the time interval $t, t + dt$. For a free particle of unit mass moving with speed v , $E = K = \frac{1}{2}v^2$ and upon substituting in Eq. (1), we recover the Langevin's

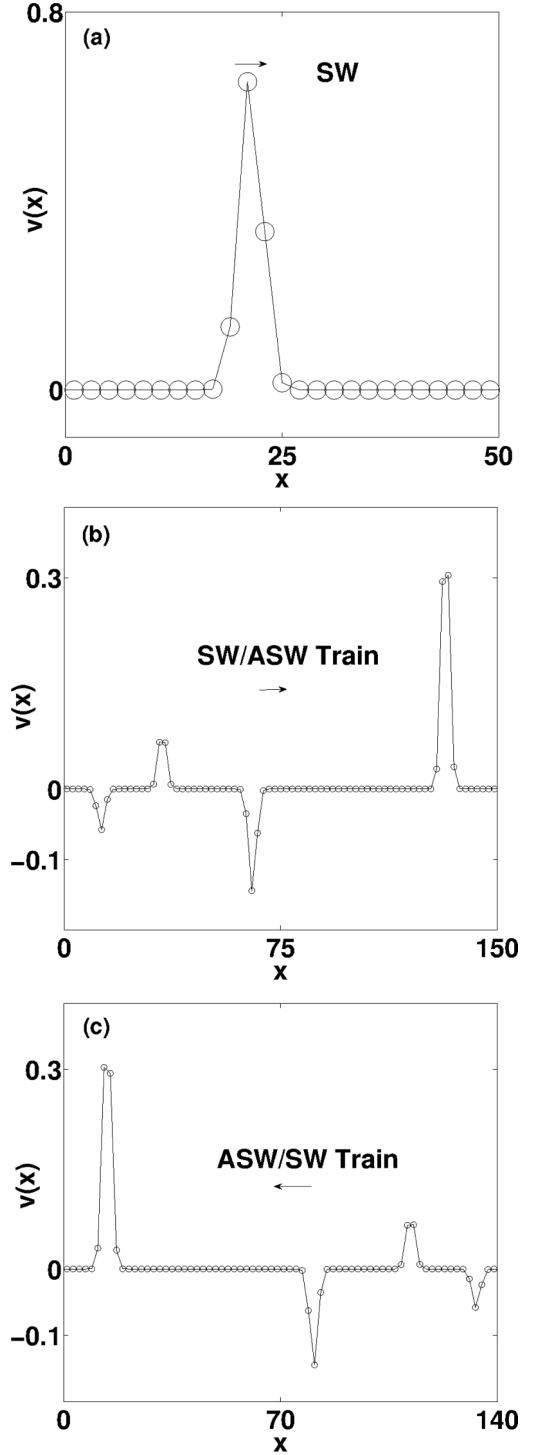


FIG. 1. Top: (a) The velocity profile of the compressive solitary wave (SW) generated through simulation in an athermal chain of beads with one sided interaction. Here the circles represent beads and we see that the solitary wave is around 5-bead diameters. (b)–(c) The velocity profiles showing the formation of a train of SW-ASW pair for two-sided nonlinear springs. A single particle is initially given an impulse to the right, generating a train led by a SW moving in the direction of the impulse (b), while simultaneously generating a symmetric train led by an ASW that moves in the opposite direction (c). Here, velocity is measured in units of ωa , where $a = 2R$ is the lattice spacing and R is the radius of the beads and $\omega = \sqrt{\frac{k}{m}a^{\alpha-2}}$.

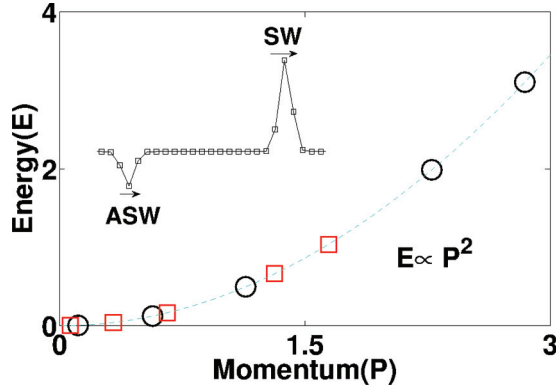


FIG. 2. (Color online) The energy momentum relation for the leading SW (black)-ASW (red) in the three cases shown in Fig. 1 following the energy (E) momentum (P) relation $E = \frac{p^2}{2m_{\text{eff}}}$. Energy is measured in units of ka^α , where k is the bare spring constant, a is the lattice spacing, and α is the exponent of the nonlinear potential. Velocity is measured in units of ωa , where $\omega = \sqrt{\frac{k}{m}}a^{\alpha-2}$. (Inset) Zoom-in of the leading SW-ASW pair from Fig. 1. We see that the SW and ASW are both around 5-bead diameters.

equation conventionally expressed as the rate of change of momentum of the particle [21].

We now derive an equation analogous to Eq. (1) for the compressive solitary wave quasiparticle. Let the displacement of a particle from its initial equilibrium position in the continuum limit be $\phi(x, t)$. If we identify the lattice spacing a as a characteristic length scale and $\omega = \sqrt{\frac{k}{m}}a^{\alpha-2}$ as an inverse time scale, then the equation of motion for the compressive displacement field $\phi(x, t)$ in dimensionless units reads

$$\phi_{tt} - \frac{1}{12}\phi_{xxtt} + [(-\phi_x)^{\alpha-1}]_x = 0, \quad (2)$$

where subscripts denote partial derivatives with respect to space x and time t . Equation (2) is a simplified form of the Nesterenko equation [1,2]; see Appendix A for details. The first two terms express the rate of change of momentum while the third term represents the force. Although the solitary wave solution to Eq. (2) is not exact (lacking compact support), Eq. (2) provides a good approximation while being analytically more tractable especially since we are interested in keeping the nonlinear exponent α general [2,3]. Note that the equation for the ASW (stretching) is obtained by modifying the third term $+ [(-\phi_x)^{\alpha-1}]_x \rightarrow - [(\phi_x)^{\alpha-1}]_x$ in Eq. (2).

In analogy with the Langevin equation for a particle, we model the coupling to a heat bath as the sum of two contributions—an external drag and a random fluctuating force, phenomenologically introduced into the equation of motion as

$$\begin{aligned} \phi_{tt} - \frac{1}{12}\phi_{xxtt} + [(-\phi_x)^{\alpha-1}]_x \\ = -\gamma \left(\phi_t - \frac{1}{12}\phi_{txx} \right) + \sqrt{\frac{2\gamma}{\alpha\Gamma}} \left(\eta(x, t; t+dt) - \frac{1}{\sqrt{12}}\eta_x(x, t; t+dt) \right), \end{aligned} \quad (3)$$

where $\gamma = \frac{\zeta}{m\omega}$ is the dimensionless drag coefficient that couples to the momentum $\Pi = (\phi_t - \frac{1}{12}\phi_{txx})$. It is useful to

define a coupling constant $\Gamma = \frac{ka^\alpha}{\alpha k_B T}$ as the ratio of potential to thermal energy in terms of which, the dimensionless diffusion coefficient is $D = \frac{2\gamma}{\alpha\Gamma}$. The last (noise) term on the right of Eq. (3) in conjunction with Π , satisfies the fluctuation dissipation theorem [22]. Here, $\eta(x, t; t+dt)$ is a Gaussian random noise during the time interval $t, t+dt$ with the moments,

$$\langle \eta(x, t; t+dt) \rangle = 0, \quad (4)$$

and

$$\langle \eta(x, t; t+dt)\eta(x', t'; t'+dt') \rangle = \delta(x-x')\delta(t-t'), \quad (5)$$

respectively, where the angular brackets denotes ensemble averaging.

To study the propagation of the SW in a background of thermal fluctuations, we now make a working assumption based on the quasiparticle approximation to the SW: Whenever the energy of the SW, $E \equiv E_{\text{SW}} \gg k_B T$, the SW functional form is unaltered and only its amplitude $A(t)$ becomes time dependent. The amplitude $A(t)$ is the collective variable for the SW quasiparticle and other properties of the solitary wave, such as its energy and momentum may be determined from it. Note, the width of the SW is independent of its amplitude and therefore we do not consider its time dependence [22].

From Eq. (2), the conserved energy is

$$E = \int dx \left(\frac{1}{2}\phi_t^2 + \frac{1}{24}\phi_{tx}^2 + \frac{1}{\alpha}(-\phi_x)^\alpha \right), \quad (6)$$

and the energy of the SW may be obtained by integrating Eq. (6) over the width of the SW of order W . (This avoids including the energy of small SW that separate from the main wave). Using Eq. (2), the rate of change of energy is

$$\begin{aligned} \frac{dE}{dt} = \sqrt{\frac{D}{dt}} \int dx \eta(x, t; t+dt) \left(\phi_t + \frac{1}{\sqrt{12}}\phi_{tx} \right) \\ - 2\gamma K + \sigma(t), \end{aligned} \quad (7)$$

where K is the kinetic part of the energy,

$$K = \int dx \left(\frac{1}{2}\phi_t^2 + \frac{1}{24}\phi_{tx}^2 \right). \quad (8)$$

The last two terms on the right of Eq. (7) describe the possible mechanisms of decay of the SW by “friction” from the heat bath (γ) and the “phonon drag” induced by the thermal motion of the chain $\sigma(t)$. The first term is the fluctuating part of the energy. In the following, we make the assumption (verified numerically) that the coupling to the heat bath is more important and therefore, ignore $\sigma(t)$.

Solving for the SW solution from Eq. (2), we find the velocity field to be

$$\phi_t(x, t) = A \operatorname{sech}^{\frac{2}{\alpha-2}} \left(\frac{x - V_s t}{W} \right), \quad (9)$$

where A is the amplitude of the SW that propagates at a speed $V_s = A^{\frac{\alpha-2}{\alpha}}$ and has a width $W = \frac{1}{\sqrt{3(\alpha-2)}}$ in units of the lattice spacing; see Appendix A 1, for details. Given the above form of the solution, the SW energy, kinetic energy, and momentum may now be expressed in terms of the collective variable A :

$$E = \int dx \phi_t^2(x, t) = A^2 I_E, \quad (10)$$

and from the virial theorem,

$$K = \frac{\alpha}{\alpha + 2} E = \frac{\alpha}{\alpha + 2} I_E A^2. \quad (11)$$

Additionally, the solitary wave momentum is

$$P = \int dx \phi_t(x, t) = A I_P. \quad (12)$$

Here,

$$I_E = \int dx \operatorname{sech}^{\frac{4}{\alpha-2}}\left(\frac{x}{W}\right), \quad (13)$$

$$I_P = \int dx \operatorname{sech}^{\frac{2}{\alpha-2}}\left(\frac{x}{W}\right) \quad (14)$$

are constants obtained by integrating over all space [2].

Substituting for E and K in terms of A , we cast Eq. (7) into the form of an ordinary Langevin equation (with additive noise) for the collective variable $A(t)$,

$$\begin{aligned} \frac{dA}{dt} = & \sqrt{\frac{2\gamma}{\alpha\Gamma I_E^2 A(t)^2 dt}} \int dx \eta(x, t; t + dt) \left(\phi_t + \frac{1}{\sqrt{12}} \phi_{tx} \right) \\ & - \frac{\alpha\gamma}{\alpha + 2} A, \end{aligned} \quad (15)$$

where, $\phi \equiv \phi(x, t)$. Equation (15) is the central result of our work whose analytical predictions we derive and test numerically in the next sections. The first term can be written as $\frac{1}{\sqrt{dt}} \eta_A(t, t + dt)$, where η_A is a white noise signal; that is, its correlations are given by $\langle \eta_A(t) \eta_A(t') \rangle = \frac{2\gamma}{(\alpha+2)I_E\Gamma} \delta(t - t')$. Using the fact that the correlations of $\eta(x, t)$ are described by delta functions, the correlations of $\eta_A(t)$ can be related to the kinetic energy Eq. (8), which can be replaced by $\frac{\alpha}{\alpha+2} I_E A(t)^2$.

IV. TIME DEPENDENCE OF MEAN AND VARIANCE

Taking the expectation value (ensemble average) of Eq. (15), we find

$$\frac{d\langle A \rangle}{dt} = -\frac{\alpha\gamma}{\alpha + 2} \langle A \rangle, \quad (16)$$

where, owing to the noise term $\eta(x, t; t + dt)$ (which acts between times $t; t + dt$) and $\phi_t(x, t)$ (which is a solution at time t) being statistically independent, the expectation value $\langle \eta(x, t; t + dt) \phi_t(x, t) \rangle = 0$. Consequently, the solitary wave amplitude decays as

$$\langle A \rangle = A_0 e^{-\frac{\alpha\gamma}{\alpha+2}t}, \quad (17)$$

where A_0 is the initial solitary wave amplitude. Note, the effective damping rate,

$$\gamma' = -\frac{\alpha\gamma}{\alpha + 2}, \quad (18)$$

is independent of the inverse temperature Γ , but rescales with the exponent of the nonlinear potential α .

Similarly, we solve for the variance of the solitary wave amplitude or equivalently, the variance in the square root of energy. Re-defining, $D = \frac{\gamma}{2\alpha\Gamma I_E^2}$, we solve for the variance in the solitary wave amplitude by first expressing the differential as

$$d[A^2] = A^2(t + dt) - A^2(t). \quad (19)$$

We obtain $A(t + dt)$ from Eq. (15),

$$\begin{aligned} A(t + dt) = & A \left(1 - \frac{\alpha\gamma}{\alpha + 2} dt \right) + \sqrt{D dt} \int dx \eta(x, t; t + dt) \\ & \times \left(\phi_t(x, t) + \frac{1}{\sqrt{12}} \phi_{tx}(x, t) \right), \end{aligned} \quad (20)$$

which when substituted into Eq. (19) gives us

$$\begin{aligned} d[A^2] = & -\frac{2\alpha\gamma}{\alpha + 2} A^2 dt + 2A\sqrt{D dt} \int dx \eta(x, t; t + dt) \\ & \times \left(\phi_t(x, t) + \frac{1}{\sqrt{12}} \phi_{tx}(x, t) \right) \\ & + D dt \iint dx dx' \left(\phi_t(x, t) + \frac{1}{\sqrt{12}} \phi_{tx}(x, t) \right) \\ & \times \left(\phi_t(x', t) + \frac{1}{\sqrt{12}} \phi_{tx'}(x', t) \right). \end{aligned} \quad (21)$$

Here, we have retained terms to order $O(dt)$ [23,24]. Taking the expectation value, the second term on the right vanishes (as discussed for the mean) and using the property that the noise term is delta correlated in space, we obtain

$$d[\langle A^2 \rangle] = -\frac{2\alpha\gamma}{\alpha + 2} \langle A^2 \rangle dt + D dt \int dx \left(\phi_t + \frac{1}{\sqrt{12}} \phi_{tx} \right)^2.$$

The last term when expanded gives twice the solitary wave kinetic energy $2K$ [see Eq. (8)], plus an integral $\frac{2}{\sqrt{12}} \int dx \phi_t \phi_{tx}$, that vanishes by symmetry for the SW solution. Moreover, the SW kinetic energy is related to its total energy via the virial relation $K = \frac{\alpha}{\alpha+2} E$. Hence, we obtain the ordinary differential equation correct to order dt ,

$$\frac{d\langle A^2 \rangle}{dt} = -\frac{2\alpha\gamma}{\alpha + 2} \langle A^2 \rangle + 2D I_E \frac{\alpha}{\alpha + 2}. \quad (22)$$

Solving, the differential equation subject to the initial condition $\langle A^2 \rangle_{t=0} = A_0^2$ and substituting for D , we obtain

$$\langle A^2 \rangle = A_0^2 e^{-\frac{2\alpha\gamma}{\alpha+2}t} + \frac{1}{2I_E\alpha\Gamma} (1 - e^{-\frac{2\alpha\gamma}{\alpha+2}t}). \quad (23)$$

Using Eq. (17), this may be expressed as

$$\operatorname{var}(A) = \langle A^2 \rangle - \langle A \rangle^2 = \frac{1}{2I_E\alpha\Gamma} (1 - e^{-\frac{2\alpha\gamma}{\alpha+2}t}). \quad (24)$$

Using the relation in Eq. (10), we rewrite the above equation as

$$\operatorname{var}(\sqrt{E}) = \frac{1}{2\alpha\Gamma} (1 - e^{-\frac{2\alpha\gamma}{\alpha+2}t}). \quad (25)$$

The coefficient $\frac{1}{2\alpha\Gamma}$ reduces to $\frac{k_B T}{2}$ when the energy is not measured in units of ka^α , so this expression is analogous to the velocity variance of a Brownian particle. Note, for large α , the SW is effectively one particle wide and thus Eq. (25) captures the correct thermal equilibration of the particle energy with the heat bath. However, for the dynamics of the SW, Eq. (25) is only useful as long as the SW is identifiable against the background thermal energy, that is, $E_{\text{SW}} \gg \Gamma^{-1}$.

V. SIMULATIONS

We consider a one-dimensional chain consisting of $N = 1024$ particles each having a mass m placed regularly on a

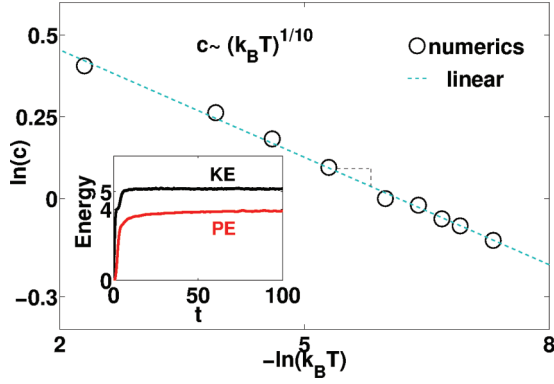


FIG. 3. (Color online) The sound speed computed from the dispersion curves for a range of Γ (inverse temperature) for $\alpha = \frac{5}{2}$. The circles are from numerical simulation while the dashed blue line is a linear fit, giving a slope of 0.11 for $\alpha = \frac{5}{2}$, close to the expected value $\frac{\alpha-2}{2\alpha} = \frac{1}{10}$. The inset shows the kinetic (KE) and potential energy (PE) approaching thermal equilibrium, where their ratio satisfies the Virial relation $\frac{\alpha}{2}$ which is 1.25 for $\alpha = \frac{5}{2}$. Here, energy is measured in units of $\frac{ka^\alpha}{10^3}$ and time in units of ωa , where k is the bare spring constant, a is the lattice spacing, and $\omega = \sqrt{\frac{k}{m}a^{\alpha-2}}$.

lattice with spacing a (spring rest length) interacting pairwise with a nearest neighbor interaction $V(\delta) = \frac{K}{\alpha}(\delta)^\alpha$, where δ is the compression and stretching induced during the dynamics. We model the coupling to the heat bath by numerically integrating Eq. (1) for each particle using the velocity-verlet algorithm [25]. In thermal equilibrium the mean kinetic energy is $\text{KE} \sim \frac{k_B T}{2}$ and potential energy is $\text{PE} \sim \frac{k_B T}{\alpha}$, where their ratio satisfies the virial relation (see Fig. 3 inset for $\alpha = \frac{5}{2}$). In the following, all numerical data is presented in dimensionless units, ensemble averaged over 1000 samples.

A. Fluctuation induced rigidity

To extract the equilibrium properties in the thermalized state, we define the longitudinal current density of particles as $j(x, t) = \frac{1}{\sqrt{N}} \sum_{i=1}^N v_i(t) \delta(x - x_i(t))$, and its Fourier transform $j(k, t) = \frac{1}{\sqrt{N}} \sum_{i=1}^N v_i(t) e^{ikx}$, where k is the longitudinal collective mode along the x direction. Thus, the corresponding longitudinal current density autocorrelation function is $C(k, t) = \langle j^*(k, 0) j(k, t) \rangle$, where the angular brackets denote ensemble averaging over the initial time. The longitudinal power spectral density is then obtained as the Fourier transform of the respective current density autocorrelation functions as, $P(k, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C(k, t)$. The Fourier transforms defined above are evaluated using fast Fourier transform from simulation data. The sound speeds in Fig. 3 correspond to the linear part of the dispersion curves, obtained by projecting the power spectral densities on the frequency (ω)—wave number (k) plane.

In Fig. 3, we plot the sound speed from the slope of the dispersion curves for $\alpha = \frac{5}{2}$ for a range of Γ . At thermal equilibrium, the mean kinetic energy and hence the temperature T satisfy the virial relation $T \sim \delta_T^\alpha$, where δ_T is the average displacement of the particles induced by thermal fluctuations. Defining the sound speed c as the second derivative of the induced potential energy leads to the relation,

$c^2 \sim T^{\frac{\alpha-2}{2\alpha}}$ [12]. For $\alpha = \frac{5}{2}$, we find $c \sim \Gamma^{-\frac{1}{10}} \sim (k_B T)^{\frac{1}{10}}$, closely matching the linear fit in Fig. 3. Thus, coupling the lattice of nonlinear springs that is initially in its state of sonic vacuum (implying the absence of linear sound) to a heat bath, leads to hydrodynamical sound modes with a linear sound speed that scales with the temperature of the heat bath [12]. Note, setting $\alpha = 2$ (harmonic springs) yields a sound speed that is independent of temperature while the limit $\alpha \rightarrow \infty$ yields $c \sim (k_B T)^{\frac{1}{2}}$, a result in agreement with the entropic elasticity for hard sphere colloidal crystals [11].

B. Comparison with analytics

Once the lattice reaches thermal equilibrium, we excite a solitary wave (SW) by imparting one of the particles an initial energy of order $E_{\text{SW}} = 0.5$ in dimensionless units. In Fig. 4, left panel, we show a snapshot of two SWs at the same time, propagating in a background of thermal fluctuations for $\alpha = 2.5$ (red) and $\alpha = 2.2$ (black). We see that the SW with lower α is wider and moves faster for the given amplitude, in qualitative agreement with the analytic widths $W \sim \frac{1}{\sqrt{3(\alpha-2)}}$ and speeds $V_s \sim A^{\frac{\alpha-2}{\alpha}}$.

In Fig. 5, left panel, we plot the numerical data (symbols) for the attenuation of the SW amplitude as a function of time for various values of γ and α and we find a very good match to the analytic expression in Eq. (17) (solid curves). For the range of Γ explored, we find the damping rate is independent of temperature (Γ) but depends on the environmental drag γ and α .

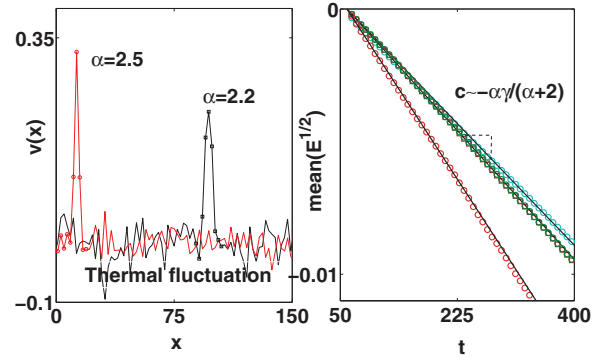


FIG. 4. (Color online) (Left) Snapshot of two leading solitary waves in a background of thermal fluctuations for $\alpha = 2.5$ (red) (narrow profile) and $\alpha = 2.2$ (black) (broader profile). The solitary waves are obtained from the velocity field $v(x)$ measured in units of ωa , where a is the lattice spacing and $\omega = \sqrt{\frac{k}{m}a^{\alpha-2}}$, while the x axis is measured in units of a . (Right) The attenuation of the solitary wave as a function of time plotted on a log-natural scale, for various values of γ , Γ , and α . The light blue circles correspond to $\alpha = 2.2, \Gamma = 10^4, \gamma = 5 \times 10^{-5}$; red circles correspond to $\alpha = 2.5, \Gamma = 10^4, \gamma = 7 \times 10^{-5}$; green circles represent $\alpha = 2.5, \Gamma = 10^4, \gamma = 5 \times 10^{-5}$; and the brown squares correspond to $\alpha = 2.5, \Gamma = 16^4, \gamma = 5 \times 10^{-5}$. The analytic estimates for these values based on Eq. (17) are shown by solid black lines. In these plots, the initial SW $E_{\text{SW}} = 0.5$ measured in units of ka^α , where k is the bare spring constant and a is the lattice spacing and time is measured in units of $\omega = \sqrt{\frac{k}{m}a^{\alpha-2}}$.

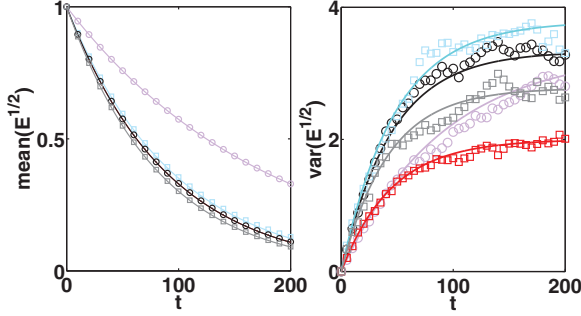


FIG. 5. (Color online) (Left) The numerically obtained mean solitary wave energy for $\alpha = 2.5, \gamma = 0.01$ (purple circles), $\alpha = 2.2, \gamma = 0.02$ (blue squares), $\alpha = 2.5, \gamma = 0.02$ (black circles), $\alpha = 3.0, \gamma = 0.02$ (gray squares) decaying exponentially compared against the analytical expression (solid curves). The mean decay rate is independent of the temperature Γ^{-1} . (Right) The numerically obtained variance of the square root of the solitary wave energy for $\alpha = 2.2, \gamma = 0.02, \Gamma = 6000$ (blue squares), $\alpha = 2.5, \gamma = 0.02, \Gamma = 6000$ (black circles), $\alpha = 3.0, \gamma = 0.02, \Gamma = 6000$ (gray squares), $\alpha = 2.5, \gamma = 0.01, \Gamma = 6000$ (purple circles), and $\alpha = 2.5, \gamma = 0.02, \Gamma = 10000$ (red squares) compared against the analytical expression Eq. (25) (solid curves). The variance has dimensions of energy expressed in units of $\frac{k\alpha^2}{10^5}$ where k is the bare spring constant and a is the lattice spacing.

In Fig. 5, right panel, we show the increase in the variance of SW amplitude (or the square root of its energy) as a function of time for multiple values of α, γ , and Γ obtained numerically (symbols) and compare them with the complete analytical solution Eq. (25) finding good agreement. Notice, the final value of the variance correctly approaches the thermal energy, as expected for a Brownian particle. However, since the solitary wave is a dynamical object that decays under the influence of the external drag, once the solitary wave energy becomes comparable to the background thermal energy, it is no longer meaningful to consider it as a Brownian particle.

VI. CONCLUSION

To conclude, we find that a lattice of two sided nonlinear springs generates a pair of solitary and antisolitary waves in response to an impulse. By coupling the lattice to a heat bath, we study the propagation of the leading compressive solitary wave that has an energy much greater than the background thermal energy, by deriving an effective Langevin equation for the solitary wave propagation. We calculated the damping rate and the growth rate of energy fluctuations, and verified our results with numerical simulations.

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APPENDIX A: CONTINUUM APPROXIMATION

In this section, we will review the Rosenau approximation to the Nesterenko solitary wave solution, that is valid for any general nonlinear potential [2,3].

Here, we adopt as our starting point the Lagrangian for a one-dimensional chain of identical spheres that are just touching each other, i.e., in the limit $\delta_0 \rightarrow 0$,

$$L = \sum_n \frac{1}{2} m \dot{u}_n^2 - \frac{K}{\alpha} \left(\frac{u_n - u_{n+1}}{a} \right)^\alpha, \quad (\text{A1})$$

where u_n is the displacement of the n th sphere from its equilibrium position, $a = 2R$ is the equilibrium lattice spacing, and K is the spring constant. In order to avoid doing a Binomial expansion in powers of α , we will define the continuum field variable as

$$a\phi'(n + \frac{1}{2}) = u_{n+1} - u_n, \quad (\text{A2})$$

where primes denote derivative with respect to x . We now take the continuum limit, i.e., $u_n \rightarrow u(x) \equiv u$ and Taylor expand the right-hand side about $x + \frac{a}{2}$:

$$a\phi'(x) \approx u + \frac{a}{2}u' + \frac{a^2}{8}u'' + \frac{a^3}{48}u''' - u + \frac{a}{2}u' - \frac{a^2}{8}u'' + \frac{a^3}{48}u'''. \quad (\text{A3})$$

Integrating both sides once with respect to x , we obtain

$$\phi(x) = u + \frac{a^2}{24}u'' \quad (\text{A4})$$

$$= \left(1 + \frac{a^2}{24} \frac{d^2}{dx^2} \right) u(x). \quad (\text{A5})$$

Inverting the differential operator we obtain

$$u(x) \approx \phi - \frac{a^2}{24}\phi''. \quad (\text{A6})$$

Thus, in the continuum limit, the Lagrangian becomes

$$\frac{L}{m} = \int dx \frac{1}{2} \dot{u}^2(x) - \frac{K}{m\alpha} (\phi'(x))^\alpha \quad (\text{A7})$$

$$= \int dx \frac{1}{2} \dot{\phi}^2 - \frac{a^2}{24} \dot{\phi} \phi'' - \frac{K}{m\alpha} (\phi')^\alpha. \quad (\text{A8})$$

By using the Euler-Lagrange equation, we find the equation of motion to be

$$\ddot{\phi} - \frac{a^2}{12} \ddot{\phi}'' + \frac{K}{m} [(-\phi')^{\alpha-1}]' = 0. \quad (\text{A9})$$

Note, ϕ here corresponds to the continuum displacement field. The corresponding equation in the strain field $\delta = -\phi'$ reads

$$\ddot{\delta} - \frac{a^2}{12} \ddot{\delta}'' - \frac{K}{m} [\delta^{\alpha-1}]'' = 0. \quad (\text{A10})$$

Upon substituting $\delta = -\phi_x$ for the compressive SW or $\delta = \phi_x$ for the expansive ASW, we find the same functional forms for the solitary wave solutions in both cases. Here, $\delta(x, t)$ represents the compression of two adjacent particles, i.e., the strain field.

1. Solitary wave solution

The solitary wave solution of Eq. (A10) can be obtained by looking for propagating solutions of the form

$$\delta(x, t) = \delta(x - V_s t);$$

$$\frac{V_s^2 a^2}{12} \delta'' - V_s^2 \delta + \frac{K}{m} \delta^{\alpha-1} = 0, \quad (\text{A11})$$

which can be expressed in the form of a Newton-like equation:

$$\delta'' = -\frac{12}{V_s^2 a^2} \left[-V_s^2 \delta + \frac{K}{m} \delta^{\alpha-1} \right] = -\frac{dW}{d\delta}. \quad (\text{A12})$$

Multiplying both sides by δ' and integrating

$$\int dx \delta' \delta'' = - \int dx \frac{dW}{d\delta} \delta', \quad (\text{A13})$$

$$\int \frac{1}{2} d(\delta')^2 = - \int dW, \quad (\text{A14})$$

$$\frac{1}{2} (\delta')^2 = -W(\delta). \quad (\text{A15})$$

Taking the square root and integrating again, we find

$$\int \frac{d\delta}{\sqrt{-2W}} = \int dx. \quad (\text{A16})$$

Substituting, $W(\delta) = \frac{12}{V_s^2 a^2} \left[\frac{K}{m\alpha} \delta^\alpha - \frac{V_s^2}{2} \delta^2 \right]$, and writing for brevity $A = \frac{12}{V_s^2 a^2} \frac{K}{m\alpha}$ and $B = \frac{6}{a^2}$, we need to integrate

$$\int \frac{d\delta}{\sqrt{2\delta\sqrt{B - A\delta^{\alpha-2}}}} = x. \quad (\text{A17})$$

Making the change of variables, $z^2 = B - A\delta^{\alpha-2}$, we find

$$\frac{-\sqrt{2}}{(\alpha-2)} \int \frac{dz}{(\sqrt{B})^2 - z^2} = x. \quad (\text{A18})$$

Therefore,

$$x = \frac{-1}{\sqrt{2B}(\alpha-2)} \left[\int \frac{dz}{\sqrt{B}-z} + \int \frac{dz}{\sqrt{B}+z} \right], \quad (\text{A19})$$

that yields

$$s = -\sqrt{2B}(\alpha-2)x = \ln \frac{\sqrt{B}+z}{\sqrt{B}-z}, \quad (\text{A20})$$

or

$$z = -\sqrt{B} \frac{1 - \exp(-s)}{1 + \exp(-s)}. \quad (\text{A21})$$

Squaring and substituting $z^2 = B - A\delta^{\alpha-2}$,

$$B - A\delta^{\alpha-2} = B \frac{\exp \frac{s}{2} - \exp -\frac{s}{2}}{\exp \frac{s}{2} + \exp -\frac{s}{2}}, \quad (\text{A22})$$

that yields

$$\delta^{\alpha-2} = \frac{B}{A} \text{sech}^2 \left(\frac{s}{2} \right). \quad (\text{A23})$$

Therefore, the solitary wave solution is

$$\delta = \left(\frac{m\alpha V_s^2}{2K} \right)^{\frac{1}{\alpha-2}} \text{sech}^{\frac{2}{\alpha-2}} \left(\frac{\sqrt{3}}{2a} (x - V_s t) \right). \quad (\text{A24})$$

APPENDIX B: SOLUTION FROM DISCRETE EQUATIONS OF MOTION

The energy and the fluctuations of the solitary wave can also be derived for a discrete chain, without making the continuum approximation. From Eq. (A1), the equation of motion is

$$m\ddot{u}_n = K(u_{n-1} - u_n)^{\alpha-1} - K(u_n - u_{n+1})^{\alpha-1}. \quad (\text{B1})$$

A solitary wave solution to the above equation of motion has the form of a wave moving at a constant speed V_s :

$$u_n(t) = \frac{A}{V_s} f(na - V_s t), \quad (\text{B2})$$

where A is the amplitude of the SW and f is a function that describes the shape of the SW. [Since we define the amplitude as the maximum speed of the particles enveloped by the solitary wave, the displacement $u_n(t)$ will be proportional to A/V_s .]

In analogy with Eq. (1), we now couple the discrete equation of motion Eq. (B1) to a source of Gaussian noise and drag:

$$m\ddot{u}_n = K(u_{n-1} - u_n)^{\alpha-1} - K(u_n - u_{n+1})^{\alpha-1} - \gamma \dot{u}_n + \sqrt{2\gamma k_B T} \eta_n(t). \quad (\text{B3})$$

Here, the noise satisfies $\langle \eta_n(t) \eta_n(t') \rangle = \delta(t - t')$. The coefficient of the noise ensures that in equilibrium the particles satisfy the fluctuation-dissipation theorem such that their average kinetic energy is $\frac{1}{2} k_B T$.

From Eq. (A1), the energy of the chain is $E = \sum_n \frac{1}{2} m \dot{u}_n^2 + \frac{K}{\alpha} (u_n - u_{n+1})^\alpha$. If we restrict the summation to particles enveloped by the solitary wave such that the sum does not include particles that are far away from the SW, then E corresponds to the energy of the SW. Multiplying Eq. (B3) by \dot{u}_n , we obtain the rate of change of energy,

$$\frac{dE}{dt} = \sum_n -\gamma \dot{u}_n^2 + \sqrt{2\gamma k_B T} \eta_n(t) \dot{u}_n, \quad (\text{B4})$$

where the contribution of terms of the form $(u_{n\pm 1} - u_n)^{\alpha-1} \dot{u}_{n\pm 1}$ (i.e., with index $n-1$ and $n+1$) cancel out upon summation over n .

Consistent with the quasiparticle interpretation of the SW, we again assume that the SW in a background of noise and drag, is still given approximately by Eq. (B2). Therefore, we write the terms in Eq. (B4) in terms of the SW amplitude. The SW energy is $E = I_E A^2$, and the first term on the right-hand side is proportional to the kinetic energy, which is $2 \frac{\alpha}{\alpha+2} E$ by the virial theorem. Thus the energy decays at a rate $\frac{\alpha}{\alpha+2}$ times the decay rate for the velocity of a single particle ($\frac{\gamma}{m}$). The SW amplitude therefore decays as

$$\dot{A} = -\frac{\gamma\alpha}{m(\alpha+2)} A - \sqrt{\frac{\gamma k_B T}{2I_E^2}} \sum_n \eta_n(t) f'(na - V_s t). \quad (\text{B5})$$

A term that compensates for the diffusion of A is omitted here (this term is derived in Ito calculus), but it is only a small amount that is negligible if $I_E A^2 \gg k_B T$. Now, the different contributions in the last term just add up to a new noise term $\lambda \eta(t) = \sqrt{\frac{\gamma T}{2I_E^2}} \sum_n \eta_n(t) f'(na - V_s t)$, which is also not correlated in time. (Assume that λ is the amplitude of

the noise while η has a noise with one unit of strength.) The original noise term $\sum \eta_n(t) \dot{x}_n$ has correlations because x_n depends on the noise at an earlier time. But if the noise mostly just changes the amplitude of the SW by a random amount, and does not cause the particles in it to be displaced randomly relative to each other, then these correlations are not too important, and that is why they cancel out in the equation for A . The variance of the noise is, therefore,

$$\lambda^2 \langle \eta(t) \eta(t') \rangle = \frac{\gamma k_B T}{2I_E^2} f'(na - V_s t)^2 \delta(t - t'), \quad (\text{B6})$$

so $\lambda^2 = \frac{\gamma T}{2I_E^2} f'(na - V_s t)^2$. This can be determined by the virial theorem since it is proportional to the kinetic energy of the SW, hence $\lambda^2 = \frac{\gamma k_B T}{I_E m} \frac{\alpha}{\alpha+2}$. Therefore the amplitude of the soliton satisfies

$$\dot{A} = -\frac{\gamma \alpha}{m(\alpha+2)} A + \sqrt{\frac{\alpha}{\alpha+2} \frac{\gamma T}{I_E m}} \eta(t). \quad (\text{B7})$$

Upon taking the mean and variance of the amplitude from Eq. (B7), we recover the solutions derived using continuum approximation.

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