Universal energy transport law for dissipative and diffusive phase transitions

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(Received 17 July 2015; revised manuscript received 29 February 2016; published 30 March 2016)

We present a scaling law for the energy and speed of transition waves in dissipative and diffusive media. By considering uniform discrete lattices and continuous solids, we show that—for arbitrary highly nonlinear many-body interactions and multistable on-site potentials—the kinetic energy per density transported by a planar transition wave front always exhibits linear scaling with wave speed and the ratio of energy difference to interface mobility between the two phases. We confirm that the resulting linear superposition applies to highly nonlinear examples from particle to continuum mechanics.

DOI: 10.1103/PhysRevB.93.104109

I. INTRODUCTION

Phase or domain boundaries are common in physical systems whose nonconvex potential energy admits more than one stable equilibrium state. Under external loads, those interfaces move, thereby producing a kink transition wave whose propagation gradually switches the system locally from one stable configuration into another. This process is observed in a myriad of physical systems spanning length and time scales from atomistic to macroscopic structures. Based on the nature of the physical process, such systems are characterized as non- or weakly dissipative, dissipative, or diffusive. Non- or weakly dissipative models have been used to explain phenomena such as dislocation motion [1], ferromagnetic domain wall motion [2], proton mobility in hydrogen-bonded chains [3], rotation of DNA bases [4], chains of rotating pendula [5], or lattices of bistable buckled, elastic structures [6]. By contrast, diffusive or dissipative kinetics play an essential role in describing the physics of, e.g., ferroelectric domain switching [7], dynamics of CNT foams [8,9], magnetic flux propagation in Josephson junctions with tunneling losses [10], pulse propagation in cardiophysiology [11] and neurophysiology [12], sliding friction [13], chemical surface adsorption [14], underdamped commensurate phase transitions [15], or defect conductivity in superionic conductors [16]. Although numerous theoretical studies have been devoted to characterizing the motion of phase boundaries particularly in 1D periodic physical, chemical, or biological systems, see, e.g. [17–24] and references therein, the lessons learned almost exclusively apply to special cases only, owing to the variety of nonlinear interaction potentials and nonconvex on-site potentials. Here, we present a surprisingly simple universal energy law that applies to diffusive and dissipative systems and uniquely links the speed and profile of transition waves to the energetics and kinetics of the periodic system.

All of the above examples of diffusive and dissipative systems, including continuous and discrete systems, essentially reduce to the same type of governing equation that describes the nonlinear wave motion. For the discrete case, this may be interpreted as the equations of motion of a periodic 1D array of N elements whose displacements $u_n(t)$ at time t satisfy (for $n = 1, \ldots, N$)

$$m\,u_{n,tt} + \alpha\,u_{n,t} + \phi'(u_n) - \sum_{j=1}^{N_b}\left[V_j'\left(\frac{u_{n+j}-u_n}{ja}\right) - V_j'\left(\frac{u_n-u_{n-j}}{ja}\right)\right] = 0, \qquad (1)$$

where m is the mass of each element, V denotes a nonlinear interaction potential (assuming long-range pairwise interactions), N_b represents the number of neighbor interactions, ϕ is the (multistable, i.e., nonconvex) on-site potential and a introduces the equilibrium spacing between masses with primes and variables following a comma in indices denoting partial derivatives.

The analogous continuous governing equation, as we will show, is obtained by taking the continuum limit of (1) as $a \to 0$. Replacing discrete variables u_n by the continuous field $u(x,t)$ such that $u_n(t) = u(na,t)$ leads to the continuous governing equation

$$\rho\,u_{,tt} + \gamma\,u_{,t} + \psi'(u) - \sum_{j=1}^{N_b} j\,u_{,xx}V_j''(u_{,x}) = 0, \qquad (2)$$

with mass density ρ and rescaled damping parameter γ and nonconvex potential ψ. The aforementioned physical, chemical, or biological systems reduce to either (1) or (2).

As in most of the examples, we consider velocity-proportional damping characterized by the dissipation parameter $\alpha > 0$ for the discrete case or $\gamma > 0$ for the continuum. For a non- or weakly dissipative system, the damping term is negligible compared to the inertial term ($|mu_{n,tt}| \gg |\alpha u_{n,t}|$ or $|\rho u_{,tt}| \gg |\gamma u_{,t}|$). The energy transport in such systems is described well by its Hamiltonian which remains approximately constant as the wave propagates. However, energy transport in dissipative ($|mu_{n,tt}| \sim |\alpha u_{n,t}|$ or $|\rho u_{,tt}| \sim |\gamma u_{,t}|$) or diffusive lattices ($|mu_{n,tt}| \ll |\alpha u_{n,t}|$ or $|\rho u_{,tt}| \ll |\gamma u_{,t}|$) is not well understood at present. Therefore, in this paper, we focus on the dynamics of diffusive and dissipative systems and derive an explicit energy transport law for such systems. We show that the law holds for both discrete and continuous systems.

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II. THEORETICAL ANALYSIS

Transition waves, i.e., the motion of phase boundaries in multistable lattices, is commonly characterized by a steady-state wave form that propagates through the medium with kinetic energy concentrated in the moving wave front. That is, away from the moving phase boundary, the system attains an equilibrium in one of the stable energy wells of ϕ. Let us begin by studying the propagation of transition waves in discrete lattice systems with governing equations of the form (1). Next, we will derive the continuum limit (2) from (1) and show that the kinetic energy transport in both types of systems is governed by the same energy scaling law.

A. Energy transport in discrete lattices

We begin by assuming a traveling wave solution of the form $u_n(t) = u(na - vt) = u(\xi)$ so that (1) becomes

$$mv^2u_{,\xi\xi} - v\alpha u_{,\xi} + \phi'(u) - \sum_{j=1}^{N_b}\left[V_j'\left(\frac{u(\xi+ja)-u(\xi)}{ja}\right) - V_j'\left(\frac{u(\xi)-u(\xi-ja)}{ja}\right)\right] = 0. \tag{3}$$

Multiplying by $u_{,\xi}$ and integrating over the real axis gives

$$\int_{-\infty}^{\infty}[mv^2u_{,\xi\xi} - v\alpha u_{,\xi} + \phi'(u)]u_{,\xi}d\xi = \sum_{j=1}^{N_b}\int_{-\infty}^{\infty}\left[V_j'\left(\frac{u(\xi+ja)-u(\xi)}{ja}\right) - V_j'\left(\frac{u(\xi)-u(\xi-ja)}{ja}\right)\right]u_{,\xi}d\xi. \tag{4}$$

Let us first examine an individual integral on the right-hand side.

Define $\eta = \xi - ja$ and redefine the integral with respect to η in the second term, thereby transforming the right-hand side terms into

$$\begin{aligned}F_j &= \int_{-\infty}^{\infty}\left[V_j'\left(\frac{u(\xi+ja)-u(\xi)}{ja}\right) - V_j'\left(\frac{u(\xi)-u(\xi-ja)}{ja}\right)\right]u_{,\xi}d\xi \\ &= \int_{-\infty}^{\infty}V_j'\left(\frac{u(\xi+ja)-u(\xi)}{ja}\right)u_{,\xi}(\xi)d\xi \\ &\quad - \int_{-\infty}^{\infty}V_j'\left(\frac{u(\eta+ja)-u(\eta)}{ja}\right)u_{,\xi}(\eta+ja)d\eta.\end{aligned} \tag{5}$$

By changing the dummy variable η back to ξ, and defining $z = \frac{u(\xi+ja)-u(\xi)}{ja}$ with $dz = \frac{u_{,\xi}(\xi+ja)-u_{,\xi}(\xi)}{ja}d\xi$, Eq. (5) reduces to

$$F_j = -ja\int_{z(\xi\to-\infty)}^{z(\xi\to\infty)}V_j'(z)dz. \tag{6}$$

Now, since the system is dissipative or diffusive, we assume that the wave profile reaches a steady state and, in particular, as $t \to \infty$ (or $\xi \to -\infty$) we have $u(\xi + ja) - u(\xi) \to 0$ and $z(\xi) \to 0$. Analogously, since the system is initially at rest, we know $u(\xi + ja) - u(\xi) \to 0$ and $z(\xi) \to 0$ as $t \to -\infty$ (or $\xi \to \infty$). Thus the system is in equilibrium and unstretched far from the wave front, in the sense that both particle velocity and relative displacement vanish in the remote fields, ahead of and behind the kink. Therefore, we must have $F_j = 0$.

By a similar argument, the integral of the inertial term on the left-hand side of (4) goes to zero.

If the transition wave switches the state variable from the initial value $u_i = \lim_{\xi\to\infty}u(\xi)$ to the final value $u_f = \lim_{\xi\to-\infty}u(\xi)$, then the on-site potential contribution becomes

$$\int_{-\infty}^{\infty}\phi'(u)u_{,\xi}d\xi = \phi(u_i) - \phi(u_f) = \Delta\phi. \tag{7}$$

Therefore (4) becomes

$$v\int_{-\infty}^{\infty}u_{,\xi}^2\,d\xi = \frac{\Delta\phi}{\alpha} = \frac{\Delta\psi}{\gamma}, \tag{8}$$

where we introduced $\psi = \phi/a$ and $\gamma = \alpha/a$ as the on-site potential per length and linear damping per length, respectively. As we will show in the continuous case below, $\gamma, \psi = O(1)$ as $a \to 0$. For large wave widths $w \gg a$, the total transported kinetic energy per mass density $\rho = m/a$ of the discrete lattice is given by

$$E_d = \sum_{i=1}^{N}\frac{1}{2}u_{i,t}^2\,a = v^2\sum_{i=1}^{N}\frac{1}{2}u_{i,\xi}^2\,a \approx \frac{v^2}{2}\int_{-\infty}^{\infty}u_{,\xi}^2d\xi\,. \tag{9}$$

Combining (8) and (9) gives a simple result for the transported energy as

$$\frac{E_d}{v} \simeq \frac{\Delta\psi}{2\gamma}. \tag{10}$$

Therefore, for a diffusive or dissipative lattice the ratio of the transported kinetic energy per density to the wave speed depends only and linearly upon the ratio of the change in the on-site potential energy to the dissipation parameter.

B. Energy transport in continuous systems

Let us first derive the continuum limit (2) of the discrete equation (1). We consider a lattice made up of N nodes with constant spacing a. Therefore, the macroscopic total length is $L = (N-1)a$. In the continuum limit, we let $N \to \infty$ while keeping the macroscopic length L fixed. Therefore, $a \to 0$ and, as $N \gg 1$, $L \simeq Na$. In the continuum limit of $a \to 0$, we first introduce Taylor expansions for u_{n+j} for each interaction potential term, which gives

$$V_j'\left(\frac{u_{n+j}-u_n}{ja}\right) = V_j'(u_{,x}) + \frac{ja}{2}\,u_{,xx}V_j''(u_{,x}) + O(a^2).$$

Insertion into (1) and division by a results in

$$\rho v^2u_{,\xi\xi} - \sum_{j=1}^{N_b}j\,V_j''(u_{,\xi})u_{,\xi\xi} + O(a) - v\frac{\alpha}{a}u_{,\xi} + \frac{1}{a}\phi'(u) = 0,$$

where $\rho = m/a$ is the mass density. When transitioning from a discrete lattice to a continuum, certain macroscopic quantities should remain finite or of $O(1)$ for physical reasons (otherwise, the continuum limit is physically nonsensical). As L is kept fixed and independent of a, we have $L = O(1)$. This results in the following scalings.

(i) The total (macroscopic) mass M must remain finite and constant:

$$M = mN \sim O(1) \Rightarrow \rho = m/a = M/L \sim O(1). \quad (11)$$

Hence the mass density remains finite and constant.

(ii) The macroscopic energy density of the on-site potential well must remain finite:

$$\sum_{i=1}^{N} \phi(u_i) \to \frac{1}{a}\int_0^L \phi(u)\,dx \sim O(1) \Rightarrow \phi(u)/a \sim O(1), \quad (12)$$

which directly leads to the conclusion that the forcing function should vary such that $\psi'(u) = \phi'(u)/a \sim O(1)$.

(iii) The macroscopic dissipation potential must remain finite:

$$\sum_{i=1}^{N} \frac{1}{2}\alpha u_{i,t}^2 \to \frac{\alpha}{a}\int_0^L \frac{1}{2}u_{,t}^2\,dx \sim O(1) \Rightarrow \alpha/a \sim O(1). \quad (13)$$

Hence we define $\gamma = \alpha/a \sim O(1)$ which must remain finite in the continuum limit.

Overall, we thus obtain the continuum balance equation (2):

$$\rho u_{,tt} - \sum_{j=1}^{N_b} j\, V_j''(u_{,x})u_{,xx} + \gamma u_{,t} + \psi'(u) = 0. \quad (14)$$

Now, assuming a traveling wave solution of the form $u(x,t) = u(x - vt) = u(\xi)$ and substituting in (14), we obtain

$$\rho v^2 u_{,\xi\xi} - \sum_{j=1}^{N_b} j\, V_j''(u_{,\xi})u_{,\xi\xi} - v\gamma u_{,\xi} + \psi'(u) = 0. \quad (15)$$

Multiplying by $u_{,\xi}$ and integrating over the real axis gives

$$\int_{-\infty}^{\infty}\left(\rho v^2 - \sum_{j=1}^{N_b} j V_j''(u_{,\xi})\right)u_{,\xi}u_{,\xi\xi}d\xi + \int_{-\infty}^{\infty}\psi'(u)u_{,\xi}d\xi = v\gamma\int_{-\infty}^{\infty}u_{,\xi}^2 d\xi. \quad (16)$$

Without loss of generality, we assume that $v > 0$ (the wave travels in the positive direction) and the system is diffusive or dissipative. Like in the discrete case, we assume that the wave profile reaches a steady state, and the particle velocity and strain vanish in the remote fields, ahead of and behind the kink, leading, again, to the conclusion that $u_{,\xi} \to 0$ as $\xi \to \pm\infty$. Consequently, we see that

$$\int_{-\infty}^{\infty}\left(\rho v^2 - \sum_{j=1}^{N_b} j V_j''(u_{,\xi})\right)u_{,\xi}\frac{du_{,\xi}}{d\xi}d\xi = 0. \quad (17)$$

If the transition wave switches the state variable from the initial value $u_i = \lim_{\xi\to\infty} u(\xi)$ to the final value $u_f = \lim_{\xi\to-\infty} u(\xi)$, then the on-site potential contribution becomes

$$\int_{-\infty}^{\infty}\psi'(u)u_{,\xi}d\xi = \psi(u_i) - \psi(u_f) = \Delta\psi \quad (18)$$

and (16) reduces to the simple relation

$$\Delta\psi = v\gamma\int_{-\infty}^{\infty}u_{,\xi}^2\,d\xi, \quad (19)$$

which can be linked to the total kinetic energy per density ρ transported by the transition wave, viz.

$$E = \int_{-\infty}^{\infty}\frac{1}{2}u_{,t}^2 dx = \frac{1}{2}v^2\int_{-\infty}^{\infty}u_{,\xi}^2\,d\xi. \quad (20)$$

By combining (19) and (20), we arrive at the universal scaling law

$$\frac{E}{v} = \frac{\Delta\psi}{2\gamma}, \quad (21)$$

which agrees with (10) for large wave widths ($E_d \approx E$).

C. Results

As shown above, the energy transport in diffusive or dissipative continua in discrete lattices and continuous media obey the same scaling law, viz. that the ratio of the transported kinetic energy per density to the wave speed is linearly proportional to the ratio of the change in the on-site potential energy to the dissipation parameter. We note that even in the limit $\rho \to 0$ the kinetic energy per unit density, E (or E_d in the discrete case), remains a finite quantity, so the law (21) applies, as long as the system response remains a traveling kink. Quantity E (or E_d) can be obtained experimentally from the particle velocities (or two snapshots from subsequent time steps).

Some of the remarkable features of this scaling law are as follows. (i) The interparticle forcing does not affect the ratio, i.e., the above law holds for any nonlinear interaction potential V. (ii) The law is independent of the number of interacting neighbors, N_b. (iii) It is independent of the topology of the on-site potential ϕ but depends only on the difference $\Delta\psi$ between the initial and final energy of a bistable transition. (iv) For $E > 0$, we must have $\Delta\psi > 0$; i.e., stable mobile transition waves can only occur when switching from higher to lower potential energy. (v) The scaling law is linear despite the governing equations being highly nonlinear. This suggests that in the case of multiwell transitions, the transported energy must follow from linear superposition of the individual two-well transitions. The law can also be interpreted as follows. The ratio of kinetic energy per unit density to the velocity is also the ratio of energy to momentum density. Therefore, the transition wave can be thought of as a localized quasiparticle with its energy scaling to its momentum density according to (21).

Finally, note that we assumed linear damping and the existence of a traveling wave solution. Both assumptions may have to be relaxed depending on the specific features of the system of interest (see the discussion in subsequent sections).

III. NUMERICAL SIMULATIONS

For numerical purposes, dimensionless forms are obtained by normalization using the characteristic length $(\phi_0/k_0)^{1/2}$, time α/k_0, and force $(\phi_0 k_0)^{1/2}$, where we defined $\phi_0 = \Delta\phi/2$ and the initial stiffness of particle interactions, $k_0 = \phi''(0)/2$.

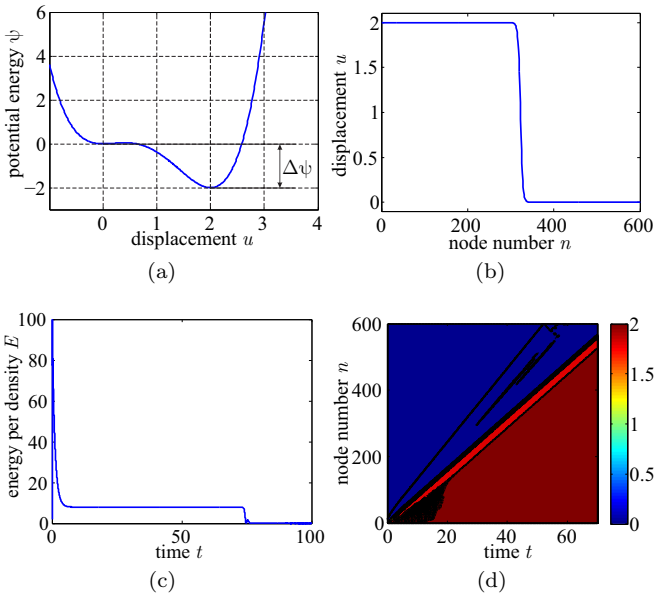

FIG. 1. Example of a moving transition wave: (a) bistable topology of the on-site potential ψ with minima at $u = 0$ and $u = 2$; (b) resulting transition wave profile (displacement vs position); (c) evolution of the kinetic energy per density vs time (the kinetic energy stabilizes at a constant value once the kink assumes a steady wave form); (d) contour plot of the wave propagation in x-t form. The phase boundary moves at a constant velocity once it assumes a steady kink wave form.

By dividing (1) by the characteristic force and normalizing all variables, we arrive at

$$\bar{m}\,\bar{u}_{n,\bar{t}\bar{t}} + \bar{\alpha}\,\bar{u}_{n,\bar{t}} + \bar{\phi}'(\bar{u}_n) - \sum_{j=1}^{N_b}\left[\bar{V}_j'\left(\frac{\bar{u}_{n+j}-\bar{u}_n}{j\bar{a}}\right) - \bar{V}_j'\left(\frac{\bar{u}_n-\bar{u}_{n-j}}{j\bar{a}}\right)\right] = 0, \quad (22)$$

where the overbars represent normalized quantities and $\bar{m} = mk_0/\alpha^2$, $\bar{\alpha} = 1$. The choice of the normalization parameters implies that $\Delta\bar{\phi} = \Delta\phi/\phi_0 = 2$ and thus $\Delta\bar{\psi}/\bar{\gamma} = 2$. Therefore, the energy law reduces to

$$\bar{E}/\bar{v} = 1. \quad (23)$$

For convenience, we omit the overbars in the subsequent numerical examples.

To verify the theoretical predictions, simulations were performed on a periodic chain of 600 particles which are governed by a variety of interaction potentials V and multistable on-site potentials ψ. The lattice is initially unstretched and at rest and loaded by displacing the leftmost particle until it transitions from one stable potential well into another. The rightmost particle is held fixed. The lattice response is computed by Newmark-β implicit time integration. After assuming a steady state, the velocity and energy of the wave remain constant over time, as shown in the example of Fig. 1.

In particular, we simulated diffusive and dissipative chains of particles exposed to the same fourth-order polynomial bistable on-site potential of Fig. 1(a) with the following interaction potentials motivated by the introductory examples: (a) linear elastic springs as in the classical Frenkel-Kontorova model of dislocation motion [1]: $V'(u) = F_0 u/a$ (with $F_0 = 100$ and $a = 1$), (b) Coulombic interactions between charged particles [20]: $V'(u) = F_0(u/a + 1)^{-2}$ (with $F_0 = 0.0015625$ and $a = 8$), (c) dipole-dipole interactions in a chain of magnets: $V'(u) = F_0(u/a + 1)^{-4}$ with ($F_0 = 0.016$ and $a = 5$), (d) nonlinear Toda interactions describing, among others, charge density waves [25]: $V'(u) = F_0(1 - e^{-\beta u/a})$ (with $F_0 = 100$, $a = 6$, and $\beta = 6$), (e) hyperelastic rubber connectors (1D incompressible neo-Hookean solid [26]): $V'(u) = F_0(1 + \frac{u}{a} - (u/a + 1)^{-2})$ (with $F_0 = 1$ and $a = 6$), and (f) Lennard-Jones (LJ) atomic interactions with varying cutoff radius: $V'(u) = F_0[(1 + u/a)^{-7} - (1 + u/a)^{-13}]$ (with $F_0 = 137.17$ and $a = 3$). Due to the short-range nature of LJ, we also computed results for long-range linear-spring interactions with up to $N_b = 4$ neighbors. The summary of results in Fig. 2 confirms that the scaling law is indeed independent of the interaction potential and of the number of neighboring interactions.

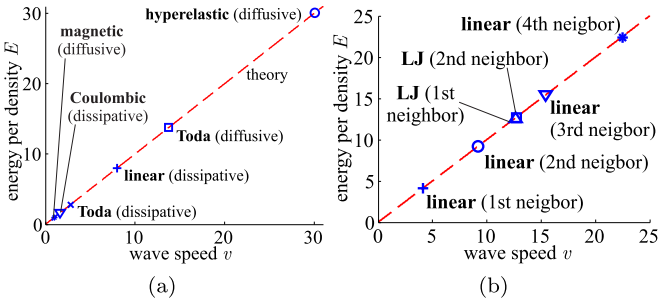

FIG. 2. Plots of the kinetic energy E of the traveling wave vs kink propagation speed v for (a) various examples of interaction potentials and (b) varying numbers of interacting neighbors. All examples use the bistable energy of Fig. 1(a) with $m = 1$ for dissipative and $m = 0.0001$ for weakly inertial or diffusive cases, and $a = 1$. All results lie almost perfectly on the predicted lines with slopes $E/v = \Delta\psi/2\gamma = 1$.

Surprisingly, the scaling law is independent of the topology of the nonconvex potential ψ. For verification, simulations were carried out on lattices with the three bistable interaction potentials shown in Fig. 3; all are fourth-order polynomials with the same value of $\Delta\psi = 2$. In analogy to Fig. 2, Fig. 3(b)

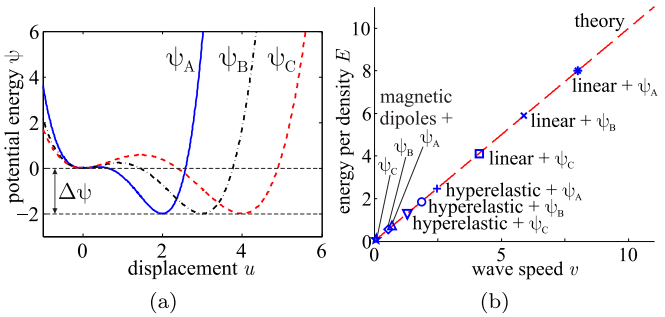

FIG. 3. (a) Three different topologies of the on-site potential ψ with different equilibrium distances but with the same energy jump $\Delta\psi$; (b) resulting energy per density E vs wave speed v for the different topologies and interaction potentials (all other parameters as in Fig. 2). Again, all computed values fall onto the predicted line with slope $E/v = \Delta\psi/2\gamma = 1$.

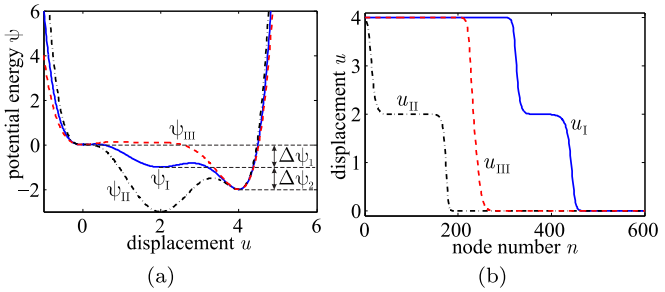

FIG. 4. (a) Three possible topologies of a triple-well potential that generate propagating kinks: (I) $\Delta\psi_1, \Delta\psi_2 > 0$, (II) $\Delta\psi_1 > 0$, $\Delta\psi_2 < 0$, and (III) $\Delta\psi_1 < 0$, $\Delta\psi_1 + \Delta\psi_2 > 0$. (b) Resulting wave forms for the three cases: (I) two transition waves travel with different velocities, (II) only one partial transition wave propagates (the other is stationary as $\Delta\psi_2 < 0$), and (III) one complete transition wave propagates with a constant velocity (the second transition drags the first along).

shows the linear relation between the computed kinetic energy of the traveling wave and the wave speed for all three bistable potentials, which confirms the energy transport law.

Since the energy law is linear, superposition can be expected in the case of multiwell transitions despite the highly nonlinear scenario. This suggests that a multiwell transition can be broken down into individual bistable transitions and analyzed separately to determine the total energy transported. To test this hypothesis, numerical experiments were performed for transitions occurring in a triple-well energy landscape as shown in Fig. 4. Results for three different interaction potentials are summarized in Table I and show excellent agreement with deviations of less than 1%, thus confirming that superposition applies indeed. However, as seen from Fig. 4(b), in the special case $\Delta\psi_1 < 0$ and $\Delta\psi_1 + \Delta\psi_2 > 0$, the second

TABLE I. Numerical results for the sixth-order tristable potential energy with energy differences $\Delta\psi_1$ (first) and $\Delta\psi_2$ (second well). Wave speeds v_i (identified from contour plots by a linear regression fit) and total kinetic energies E are compared to the superposed theoretical predictions of the linear energy law (recall that traveling waves require $\Delta\psi_i > 0$).

Interaction	$\Delta\psi_1$	$\Delta\psi_2$	v_1	v_2	$\frac{\Delta\psi_1 v_1 + \Delta\psi_2 v_2}{2\gamma}$	E
Linear	0	2	4.5051	4.5051	4.5051	4.5029
	0.5	1.5	5.6130	5.6130	5.6130	5.6146
	1	1	7.2538	5.6741	6.4640	6.4114
	1.5	0.5	8.1123	3.1141	6.8628	6.8637
	2	0	8.5710	0.0307	8.5710	8.5760
Hyperelastic	0	2	1.4241	1.4240	1.4241	1.4231
	0.5	1.5	1.7733	1.7732	1.7732	1.7697
	1	1	2.2778	1.7762	2.0270	2.0089
	1.5	0.5	2.5308	0.9760	2.2421	2.1424
	2	0	2.6660	0.0132	2.6660	2.6670
Coulombic	0	2	0.9434	0.9434	0.9434	0.9429
	0.5	1.5	1.1476	1.1476	1.1476	1.1480
	1	1	1.4635	1.1492	1.3064	1.2964
	1.5	0.5	1.6398	0.6307	1.3875	1.3877
	2	0	1.7454	0.0000	1.7454	1.7464

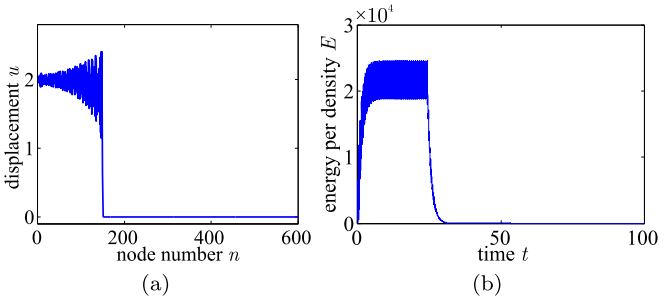

FIG. 5. (a) Displacement profile and (b) kinetic energy when discreteness effects dominate and the wave profile is not smooth ($m = 1000$ with the hyperelastic interaction potential).

transition drags the first along, causing both transitions to move at the same speed. Therefore, for multiple transitions, to preserve single-valuedness of the solution, we conclude that $v_k \geqslant v_{k+1}$, where v_k is the velocity of the kth transition.

IV. DISCRETENESS EFFECTS

Discreteness effects become important in discrete systems when the width w of the transition wave is on the order of the lattice spacing (i.e., $w \sim a$). The continuum limit (14) of the discrete lattice model holds if the wave profile remains smooth. Smoothness is observed if dissipative effects dominate over inertial effects of the lattice ($\alpha^2 \gg mk_0$). However, in case of small dissipation and significant inertia ($mk_0 \gg \alpha^2$), the displacement profile displays rapid oscillations (twinkling modes) [18] in the wake of the traveling kink and the kinetic energy of the wave oscillates with a period $T = a/v$. An example of a weakly dissipative discrete system is shown in Fig. 5. Here, the higher-order terms cannot be neglected when taking the continuum limit and hence the approximation in (9) fails to hold. In such cases, the energy law still applies if the energy E is replaced by its time average

$$\langle E \rangle = \frac{1}{T}\int_{t_0}^{t_0+T} E\,dt' = v\int_{t_0}^{t_0+T}\sum_{i=1}^{N}\frac{1}{2}u_{i,t'}^2\,dt', \qquad (24)$$

where $[t_0, t_0 + T)$ represents one time period. The difference between the maximum energy level and the average energy is a measure of the kinetic energy barrier which is equivalent to the Peierls-Nabarro (PN) barrier that is created due to the discreteness of a lattice [27,28]. As seen from Fig. 5, the energy oscillates about an average value as the wave travels through the lattice, and this average indeed equals the energy computed from the transport law (21).

V. GENERALIZATIONS

A. Nonlinear damping

In case of nonlinear velocity-dependent on-site damping, the governing equation (1) changes into

$$m\,u_{n,tt} + F(u_{n,t}) + \phi'(u_n) - \sum_{j=1}^{N_b}\left[V_j'\left(\frac{u_{n+j}-u_n}{ja}\right) - V_j'\left(\frac{u_n - u_{n-j}}{ja}\right)\right] = 0, \qquad (25)$$

where $F(u_{n,t})$ is a generalized drag force. Following a similar procedure as that of Sec. II A shows that

$$v\,\Delta\psi = -\frac{1}{a}\int_{-\infty}^{\infty} F(-vu_{,\xi})vu_{,\xi}d\xi \simeq \sum_{n=1}^{N} F(u_{n,t})u_{n,t}. \quad (26)$$

The right-hand side represents the total power dissipated by the nonlinear damping and reduces to $2\gamma E$ in the case of linear damping, i.e., for $F(u_{,t}) = \alpha u_{,t}$. As the second law forces the dissipation to constantly drain energy from the system,

$$\sum_{n=1}^{N} F(u_{n,t})u_{n,t} \geqslant 0 \Rightarrow v\,\Delta\psi \geqslant 0. \quad (27)$$

The above result is analogous to the entropy condition in phase boundary propagation [22], where $\Delta\psi$ is the driving force on the phase front. Therefore, the above analysis may be interpreted as a derivation of the entropy condition for phase boundary propagation, in a general case. In the common case of linear damping, the power dissipated is proportional to the kinetic energy transported by the phase boundary. It is interesting to note that for linear on-site damping the dissipation removes only the contribution of the potential energy while preserving the kinetic energy.

B. Higher dimensions

Even though formulated in 1D, the above concepts also apply to general plane waves in higher dimensions.

Consider, e.g., the time evolution of the polarization vector $\boldsymbol{p}$, a diffusive phase-field variable, in ferroelectric ceramics. The potential energy density is commonly written as $W = \psi(\boldsymbol{p}) + \frac{\kappa}{2}|\nabla \boldsymbol{p}|^2$ with nonconvex $\psi(\boldsymbol{p})$ and the nonlocal term representing energy stored in ferroelectric domain walls. One often derives the kinetics of domain switching from the gradient flow assumption [29,30] with a drag coefficient γ, i.e.,

$$\gamma\,\dot{\boldsymbol{p}} = -\frac{\delta W}{\delta \boldsymbol{p}} = -\frac{\partial \psi}{\partial \boldsymbol{p}} + \kappa\,\nabla^2 \boldsymbol{p}. \quad (28)$$

Ferroelectric switching is accommodated by the motion of planar domain walls which can be expressed as a plane wave $\boldsymbol{p}(\boldsymbol{x},t) = \boldsymbol{p}(\boldsymbol{x}\cdot\boldsymbol{k} - vt) = \boldsymbol{p}(\xi)$, so that (28) becomes

$$-\kappa\,|\boldsymbol{k}|^2 p_{i,\xi\xi} - v\,\gamma\,p_{i,\xi} + \psi_{,i} = 0, \quad (29)$$

using indicial notation. Thus we recover the general form of governing equation (2). Multiplying by $p_{i,\xi}$ and integrating over time with $p_{i,\xi} = 0$ as $\xi \to \pm\infty$ yields

$$v\,\gamma\int_{-\infty}^{\infty} p_{i,\xi}\,p_{i,\xi}\,d\xi = \Delta\psi, \quad (30)$$

which leads to a restatement of the energy scaling law (21). Here, we observe that the speed of domain walls is related linearly to drag coefficient γ, the energy difference between the domains, and the shape of the domain wall (expressed by the above integral). This derivation also holds true if domain switching in a fully electromechanically coupled fashion is considered (with polarization $\boldsymbol{p}$, electric field $\boldsymbol{e}$, and mechanical strain $\boldsymbol{\epsilon}$ all represented as moving transition waves).

As a second example, consider the complex Ginzburg-Landau equation for Poiseuille flow or reaction-diffusion systems [31],

$$A_{,t} = A + (1+i\alpha)\nabla^2 A - (1+i\beta)|A|^2 A. \quad (31)$$

Applied to plane waves $A(\boldsymbol{x},t) = A(\boldsymbol{k}\cdot\boldsymbol{x} - vt) = A(\xi)$, this leads to the diffusive governing equation

$$(1+i\alpha)|\boldsymbol{k}|^2 A_{\xi\xi} - v\,A_{\xi} + [A - (1+i\beta)|A|^2 A] = 0, \quad (32)$$

which is again of the same type as (2) and can be treated using the above procedures. In summary, even though derived for discrete 1D systems, the applicability of the energy scaling law is more general and applies to plane waves in both discrete and continuous systems.

VI. CONCLUSIONS

We have derived an energy scaling law that applies to general nonlinear dissipative and diffusive lattices as well as to continuous systems, for arbitrary interaction potentials and nonconvex on-site potentials. As a unique feature, linear superposition applies for multiple transitions even though the governing equations are highly nonlinear. Besides its surprising simplicity, the energy law is valuable to extract the speed, mobility, or transported energy of a transition wave from experimental data when only a subset of the latter is known.

ACKNOWLEDGMENTS

N.N. and C.D. acknowledge support from the National Science Foundation (NSF) under Grant No. CMMI-1200319. D.M.K. acknowledges support from the NSF through CAREER Award No. CMMI-1254424.

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