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Prototypical Lattice Model of a Moving Defect: The Role of Environmental Viscosity[1,2]

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Abstract—The goal of this short note is to present a simple discrete micromodel of a moving crystalline defect allowing one to compute in closed form the functional relation between the macroscopic driving force and the velocity of the defect (the kinetic relation). To make the description more realistic, we augmented the Hamiltonian lattice model by adding an environmental viscous dissipation.

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1. INTRODUCTION

In this paper, we study the kinetics of a prototypical lattice defect in media with environmental damping. To emphasize our ideas, we consider the simplest setting: an array of linearly coupled bistable elements. To drive the system, we apply to the elements an external force that creates a bias towards one of the energy wells and makes the propagation of a switching wave (kink) energetically favorable. Our goal then is to compute the relation between the external loading and the velocity of the defect.

Our prototypical model represents a two-well adaptation of the well-known discrete Frenkel–Kontorova (FK) model [Frenkel and Kontorova, 1938]. Following the pioneering work of Weiner [1964], we chose the energy of the bistable springs to be biparabolic with equal elastic moduli. The advantage of this “symmetric” piecewise linear approximation is that it lends itself to fully analytical treatment through a direct Fourier transform. In its original spatially periodic form, the FK model has been used repeatedly for the description of dynamic dislocations (see [Braun and Kivshar, 1998] for a recent review). Typically the system is viewed either as Hamiltonian (e.g., [Atkinson and Cabrera, 1965; Peyrard and Kruskal, 1984; Kresse and Truskinovsky, 2003]) or as overdamped (e.g., [Fath, 1988; Cahn et al., 1999]). The main focus of this paper is on the intermediate case of an underdamped viscous system, which has some features differing from those of any of the limiting cases. Previous numerical work along similar lines was done by Ishioka [1973] and Elmer and Van Vleck [1996]. In the context of fracture mechanics, the effects of viscoelasticity in lattice models have been studied by Slepyan [2002] and Pechenik et al. [2002]. Here we mostly follow the PhD work of Kresse [2002]; in a recent independent study, Carpio and Bonilla [2003] have partially rediscovered some of our results.

The environmental viscosity in the 1-D lattice model can be understood in several ways. Recall that the full 3-D energy of the lattice depends on parameters that have been neglected in our simple model. By focusing on the 1-D setting, we are left with the task of implicitly describing the energy losses due to the “missing” dimensions. The possibility of excluding the corresponding degrees of freedom constitutes the essence of the adiabatic approximation, which can be applied to harmonic oscillations and to vibrations with small anharmonicity. If the motion is fast and the adjustment is not instantaneous, the energy transfer towards the additional degrees of freedom, both atomic and electronic, must be taken into account. The corresponding “losses” in the low-parametric model in the first approximation can be modeled in terms of the bulk viscosity. In addition to such effective viscosity, there are other mechanisms that can damp the motion of defects (e.g., scattering of lattice waves or interaction with impurities) and affect the value of the viscosity constant.

The main result of the paper is a set of exact solutions of the traveling wave problem. The obtained solutions show explicitly how, in a medium with a structure (a discrete lattice), the propagation of a defect proceeds through the autocatalytic development of internal instabilities. This process generates short wave lattice oscillations that carry energy away from the moving front and produces radiative damping even in the Hamiltonian setting (e.g., [Kresse and Truskinovsky, 2003]). Taking environmental damping into account allows us to eliminate the infinite resonances observed in the con-

[1] In memory of V.P. Myasnikov.

[2] The text was submitted by the authors in English.

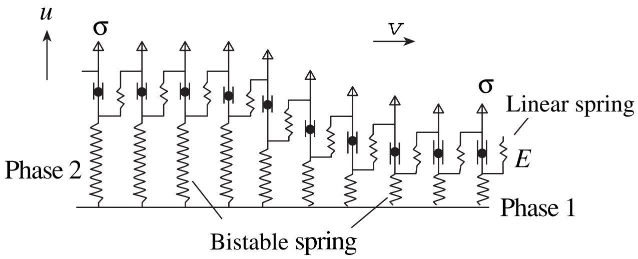

Fig. 1. Schematic configuration of particles around a defect moving to the right with velocity v.

servative setting and makes the resulting kinetic curves look much more realistic.

2. THE MODEL

Consider a highly idealized mechanical model intended to describe a prototypical moving defect. It can be viewed as an array of bistable springs supporting a chain of particles with harmonic nearest neighbor interactions (Fig. 1). Suppose that $\tilde{u}_n$ is the (vertical) displacement of the particle with the index n from its reference position. The energy $w(\tilde{u}_n)$ of the bistable springs is selected to be piecewise quadratic,

$$w(\tilde{u}_n) = \begin{cases} \frac{1}{2}c\tilde{u}_n^2, & \tilde{u}_n < a/2 \\ \frac{1}{2}c(\tilde{u}_n - a)^2, & \tilde{u}_n > a/2, \end{cases} \tag{1}$$

with equal moduli. To bias one of the energy wells, we introduce an external force per unit length $\tilde{\sigma}$, acting in the direction of the displacement $\tilde{u}_n$ and independent of the position of the particle. The equations of motion take the form

$$\rho\varepsilon\ddot{\tilde{u}}_n - E\varepsilon^{-1}(\tilde{u}_{n+1} - 2\tilde{u}_n + \tilde{u}_{n-1}) + \tilde{\alpha}\dot{\tilde{u}}_n = \begin{cases} \varepsilon(\tilde{\sigma} - c\tilde{u}_n), & \tilde{u}_n < a/2 \\ \varepsilon[\tilde{\sigma} - c(\tilde{u}_n - a)], & \tilde{u}_n > a/2, \end{cases} \tag{2}$$

where ε is the reference length of the linear springs, which will be considered a small parameter; E is the corresponding elastic modulus; and ρ is the mass density per unit spring length. To make the description more realistic, we have also included viscous dissipation due to the surrounding medium.

Consider next a special class of steady-state motion of the chain in the form of traveling waves moving with the prescribed velocity $\tilde{v}$. This means $\tilde{u}_n(t) = \tilde{u}(\varepsilon n - \tilde{v}t)$. We also assume that all springs located at $\tilde{x} > 0$ are in one energy well (phase 1) and all springs located at $\tilde{x} < 0$ are in the other energy well (phase 2). Then, by using nondimensional variables

$$x = \frac{\tilde{x}}{\varepsilon}, \quad u = \frac{\tilde{u}}{a}, \quad v = \tilde{v}\sqrt{\frac{\rho}{E}}, \quad \sigma = \frac{\tilde{\sigma}}{ac}, \tag{3}$$

we obtain the following equation:

$$v^2\frac{d^2u}{dx^2} - [u(x+1) - 2u(x) + u(x-1)] - \alpha v\frac{du}{dx} + \Omega_0^2[u(x) - \sigma] - H(-x)\Omega_0^2 = 0, \tag{4}$$

where $H(x)$ is the Heaviside function, $H(x) = 0$ for $x < 0$, and $H(x) = 1$ for $x > 0$. The main dimensionless parameters of the problem are

$$\Omega_0 = \varepsilon\sqrt{\frac{c}{E}}; \quad \alpha = \frac{\tilde{\alpha}}{\sqrt{E\rho}}. \tag{5}$$

For consistency of the model, we must require that

$$u(0) = 1/2, \tag{6}$$

and

$$u(x) < 1/2, \quad x > 0; \quad u(x) > 1/2, \quad x < 0. \tag{7}$$

Configurations of the chain at $x = \pm\infty$ must correspond to the (trivial) static equilibrium, where all particles are in either one or the other well. By selecting the two limiting states in different wells, we obtain the following boundary conditions:

$$u(x) \longrightarrow \begin{cases} \sigma, & x \longrightarrow \infty \\ 1 + \sigma, & x \longrightarrow -\infty. \end{cases} \tag{8}$$

3. ANALYTICAL SOLUTION

Equation (4) is linear and can be solved by the Fourier transform. We omit the details of the method, which are straightforward, and write the solution in the form

$$u(x) = \sigma - \frac{\Omega_0^2}{2\pi i}\int_\gamma \frac{e^{ikx}}{kN(k)}dk, \tag{9}$$

where the contour γ goes along the real axis and passes above the singularity at the origin. The zeros of the function

$$N(k) = \Omega_0^2 + 4\sin^2\frac{k}{2} - v^2k^2 - ik\alpha v \tag{10}$$

define the wave numbers contributing to the solution (the dispersion spectrum). In terms of those wave numbers, we can write

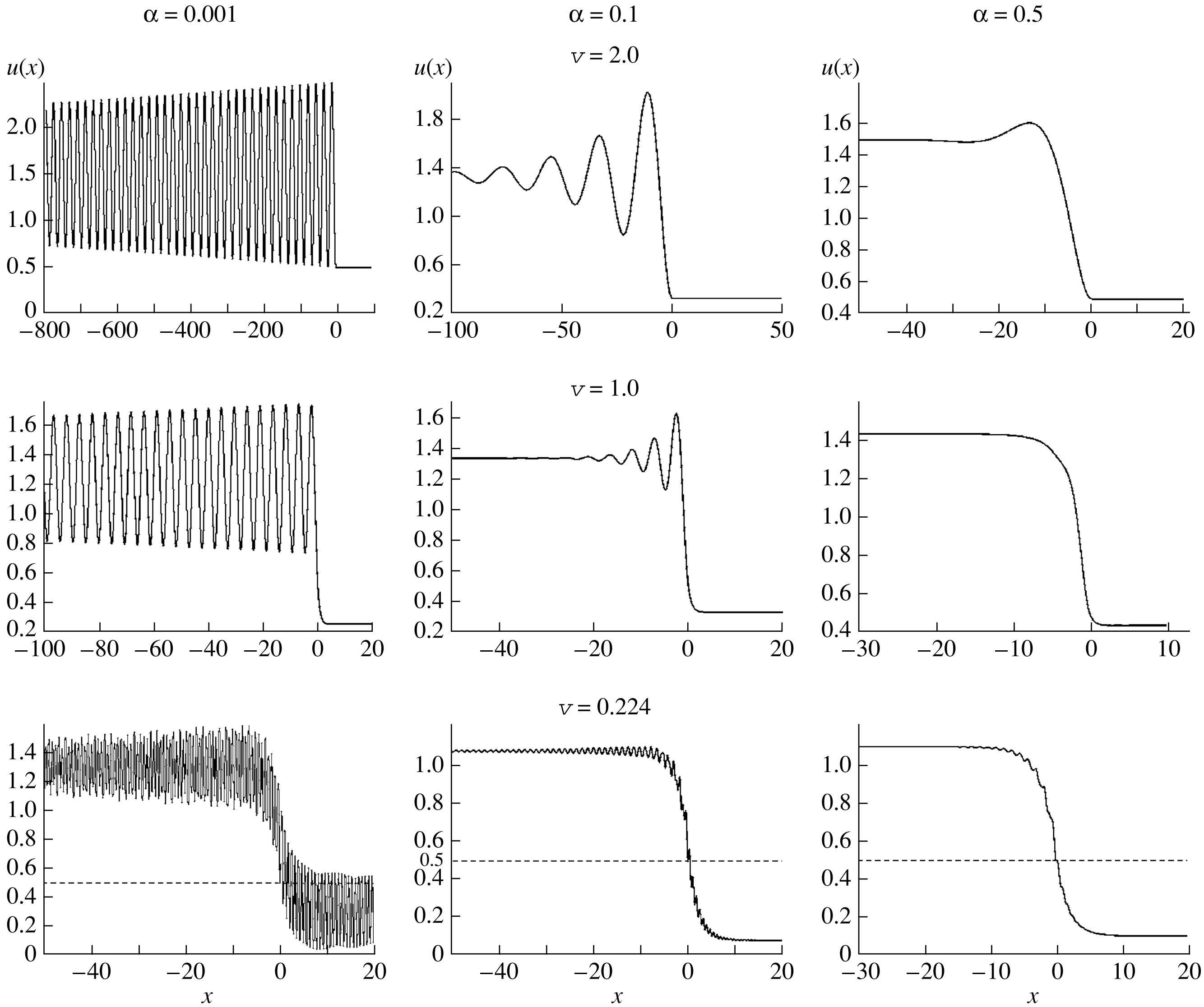

Fig. 2. Comparison of the displacement profiles at different α and v.

$$u(x) = \begin{cases} \sigma - \Omega_0^2 \sum_{\tilde{M}_+} \frac{e^{ikx}}{kN'(k)}, & x > 0 \\ \sigma + 1 + \Omega_0^2 \sum_{\tilde{M}_-} \frac{e^{ikx}}{kN'(k)}, & x < 0, \end{cases} \quad (11)$$

where

$$\tilde{M}_+ = \{k: N(k) = 0, \mathrm{Im}k > 0\},$$
$$\tilde{M}_- = \{k: N(k) = 0, \mathrm{Im}k < 0\}. \quad (12)$$

To explicitly compute solution (11), we need to find the applied force σ corresponding to the given value of the velocity v. The structure of displacement field (11) at different values of α is shown in Fig. 2. Comparing these figures with the corresponding figures for the case where $\alpha > 0$ [Kresse and Truskinovsky, 2003], one observes that the motion is damped at ±∞. We can also conclude that the inclusion of damping makes the interval of admissible velocities wider. For instance, by analyzing the displacement field near the core region of the defect at $0.130 < v < 0.248$ and $\alpha = 0.001$, one can show that most solutions in this interval of velocities are not admissible. If we increase the value of α, the domain of nonexistence of a solution becomes narrower. In a separate publication, we will show that, above some critical value of viscosity, the traveling wave solution becomes admissible in the whole range of velocities.

The relation between the applied force and the velocity of the phase boundary can be obtained from the condition $u(0) = 1/2$. It gives

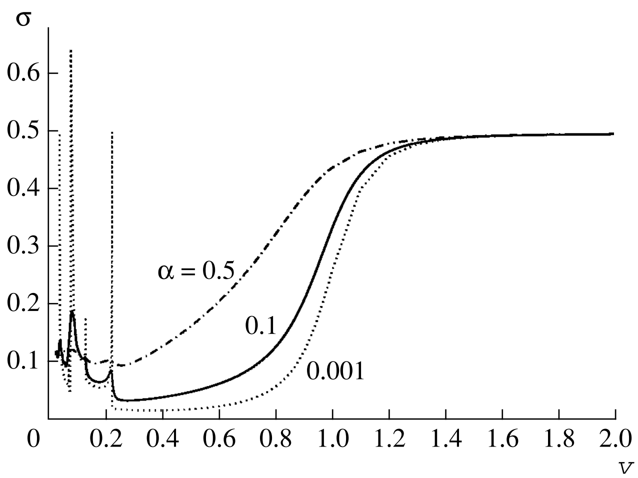

Fig. 3. Applied force as a function of velocity for different values of viscosity α ($\Omega_0 = 0.5$).

$$\sigma = \frac{1}{2} + \Omega_0^2 \sum_{\tilde{M}_+} \frac{1}{kN'(k)}. \qquad (13)$$

Representative force–velocity relations are shown in Fig. 3. One can see that an increase in α leads to the smoothening of the resonances at critical velocities. One can also observe that the limiting behavior of the force–velocity relation at $v \longrightarrow \infty$ and $v \longrightarrow 0$ does not depend on the value of α and is the same as in the case without damping. More precisely, when $v \longrightarrow \infty$, the force for every value of α tends to the ultimate threshold $\sigma \longrightarrow \sigma_0 = 1/2$. Similarly, when $v \longrightarrow 0$, we have $\sigma \longrightarrow \sigma_p$, where σ_p is the Peierls force for our system, computed, for instance, in Kresse and Truskinovsky [2003].

4. CONCLUSIONS

In this paper, we presented an exact solution of a two-well adaptation of the FK model illustrating the role of environmental viscosity on the steady-state propagation of a generic lattice defect. Following some previous work on fracture and plasticity, we used piecewise quadratic approximation for the on-site potential, which allowed us to apply the Fourier method and to construct an explicit solution of the discrete problem in the form of a traveling wave. The relation between the applied force and the velocity of the defect was shown to be influenced by the viscous properties of the material. In particular, as expected, the introduction of damping replaced the infinite resonances of the applied force by finite peaks.

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