Beyond kinetic relations

Lev Truskinovsky * Anna Vainchtein †

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Abstract

We introduce the concept of kinetic equations representing a natural extension of the more conventional notion of a kinetic relation. Algebraic kinetic relations, widely used to model dynamics of dislocations, cracks and phase boundaries, link the instantaneous value of the velocity of a defect with an instantaneous value of the driving force. The new approach generalizes kinetic relations by implying a relation between the velocity and the driving force which is nonlocal in time. To make this relations explicit one needs to integrate the system of kinetic equations. We illustrate the difference between kinetic relation and kinetic equations by working out in full detail a prototypical model of an overdamped defect in a one-dimensional discrete lattice. We show that the minimal nonlocal kinetic description containing now an internal time scale is furnished by a system of two ordinary differential equations coupling the spatial location of defect with another internal parameter that describes configuration of the core region.

Keywords: martensitic phase transitions, lattice dynamics, kinetic relations, kinks, defects, quasicontinuum models, dispersion, nonlinear waves

1 Introduction

Kinetic relations attributing a particular value of velocity to a given value of the driving force are widely used in continuum mechanics as a constitutive description of such lattice defects as phase boundaries, dislocations and cracks (see the reviews [2, 15, 26, 28]). These algebraic relations form independent postulates that serve as closing conditions specifying

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* Laboratoire de Mécanique des Solides, CNRS-UMR 7649, Ecole Polytechnique, 91128, Palaiseau, France
† Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15260
singular solutions in the classical continuum theories. Since kinetic relations replace the
detailed modeling of the core regions of the defects, they represent a condensed description
of the complex physical behavior at the microscale. In practice, kinetic relations are either
taken from experiment or deduced from the solutions of auxiliary microscale problems.
Characteristically, these auxiliary problems always assume constant values of both the
macroscopic velocity of the defect and of the corresponding driving force.

Due to the implicit assumption that the defect is in a steady motion, the kinetic
relations-based description misses the details of a nonsteady internal dynamics of the core
region. In particular, the internal pulsations originating from the defect interaction with
localized micro-inhomogeneities become averaged out. This is in contradiction with the
presence of accelerated motions of defects at all scales, as revealed, for instance, by the
power law acoustic emission accompanying plasticity, martensitic phase transitions and
fracture (e.g. [21]).

To partially recover the missing information we propose in this paper to replace alge-
braic kinetic relations by differential *kinetic equations*. The aim of these equations is to
capture the transient phases of the defect evolution in response to nonsteady driving. In
the language of constitutive theory we propose to replace the instantaneous rheological
relations on the phase boundary by nonlocal memory functionals originating from a local
description in terms of internal variables. Such extension brings into the conventional
theory an internal time scale and allows one to deal with the so-called “rate effects”. An
example of a similar development is provided by the rate-dependent constitutive laws in
the theory of friction, where the set of internal state variables is also assumed to satisfy
differential constitutive relations (e.g. [31, 32]).

In order to show the possibility of a systematic derivation of kinetic equations from
a micromodel we consider a prototypical overdamped defect moving in a lattice. We de-
velop a low-parametric description of the internal dynamics of this defect involving some
specially selected internal variables which characterize the structure of the core region.
Our approach can be viewed as an example of a quasicontinuum method in the sense of
[4, 27, 35] whose goal is to match the macroscopic continuum description outside singular-
ities with a more detailed atomistic resolution of the core regions. The zero-order model
of this type produces kinetic relations and implies instantaneous and universal response
of the core region to external perturbations (autonomous core region). The first-order ap-
proximation leads to kinetic equations which already capture some nonuniversal features
of the microscopic dynamics. For consistency of the two approximations, kinetic equa-
tions must of course reduce to the kinetic relation when the variation of the macroscopic
parameters is sufficiently slow.

To illustrate the main idea of our approach consider a toy model describing an over-
damped dynamics of a configurational point in a one-dimensional energy landscape:

\[
\frac{\partial \nu}{\partial \tau} = -\frac{\partial \Phi(\nu; G(t))}{\partial \nu}.
\]  

(1)

Here \( \nu \) is a variable defining the microstate of the system and \( G(t) \) is a sufficiently slow varying macroscopic driving force which depends on slow time \( t \). The fast time is defined as \( \tau = t/\epsilon \), where \( \epsilon \ll 1 \) is a small parameter. We assume that the gradient of the energy landscape \( \Phi(\nu; G) \) is periodic in \( \nu \). The method of kinetic relations postulates the existence of an algebraic relation between the driving force \( G \) and the macroscopic velocity

\[
V(t) = \left\langle \frac{\partial \nu}{\partial \tau} \right\rangle_{\tau} = \lim_{\epsilon \to 0} \epsilon \int_{0}^{1/\epsilon} \frac{\partial \nu}{\partial \tau} d\tau.
\]

(2)

Such relation, which we write as \( V(t) = \Gamma(G(t)) \), can be computed explicitly if \( G \) is a tilt of the energy landscape

\[
\Phi(\nu; G) = G_P \cos \nu - G \nu.
\]

(3)

Then a direct computation gives (e.g. [14, 11])

\[
V = \Gamma(G) = \begin{cases} 
0 & |G| \leq G_P \\
\text{sgn}(G - G_P) \sqrt{G^2 - G_P^2} & |G| \geq G_P.
\end{cases}
\]

(4)

In the realistic situations the microscopic description of the type (1) is too complex because it involves a huge number of variables. In contrast, the macroscopic description (4) is too schematic and cannot be trusted when one deals with the problems where slow and fast time scales cannot be separated. This point has been often overlooked, and kinetic relations implying a universal elimination of microscopic variables were used in situations where both \( G \) and \( V \) are changing fast as, for instance, in the case of pinning-depinning phenomena.

In what follows we present a detailed adaptation of the above ideas to the case of a martensitic phase transition. Martensitic phase boundaries are particularly convenient for the demonstration of the main principles of our approach because these plane defects may be adequately represented already in one-dimensional models. To emphasize ideas we consider the simplest case of a phase boundary with overdamped dynamics. At the microscale, the analysis of the non-steady evolution of the core region of such phase boundaries requires a study of a dynamical system with an infinite number of degrees of freedom. At the macroscale the phase transition is modeled as a singular surface (jump discontinuity) whose evolution is governed by a kinetic relation [36].

We pose the question of whether an intermediate description is possible when the interface is equipped with a small number of “mesoscopic” degrees of freedom whose dynamics
reproduces the main transient effects. An early example of such a reduced description can be found in the theory of dislocations where static defects are often represented as effective particles in the Peierls-Nabarro (PN) landscape [7]. The static PN landscape is obtained by relaxing all microscopic variables other than one collective variable interpreted as the macroscopically observable location of the core. The idea of a tilted PN landscape has been heuristically applied to the description of dynamic dislocations in close to continuum limit [12, 16, 17, 18, 19, 25, 30, 43]. This approach, however, cannot be used in principle in the strongly discrete case when the dislocation core is atomically narrow [13, 20]. In order to deal with this limit it is natural to abandon the idea of macroscopic collective variables and trace instead the dynamics of the particular discrete elements while again enslaving all others. Such elements were called “localized normal modes” in [42] and “active points” in [23]. In some special cases it has been proven rigorously that dynamics of “active points” corresponds to the motion along the center manifold of the infinite-dimensional dynamical system [9].

In this paper we extend the approach of “active points” from the immediate vicinity of the depinning point where it has been formally justified to a broader class of nonsteady motions of defects. The key to our method is the assumption that the dynamics of only a few bonds located in the core region has to be resolved fully. The other bonds remain confined to near bottoms of their respective potential wells, and their small adjustment to the changing conditions can be treated as instantaneous.

The main question confronted by such theory concerns the minimal number of internal variables which is sufficient to capture the response of a defect to a particular class of external perturbations. In this paper we propose to base the selection of the minimal set of internal variables on the careful analysis of the relative “activity” of the variables in the traveling wave solution. As a result, we obtain kinetic equations which describe faithfully only small deviations from such steady states. Strong deviations from the traveling wave ansatz have been rigorously studied for several classes of nonlinear equations in the case of periodic obstacles (pulsating traveling fronts, e.g. [5, 10]). Our approach deals with the singular limit of such problems (localization of the fronts), which, as far as we know, has not yet been studied in the mathematical literature.

In our construction we use essentially the fact that the exact traveling wave solution of our discrete problem is known in the case of a piecewise quadratic interaction potential [40, 41]. Using this solution as a benchmark, we construct a simple two-dimensional dynamical system which in the case of a constant macroscopic driving force generates a remarkably good approximation for the kinetic relation originating from the study of the full infinite-dimensional dynamical system. We then apply this low-parametric description to the case when the driving force is a given function of time and show how it can be used to obtain a rheological model of the transformation kinetics which is nonlocal in time. We also provide an example showing that depending on the rate of external driving
the responses of the phase boundary based on the kinetic relation and on the associated kinetic equations can be markedly different. A systematic application of the obtained kinetic equations to solutions of the particular macroscopic boundary value problems involving strongly inhomogeneous media will be given elsewhere.

The paper is organized as follows. In Section 2 we formulate the singular macroscopic problem which requires a microscopic closure. In search for such a closure we turn in Section 3 to a specific microscopic model. To illustrate the existing methods of model reduction in relation to moving defects, we construct in Section 4 the static PN landscape and then use its tilted version in Section 5 to describe the steady state dynamics of phase boundaries. Since this approach is not satisfactory, we develop in Section 6 a more systematic one-parametric kinetic equation and introduce a concept of dynamic PN landscape. We then find that the one-parametric model is only adequate in the immediate vicinity of the depinning point and proceed in Section 7 with the systematic derivation of the two-dimensional system of kinetic equations. We find that such description works well in the whole interval of admissible velocities. In Section 8 we choose a specific loading program and compare the predictions of the nonlocal model with the predictions based on the classical kinetic relations. Our concluding remarks are collected in Section 9. To make the exposition self-contained, we present in the Appendix a concise derivation of the exact kinetic relation.

2 Macroscopic model

Let \( u(x, t) \) be the one-dimensional continuum displacement field. The macroscopic energy of a bar undergoing martensitic phase transition can be written as

\[
\mathcal{E} = \int \left[ \frac{\rho u_t^2}{2} + \phi(u_x) \right] dx. \tag{5}
\]

Here \( u_t \equiv \partial u / \partial t \) is the macroscopic velocity, \( u_x \equiv \partial u / \partial x \) is the macroscopic strain, \( \rho > 0 \) is the reference mass density, and the energy density \( \phi(u_x) \) is represented by a double-well potential which will be specified later.

The dynamic equation corresponding to the energy (5) is

\[
\rho u_{tt} = (\dot{\sigma}(u_x))_x, \tag{6}
\]

where \( \dot{\sigma}(u_x) = \phi'(u_x) \) is the stress-strain relation. On discontinuities, the equation (6) must be supplemented with the jump conditions. Let \( f_- \) and \( f_+ \) denote the values of \( f(x) \) to the left and to the right of the interface, and introduce the notations \( [f] \equiv f_+ - f_- \) for the jump and \( \{f\} \equiv (f_+ + f_-)/2 \) for the average of \( f \) across the discontinuity. Then the
parameters on a discontinuity must satisfy the classical Rankine-Hugoniot jump conditions

\[ [u_t] + V[u_x] = 0, \quad \rho V[u_t] + [\hat{\sigma}(u_x)] = 0. \]  

(7)

The entropy inequality, which must also hold on the jump, can be written in the form

\[ \mathcal{R} = GV \geq 0, \]  

(8)

where \( \mathcal{R} \) is the rate of energy dissipation and

\[ G = [\phi] - \{\hat{\sigma}(u_x)\}[u_x] \]  

(9)

is the configurational (driving) force. In one-dimensional problems imposing the entropy inequality can remedy local nonuniqueness only in the case of supersonic discontinuities (shock waves). For subsonic phase boundaries one must specify the rate of entropy production as well. This is usually done phenomenologically through the kinetic relation \( G = G(V) \) between the driving force and the velocity [3, 36, 37]. If the microscopic model is known one can instead compute the function \( G(V) \) directly from the microscopic traveling wave solution (e.g. [33, 34, 36, 40, 41]).

Behind the assumption that there exists an algebraic relation between the driving force \( G \) and the velocity \( V \) lies the idea that the width of the transition layer is so small that the internal relaxation to the traveling wave profile takes place much faster than the variation of the driving force. However, the convergence to the sharp interface limit is expected to be nonuniform with respect to the parameter describing the rate of configurational loading. For instance, if the phase boundary interacts with an obstacle, the structure of this obstacle should be sufficiently diffuse for the algebraic kinetic relation to hold within certain error bars. If the profile of the obstacle is sufficiently sharp, the time scales of internal relaxation and of external driving are comparable and the traveling wave profile is not an adequate ansatz. In this case one can expect a uniform double-parametric asymptotics in the spirit of [6] to be more complex than is assumed by the computations based on the traveling waves.

In what follows we do not attempt a rigorous asymptotic analysis in the general situation and instead choose a simple microscopic model and formally derive a set of differential kinetic equations describing the transient response for the inner structure of a phase boundary.

### 3 Microscopic model

Consider an infinite chain of particles, connected to their nearest neighbors (NN) through viscoelastic springs and to their next-to-nearest neighbors (NNN) by elastic springs (see
Figure 1: The discrete microstructure with viscoelastic nearest and elastic next-to-nearest-neighbor interactions.

Suppose that in the undeformed configuration the NN and NNN springs have lengths $\varepsilon$ and $2\varepsilon$, respectively. Let $u_n(t)$ denote the displacement of $n$th particle at time $t$ with respect to the reference configuration. We associate with the deformation of $n$th NN spring a discrete measure of strain

$$w_n = \frac{u_n - u_{n-1}}{\varepsilon}. \quad (10)$$

For the viscoelastic NN springs we assume the following constitutive relation:

$$f_{\text{NN}}(w, \dot{w}) = \phi_{\text{NN}}'(w) + \xi \dot{w}, \quad (11)$$

where $\xi > 0$ is the viscosity coefficient. To describe domain boundaries the function $\phi_{\text{NN}}(w)$ must be at least a double-well potential; to obtain explicit solutions, we assume that this function is biquadratic:

$$\phi_{\text{NN}}(w) = \begin{cases} 
\frac{1}{2} \mu w^2, & w \leq w_c \\
\frac{1}{2} \mu (w - a)^2 + \mu a \left( w_c - \frac{a}{2} \right), & w \geq w_c.
\end{cases} \quad (12)$$

Under these assumptions the NN elastic units can be in two different phases, depending on whether the strain is below (phase I) or above (phase II) the critical value $w_c$. The elastic modulus in each phase is $\mu > 0$, and the parameter $a > 0$ measures the transformation strain. To simplify calculations, we assume that the NNN interactions are linearly elastic:

$$f_{\text{NNN}}(\hat{w}) = 2\gamma \hat{w}. \quad (13)$$

Here we defined $\hat{w}_n = (w_{n+1} + w_n)/2$ as the strain in the NNN spring connecting $(n+1)$th and $(n-1)$th particles.

The dynamics of the chain is governed by the following system of ordinary differential equations:

$$\rho \varepsilon \ddot{u}_n = \mu [w_{n+1} - w_n - \theta (w_{n+1} - w_c)a + \theta (w_n - w_c)a] + \gamma (w_{n+2} + w_{n+1} - w_n - w_{n-1}) + \xi (\hat{w}_{n+1} - \hat{w}_n). \quad (14)$$
Here $\rho > 0$ is the mass density of the chain and $\theta(x)$ is the unit step function. To ensure stability of the chain we require that

$$E = \mu + 4\gamma > 0,$$

where $E$ is the homogenized macroscopic elastic modulus; following [38, 39], we also assume that the NNN interactions are of ferromagnetic type, meaning that $\gamma \leq 0$. In the limit $\varepsilon/L \to 0$, where $L$ is a macroscopic length scale, we recover (6) with the homogenized stress-strain law [41]

$$\hat{\sigma}(w) = E(w - \Delta \theta(w - w_c)).$$

Here $\Delta$ is the macroscopic transformation strain:

$$\Delta = \frac{a\mu}{E}. \quad (16)$$

There are two time scales associated with this problem: the time scale of inertia, $T_{in} = \varepsilon \sqrt{\rho/E}$, and the viscosity time scale, $T_{visc} = \xi/E$. In this paper we consider the overdamped limit when $T_{visc} >> T_{in}$, i.e.

$$\xi >> \varepsilon \sqrt{\rho E}. \quad (17)$$

We can nondimensionalize the problem using $T_{visc}$ as the time scale and letting

$$\bar{t} = \frac{tE}{\xi}, \quad \bar{u}_n = \frac{u_n}{\Delta \varepsilon}, \quad \bar{w}_n = \frac{w_n}{\Delta}, \quad \bar{w}_c = \frac{w_c}{\Delta}. \quad (18)$$

Dropping the bars on the new variables, we obtain dimensionless system equations:

$$\dot{w}_n - \dot{w}_{n+1} + 1 = \hat{\sigma}(w_{n+1}) - \hat{\sigma}(w_n) + \hat{D}(w_{n+2} + w_{n+1} - w_n - w_{n-1}), \quad (19)$$

where

$$\hat{\sigma}(w) = w - \theta(w - w_c) \quad (20)$$

is the rescaled macroscopic stress-strain law. The dimensionless parameter

$$D = -\frac{\gamma}{E} \geq 0 \quad (21)$$

measures the relative strength of NN and NNN interactions. In what follows it will also be interpreted as a measure of coupling of the bistable units.

Observe that system (19) can be “integrated”, yielding

$$\dot{w}_n = D(w_{n+1} - 2w_n + w_{n-1}) - \hat{\sigma}(w_n) + \sigma. \quad (22)$$
Here $\sigma = \sigma(t)$ is the time-dependent applied stress. One can see that (22) also governs the overdamped Frenkel-Kontorova model [9, 11, 22, 24]; a subtle but important distinction of the present setting is that here the coupling coefficient $D$ is independent of $\varepsilon$.

In the overdamped limit the macroscale governing equations (6) reduce to $(\sigma'(u_x))_x = 0$, or $\sigma(u_x) = \sigma(t)$, while the jump conditions take the form $[\sigma'(u_x)] = 0$ [11]. The driving force (9) is then a function of time:

$$G(t) = \sigma(t) - \sigma_M,$$

where

$$\sigma_M = w_c - 1/2$$

is the Maxwell stress. The function $G(t)$ also enters the microscopic equation (22) which can be rewritten in the gradient-flow form

$$\dot{w} = -\nabla W(w; G(t)).$$

Here $w \in \mathbb{R}^\infty$ is the vector of strains, the gradient is taken with respect to $w$, and

$$W = \sum_{n=-\infty}^{\infty} \left( \frac{1}{2} w_n^2 - (w_n - w_c)\theta(w_n - w_c) + D(w_{n+1} - w_n)^2 - (\sigma_M + G(t)) w_n \right),$$

is the dimensionless energy of the system.

Our main goal will be to approximate the infinite-dimensional dynamical system (24) by a finite-dimensional reduced dynamical system of the type

$$\dot{\nu} = -\alpha \nabla \Phi(\nu; G(t)),$$

where $\alpha$ is the effective mobility matrix. The gradient is taken with respect to the order parameter $\nu \in \mathbb{R}^K$ where the integer-valued parameter $K$ defines the dimensionality of the reduced system. After the solution of the vector equation (24) is known, the approximation of the discrete field (24) should be recoverable from the auxiliary relations $w_n(t) = w_n(\nu_1(t), \ldots, \nu_K(t))$ describing the recovery of relaxed “non-order-parameter” variables.

In the absence of a rigorous method condensing (24) to (26) we base our formal reduction on the detailed study of a traveling wave solution of (24) in the form $w_n(t) = w(n - V t)$. This solution, which is known explicitly (see Appendix), corresponds to the case when $G(t) = \text{const}$ and describes a steadily propagating phase boundary. We emphasize that in our method the $G = \text{const}$ solution is used only to suggest the dimensionality of the reduced system, while the actual behavior of the resulting dynamical system is fully driven by the time-dependent $G(t)$.
4 Classical PN landscape

The simplest one-parametric ($K = 1$) reduction of the infinite-dimensional system (24) is based on the idea of Peierls-Nabarro (PN) energy landscape which was first developed for dislocations (see the review [29]) and then generalized to phase boundaries in [38]. The construction is fully static and therefore restricted to the case of sufficiently small $G$. Since the ideas behind the construction of the PN landscape are used later to obtain the approximate kinetic equations, we outline the main steps below; see [38] for more details.

Assume that $G = \sigma - \sigma_M = \text{const}$ and compute stable monotone solutions of the equilibrium difference equations (24). For the phase boundary located at $n = m$ we obtain (see also [11, 16]):

$$w_m^m(G) = \sigma_M + \begin{cases} G + 1 - \frac{\exp(\lambda(n - m - 1/2))}{2 \cosh(\lambda/2)}, & n < m \\ G + \frac{\exp(-\lambda(n - m - 1/2))}{2 \cosh(\lambda/2)}, & n \geq m, \end{cases}$$

(27)

where

$$\lambda(D) = \text{arccosh}\left(1 + \frac{1}{2D}\right).$$

(28)

The admissibility constraints

$$w_n^m \geq w_c \quad \text{for } n \leq m, \quad w_n^m \leq w_c \quad \text{for } n \geq m + 1$$

(29)

determine the constraints on $G$; the set of driving forces satisfying these constraints constitutes the trapping region. One can show that for $D > 0$ the strain profile (27) is monotone, so the constraints (29) can be replaced by $w_n^m \geq w_c$ and $w_n^{m+1} \leq w_c$. The trapping region is then given by

$$|G| \leq G_P,$$

(30)

where

$$G_P(D) = \frac{1}{2} \tanh \frac{\lambda}{2} = \frac{1}{2 \sqrt{1 + 4D}}$$

(31)

is the desired expression for the Peierls threshold [8, 38].

One can see that at $|G| \leq G_P$ the phase boundary can be in an infinite number of stable equilibrium configurations (27) parameterized by $m$. In order to connect these stable states one needs to consider a path involving non-equilibrium intermediate configurations. For instance, take two equilibrium configurations, one with the phase boundary located at $n = i - 1$ and the other one at $n = i$. Suppose that phase II is located behind the phase boundary and consider all paths connecting the two equilibria along which the $i$th NN spring is the only one that changes phase, while all other springs stay in their respective
energy wells. As the \( i \)th NN spring crosses the critical value of strain \( w_c \) the system goes through an energy barrier and the next task is to select the path that involves the minimal barrier.

To this end we fix \( w_i \) and minimize the energy of the chain with respect to all strains \( w_k \) with \( k \neq i \). We obtain:

\[
(1 + 2D)w_k - D(w_{k+1} + w_{k-1}) = \sigma_M + \begin{cases} 
G + 1, & k \leq i - 1 \\
G, & k \geq i + 1.
\end{cases}
\] (32)

Solving equations (32) at \( k \leq i - 1 \) and \( k \geq i + 1 \) and requiring that the corresponding solutions, when extended to \( k = i \), both equal \( w_i \), we obtain the following strains along the path connecting the two equilibrium states:

\[
w_k = \sigma_M + \begin{cases} 
G + 1 + e^{\lambda(k-i)}(w_i - \sigma_M - G - 1), & k \leq i \\
G + e^{-\lambda(k-i)}(w_i - \sigma_M - G), & k \geq i.
\end{cases}
\] (33)

At the saddle point \( w_i = w_c \) the energy reaches its maximal value; due to the nonsmoothness of the biquadratic potential at \( w = w_c \), the corresponding states are singular.

The next step is to construct a global path that connects not just two but all equivalent equilibrium points. To this end we replace the order parameters \( w_i \) which were operative in the consecutive segments of the path by a global order parameter \( \nu \) defined implicitly by

\[
w_{[\nu]} = w^*(\nu) = \sigma_M + G + \frac{\exp(-\lambda/2)}{2 \cosh(\lambda/2)} + (\nu - [\nu]) \tanh(\lambda/2).
\] (34)

Here \([\nu]\) denotes the integer part of \( \nu \). At the integer values of \( \nu \) we have \( w_{[\nu]} = w_L \), and as \( \nu \) approaches \([\nu] + 1\) from below, \( w_{[\nu]} \) linearly increases to \( w_U \). The function \( w^*(\nu) \) is periodic with period 1 and has jump discontinuities at \( \nu = [\nu] \). One can see that \( \nu \) can be interpreted as the macroscopic location of the interface.

Using (34) and recalling (33), we obtain strains along the path that are now parametrized by \( \nu \):

\[
w_k = \sigma_M + \begin{cases} 
G + 1 + e^{\lambda[k-[\nu]}(w^*(\nu) - \sigma_M - G - 1), & k \leq [\nu] \\
G + \frac{\exp(-\lambda(k-[\nu]))}{2 \cosh(\lambda/2)}(w^*(\nu) - \sigma_M - G), & k \geq [\nu].
\end{cases}
\] (35)

To evaluate the energy \( W \) along the path (35) we first renormalized it as \( \Phi(\nu; G) = W(\nu) - W(0) \). Substituting (35) in (25), we obtain (recall that \( 0 \leq G \leq G_P \)):

\[
\Phi(\nu; G) = G_P(\nu - [\nu])^2 - G[\nu] - (G - G_P + 2(\nu - [\nu])G_P)\theta(\nu - [\nu] - \frac{G_P - G}{2G_P}).
\] (36)
Figure 2: One-dimensional energy landscape $\Phi(\nu; G)$ at $D = 0.5$ and different $G$. The classical static PN landscape corresponds to $G \leq G_P$. The dynamic potential above the Periels threshold $G > G_P$ was constructed using the $K = 1$ approximation.

Observe that the minima of the resulting PN landscape $\Phi(\nu; G)$ are located at the integer values of $\nu$ and correspond to stable equilibrium states, while the singularities at $\nu = \nu_i$ represent unstable equilibria (saddle points) where $w_i(\nu_i) = w_c$ (see Fig. 2). The energy barriers separating equilibria at $\nu = i$ and $\nu = i + 1$ are independent of $i$:

$$\Phi(\nu_i) - \Phi(i) = \frac{(G_P - G)^2}{4G_P}.$$ 

At $G = G_P$ the stable equilibria become marginally stable; see the curve $G = G_P$ in Fig. 2. Above the Peierls threshold ($G_P < G < G_S$), the stable equilibria cease to exist, and the above construction of the PN landscape becomes invalid.

5 Dynamics on a tilted PN landscape

One very heuristic but rather common way to extend the idea of the PN landscape to dynamics is to take the classical PN landscape at $G = 0$ and tilt it to account for nonzero $G$. Then one can obtain an approximate kinetic relation by considering the overdamped motion of a material point on this tilted landscape and studying the dependence of the average velocity on the driving force $[7]$.

The tilted PN landscape can be defined as follows

$$\Phi_T(\nu; G) = \Phi(\nu + 1/2; 0) - G\nu - \frac{G_P}{4},$$

(37)

where we have added a constant to ensure that $\Phi_T(0; G) = 0$. It is not hard to see that at $G \leq G_P$ the energy (36) agrees with (37) up to the appropriate shifts in horizontal and
Figure 3: (a) The tilted energy landscape (grey) and the DPN landscape for $K = 1$ (black) at $D = 0.5$. The two landscapes coincide at $G = G_P$. (b) The exact kinetic relation $G(V)$ from the Appendix (solid curve) and its approximations via the tilted landscape (grey curve), $K = 1$ approximation (dotted curve) and $K = 2$ approximation (dashed curve).

vertical directions:

$$
\Phi\left(\nu + \frac{G_P - G}{2G_P} ; G \right) - \frac{(G_P - G)^2}{4G_P} = \Phi_T(\nu; G), \quad 0 \leq G \leq G_P.
$$

Note that the two landscapes coincide exactly only at the Peierls threshold. Indeed, in the actual PN landscape [36] the local energy minima are always located at the integer values of $\nu$, reflecting the fact that in a discrete system position of a phase boundary always coincides with a lattice point. As $G$ approaches the value $G_P$ the points of local maxima of the PN landscape also move towards integer values and eventually the minimum and maximum points merge. Meanwhile, in the case of the tilted PN landscape [37] the local maxima are always fixed at the integer values, and the minimum points move instead.

Despite these deficiencies, the tilted PN landscape has a strong advantage: it can be formally extended beyond the Peierls threshold $G = G_P$. One can then try to model the dynamics of a phase boundary by the overdamped motion of a particle in the tilted landscape (see the grey curve in Figure 3a). The equation of motion takes the form

$$
\dot{\nu} = -\alpha \Phi_T'(\nu; G) = -\alpha (2G_P(\nu - \lceil \nu \rceil - 1/2) - G).
$$

Solving this equation subject to the condition $\nu([Vt]/V) = [Vt]$ yields

$$
\nu(t) = [Vt] + \frac{G + G_P}{2G_P} \left(1 - e^{-2\alpha G_P(t-[Vt]/V)}\right).
$$
Imposing the periodicity condition \( \nu(([Vt] + 1)/V) = [Vt] + 1 \), we obtain the desired kinetic relation

\[
G(V) = G_P \frac{1 + e^{-2\alpha G_P/V}}{1 - e^{-2\alpha G_P/V}}.
\]  

(38)

As expected, it gives the correct limit \( G \to G_P \) when \( V \to 0 \). However, in contrast to the exact kinetic relation obtained in the Appendix (see (85)) the function (38) is unbounded: at large \( V \) it grows as \( G(V) \approx V/\alpha \) (see Figure 3b). In addition, since the physical meaning of the dynamic variable \( \nu(t) \) is obscure, it is not clear how one can recover the strains \( w_n(t) \). We therefore abandon this heuristic path and search for a more adequate representation of the actual dynamics of the chain.

6 Reduced model with one internal variable

We now take a more systematic point of view, choose a single variable and follow its exact dynamics while minimizing the energy with respect to all remaining variables. The resulting model is similar to the “single-active-site theory” of [9, 23].

6.1 \( K = 1 \) model

Suppose that \( G = \text{const} \) and assume that the motion in the reduced system is periodic. Assume also that during each period dynamics of only a single NN spring, located right behind the phase transition front and actually changing the energy well during this period, needs to be traced in all the detail, while all other springs can be “enslaved”. We can always assume that at \( t = 0 \) the 0th NN spring has just switched to phase II: \( w_0(0) = w_c \).

Therefore, during the time period \( 0 \leq t < 1/V \) the “active strain” is \( w_0 \). Minimizing the energy with respect to all other strain variables, we obtain

\[
w_n = w_c - 1/2 + G + \begin{cases} 
1 + (w_0 - w_c - G - 1/2)e^{\lambda n}, & n \leq 0 \\
(w_0 - w_c - G + 1/2)e^{-\lambda n}, & n \geq 1.
\end{cases}
\]  

(39)

Substituting these expressions in (22) for \( n = 0 \), we obtain a single equation governing the dynamics of the active point:

\[
\dot{w}_0 = -w_0\{1 + 2D(1 - e^{-\lambda})\} + w_c + G + 1/2 + 2D(G + w_c)(1 - e^{-\lambda}).
\]  

(40)

6.2 \( K = 1 \) kinetic relation

To see whether the ensuing dynamics is compatible with the exact kinetic relation (85) in the Appendix, we solve (40) subject to the boundary condition \( w_0(0) = w_c \), obtaining

\[
w_0(t) = w_c + (G + G_P)\left\{1 - \exp\left(-\frac{t}{2G_P}\right)\right\},
\]  

(41)
Then, setting $n = 1$ in (39), we find

$$w_1(t) = w_c + G - G_P - e^{-\lambda}(G + G_P) \exp\left(-\frac{t}{2G_P}\right).$$

The second boundary condition $w_1(1/V) = w_c$ yields the desired approximation of the kinetic relation:

$$G(V) = G_P + \frac{(1 - e^{-\lambda})(G_S - G_P)}{\exp\left(\frac{1}{2G_P V}\right) - \exp(-\lambda)}. \quad (42)$$

Clearly, $G(V) \to G_P$ as $V \to 0$, and in agreement with (35) $G(V)$ tends to the spinodal value $G_S = 1/2$ as $V$ goes to infinity. Note, however, that the asymptotic behavior at small $V$, $G - G_P \sim \exp\left(-\frac{1}{2G_P V}\right)$, differs from the exact asymptotics

$$G - G_P \approx \frac{\sqrt{V}\exp(-1/V)}{\sqrt{4\pi D}}. \quad (43)$$

obtained in [11].

6.3 $K = 1$ dynamic PN landscape

To construct the dynamic PN landscape we need to to patch different segments of the dynamic trajectory into one by introducing a single order parameter. Recall that during each time period $k/V \leq t \leq (k + 1)/V$ the active strain is $w_k(t)$, and the corresponding solution can be obtained by replacing $n$ in the expressions above for $k = 0$ by $n - k$ and $t$ by $t - k/V$. Introduce a new continuous monotonically increasing function $\nu(t)$:

$$\nu(t) = [Vt] + \frac{1 - \exp\left(-\frac{1}{2G_P}(t - \frac{[Vt]}{V})\right)}{1 - \exp(-\frac{1}{2G_P})} = [Vt] + \frac{G + G_P}{(G_S - G)(e^\lambda - 1)} \left\{1 - \exp\left(-\frac{1}{2G_P}\left(t - \frac{[Vt]}{V}\right)\right)\right\}, \quad (44)$$

where $[\nu] = [Vt]$ and note that $\nu(t)$ takes consecutive integer values at the beginning of each time period. Therefore, it is exactly the dynamic extension of the parameter $\nu$ which we used to obtain the static PN landscape. In terms of this new “global” order parameter, we obtain the following expression for an active strain $w_{[\nu]}(t)$ (over the time period $[\nu]/V \leq t \leq ([\nu] + 1)/V$):

$$w_{[\nu]}(t) = w_c + (e^\lambda - 1)(G_S - G)(\nu(t) - [\nu(t)]).$$
Figure 4: (a) Kinetic relations \( G(V) \) for infinite-dimensional dynamics (solid curve), its small-velocity approximation (grey curve) and \( K = 1 \) approximation (dotted curve). (b) Comparison of strain trajectories obtained in the \( K = 1 \) reduced model (dotted curves) and in the original infinite-dimensional model (solid curves). Parameters: \( V = 0.1, D = 0.5, w_c = 1. \)

Time evolution of all strains can be then written in terms of \( \nu \) as

\[
w_n(t) = w_c - \frac{1}{2} + G + \begin{cases} 
1 + \left((e^\lambda - 1)(G_S - G)(\nu(t) - [Vt]) - G - G_S\right)e^{\lambda(n-[Vt])}, & n \leq [Vt] \\
\left((e^\lambda - 1)(G_S - G)(\nu(t) - [Vt]) - G + G_S\right)e^{-\lambda(n-[Vt])} & n \geq [Vt] + 1.
\end{cases}
\] (45)

Now we are in a position to construct the global DPN potential \( \Phi(\nu; G) \) which serves as a landscape for the overdamped dynamics of \( \nu(t) \):

\[
\dot{\nu} = -\alpha \Phi'(\nu; G).
\] (46)

The potential \( \Phi(\nu; G) \) is piecewise quadratic and we can select the coefficient \( \alpha = 1/(4G_P^2) \) to ensure that the function (44) is the solution of (46). As the result, we obtain

\[
\Phi(\nu; G) = G_P \left( (\nu - [\nu])^2 - \frac{2(G + G_P)}{(e^\lambda - 1)(G_S - G)} \nu + [\nu] \right).
\] (47)

---

Although \( \nu(t) \) is by construction a continuous function of time, the strain variables have jump discontinuities at \( t = n/V, n = 1, 2, \ldots \). This is due to the fact that our approximation treats non-active strains as if they were equilibrated and neglects their real dynamics. As a result, at the end of each time period when we switch to the new active strain, the old one has to increase its value discontinuously in order to reach equilibrium with the new active point. The associated jumps can be computed explicitly:

\[
[w_n]_{t=(n+1)/V} = [w_0]_{t=1/V} = w_0(1/V + 0) - w_0(1/V - 0) = 2 \sinh \lambda(G - G_P).
\]
Notice that this potential coincides with the equilibrium PN landscape at $G = G_P$ (see Figure 2).

In Figure 4b we compare the one-dimensional dynamics (46) with the full infinite-dimensional dynamics at $G = \text{const}$ (see Appendix). As expected, the evolution of the active strain is captured quite well, but there is a visible deviation from the actual values for the strains whose adjustment was assumed to be instantaneous. The corresponding kinetic relations are compared in Figure 4a. One can see that the reduced model with $K = 1$ provides a good quantitative approximation of the exact kinetic relation until $V = 0.2$. At higher velocities it deviates substantially from the exact relation, although both tend to the same spinodal limit $G_S$ at infinite $V$. The observed discrepancies in the case $G = \text{const}$ suggest that the reduced model with $K = 1$ is oversimplified and cannot be used as the base for the construction of kinetic equations.

7 Reduced model with two internal variables

To obtain a reduced model which works well in the whole range of admissible velocities, we need to consider more “active points” in the core region of the defect. From Figure 4b one can see that in each period the natural choice for the expanded set of order parameters would be $w_{-1}, w_0$ and $w_1$.

7.1 $K = 2$ model

Assume again that $G = \text{const}$ and minimize the energy with respect to all strain variables other than $w_{-1}, w_0$ and $w_1$. We obtain the following recovery relations

$$w_n = \begin{cases} 
w_{c} + G + 1/2 + (w_{-1} - w_{c} - G - 1/2)e^{\lambda(n+1)}, & n \leq -1 \\
w_0, & n = 0 \\
w_{c} + G - 1/2 + (w_1 - w_{c} - G + 1/2)e^{\lambda(1-n)}, & n \geq 1. 
\end{cases}$$

(48)

Observe that the dynamics of the variables $w_{-1}(t), w_0(t)$ and $w_1(t)$ in (48) is not independent. Indeed, the three active points satisfy the dynamic equations

$$\begin{align*}
\dot{w}_{-1} &= D(w_0 - 2w_{-1} + w_{-2}) - w_{-1} + w_{c} + G + 1/2 \\
\dot{w}_0 &= D(w_1 - 2w_0 + w_{-1}) - w_0 + w_{c} + G + 1/2 \\
\dot{w}_1 &= D(w_2 - 2w_1 + w_0) - w_1 + w_{c} + G - 1/2
\end{align*}$$

(49)

Notice that instead of minimizing out the “enslaved” variables at each value of $G$ we could have also used the tails of the known traveling wave solution (see Appendix). However this leads to very complicated implicit algebraic relations and in the interest of transparency we decided not to pursue this more rigorous approach in this paper.
Substituting the expressions for $w_2$ and $w_{-2}$ from (48) in (49), we obtain

$$
\begin{align*}
\dot{w}_{-1} &= (-2D - 1 + e^{-\lambda}D)w_{-1} + Dw_0 + (w_c + G + 1/2)(1 + D(1 - e^{-\lambda})) \\
\dot{w}_0 &= (-2D - 1)w_0 + Dw_1 + Dw_{-1} + w_c + G + 1/2 \\
\dot{w}_1 &= (-2D - 1 + e^{-\lambda}D)w_{-1} + Dw_0 + (w_c + G - 1/2)(1 + D(1 - e^{-\lambda}))
\end{align*}
$$

(50)

If we now compare the equations governing the dynamics of $w_{-1}(t)$ and $w_1(t)$, we see that they differ only by a constant term in the right hand side. This allows us to reduce (50) to a two-dimensional system for

$$
\begin{align*}
x(t) &= w_0(t), \\
y(t) &= \frac{w_{-1}(t) + w_1(t)}{2}.
\end{align*}
$$

(51)

Note that

$$
w_{\pm 1}(t) = y(t) \pm \frac{1 + D(1 - e^{-\lambda})}{2(1 + D(2 - e^{-\lambda}))} = y(t) \pm \frac{1 - e^{-\lambda}}{2},
$$

where we used (28) to obtain the second equality. The two variables: $x(t)$, describing the dynamics of the transforming spring, and $y(t)$, describing the average strain in the core region, must satisfy the following system of equations:

$$
\dot{x} = (-2D - 1)x + 2Dy + w_c + G + 1/2
$$

(52)

$$
\dot{y} = Dx + (-2D - 1 + e^{-\lambda}D)y + (w_c + G)(1 + D(1 - e^{-\lambda})).
$$

(53)

This system will be used as an approximation of the full infinite-dimensional dynamics.

7.2 $K = 2$ kinetic relation

We first check that the traveling wave solutions of the original system (see Appendix) can be reproduced by the reduced system (52), (53). Such solution must be subjected to the following constraints. First, we must require that

$$
x(0) = w_c,
$$

(54)

a condition that ensures that the 0th NN spring (recall that $x = w_0$) has just transformed to the new phase at $t = 0$. Second, we require that

$$
w_1(1/V) = w_c,
$$

or

$$
y(1/V) = w_c + \frac{1 - e^{-\lambda}}{2}.
$$

(55)
Figure 5: (a) Kinetic relations $G(V)$: infinite-dimensional system $[55]$ (solid curve), its small-velocity approximation $[53]$ (grey curve) and $K = 2$ approximation (dashed curve); (b) Comparison of the strain trajectories obtained in the $K = 2$ model (dashed curves) and in the infinite-dimensional model (solid curves). Parameters: $V = 0.1$, $D = 0.5$, $w_c = 1$.

This means that at $t = 1/V$ the first NN spring reaches the critical strain, marking the end of the period. Finally, periodicity requires that

$$w_1(0) = w_2(1/V).$$

Using $[48]$ at $n = 2$ together with $[55]$, we can see that this boundary condition reduces to

$$w_1(0) = w_c - (G_S - G)(1 - e^{-\lambda}),$$

or

$$y(0) = w_c + G(1 - e^{-\lambda}).$$

Next, by solving the system $[52], [53]$ subject to the initial conditions $[54]$ and $[56]$, we obtain

$$x(t) = w_c + G + G_P + c_1e^{r_1t} + c_2e^{r_2t}$$

$$y(t) = w_c + e^{-\lambda}G_P + \frac{e^{-\lambda}}{4}(c_1(1 + \sqrt{1 + 8e^{2\lambda}})e^{r_1t} + c_2(1 - \sqrt{1 + 8e^{2\lambda}})e^{r_2t}),$$

where

$$r_{1,2} = -\frac{e^\lambda}{4\sinh^2(\lambda/2)}\left(1 + \frac{1}{2}e^{-2\lambda}(1 + \sqrt{1 + 8e^{2\lambda}})\right)$$

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Figure 6: The error in the approximation of the exact kinetic relation $G_{\text{ex}}(V)$ by the reduced models with $K = 1$ and $K = 2$ generating approximate kinetic relation $G_{\text{ap}}(V)$. (note that $r_2 < r_1 < 0$) and

$$c_1 = \frac{(3 + \sqrt{1 + 8e^{2\lambda}})(2G - 1 + e^\lambda(1 + 2G))}{4(1 + e^\lambda)\sqrt{1 + 8e^{2\lambda}}}$$

$$c_2 = \frac{(\sqrt{1 + 8e^{2\lambda}} - 3)(2G - 1 + e^\lambda(1 + 2G))}{4(1 + e^\lambda)\sqrt{1 + 8e^{2\lambda}}}.$$  

The application of the boundary condition (55) yields the desired approximation of the exact kinetic relation:

$$G(V) = G_P + \frac{1 - e^{-\lambda}}{4(1 + e^\lambda)\sqrt{1 + 8e^{2\lambda}}} \left( (1 + 2e^{2\lambda} + \sqrt{1 + 8e^{2\lambda}})e^{r_1/V} + \left( \sqrt{1 + 8e^{2\lambda}} - 2e^{2\lambda} - 1 \right)e^{r_2/V} \right)$$

$$1 - \frac{e^{-\lambda}}{2\sqrt{1 + 8e^{2\lambda}}} \left( (1 + 2e^{2\lambda} + \sqrt{1 + 8e^{2\lambda}})e^{r_1/V} + \left( \sqrt{1 + 8e^{2\lambda}} - 2e^{2\lambda} - 1 \right)e^{r_2/V} \right).$$  

(59)

First we notice that the approximate kinetic relation (59) satisfies the constraint $G(0) = G_P$. Then, as $V$ tends to infinity, $G(V) \to G_S = 1/2$ with the asymptotics $G - G_s \sim \exp(-|r_1|/V)$. The global comparison of the approximate and exact (see Appendix) kinetic relations is presented in Figure 5. One can see that in view of how few degrees of freedom are involved in the approximation, the agreement is remarkable, at least for small (strongly discrete limit) to moderate values of $D$ (see Figure 6).

---

4At larger $D$ (strong coupling limit) the core region delocalizes and more and more active points need to be included [9]. Another possibility is to change the type of the approximation from “active points” to “collective variables”, which is more in tune with a close to continuum character of the model in this limit. We will not pursue these ideas in the present paper.
Figure 7: (a) Two-dimensional energy landscape \( \Phi(\nu_1,\nu_2) \). (b) Level sets of the energy along with the path of the effective particle \( \nu(t) \). Parameters: \( V = 0.1, D = 0.5, w_c = 1 \).

7.3 \( K = 2 \) dynamic PN landscape

We can now introduce the global order parameter and reformulate the \( G = \text{const} \) dynamics in the form of a gradient flow on a fixed two-dimensional DPN landscape. Recall that expressions (57), (51) and (48) define the strain trajectories \( w_n(t) \) only over the time period \( 0 \leq t \leq 1/V \). The extension of this solution for \( k/V \leq t \leq (k + 1)/V \) is obtained by replacing \( n \) in the above formulas by \( n-k \) and \( t \) by \( t-k/V \). To patch together different periods we need to introduce a set of two order parameters that change continuously and monotonically with \( t \). We denote these variables as \( \check{\nu}_1(t) \) and \( \check{\nu}_2(t) \) and define them by the conditions \[ [\check{\nu}_1(t)] = [\check{\nu}_2(t)] = [Vt]. \] Then the variables \( x(t) \) and \( y(t) \) can be extended periodically to any \( t \geq 0 \) as follows: \[ x(t) = w_c + (\check{\nu}_1(t) - [Vt])(x(1/V) - w_c) \] and \[ y(t) = y(0) + (\check{\nu}_2(t) - [Vt])(y(1/V) - y(0)). \] Under the assumption that \( V = \Gamma(G) \), where \( \Gamma(G) \) is the inverse of \( G(V) \) from (59), the dynamics of the vector field \( \check{\nu}(t) = (\check{\nu}_1(t), \check{\nu}_2(t)) \) can be represented in the form

\[ \frac{d}{dt} \check{\nu} = -\check{\alpha} \nabla \check{\Phi}(\check{\nu}; G). \quad (60) \]

Here we introduced a mobility matrix \( \check{\alpha} \) and a two-dimensional effective DPN potential \( \check{\Phi}(\check{\nu}; G) \).

We can further simplify the system (60) by diagonalizing the mobility matrix \( \check{\alpha} \). Observe that in (58) we have \( |r_2| > |r_1| > 0 \), so that the eigenvector \((\frac{e^{-\lambda}}{4}(\sqrt{1 + 8e^{2\lambda}} + 1), 1)\) corresponding the eigenvalue \( r_2 \) is the slow direction, while the eigenvector \((\frac{e^{-\lambda}}{4}(1 - \frac{e^{-\lambda}}{4}(\sqrt{1 + 8e^{2\lambda}} + 1), 1)\)
\[ \nu_1(t) = [Vt] + \frac{1 - \exp(r_1(t - [Vt]/V))}{1 - \exp(r_1/V)} \]

and the fast variable

\[ \nu_2(t) = [Vt] + \frac{1 - \exp(r_2(t - [Vt]/V))}{1 - \exp(r_2/V)}. \]

In terms of the new variables, the time evolution of all strains is given by

\[
\begin{cases}
  w_c + G + 1/2 + \left\{ G_P - 1/2 + \frac{1}{4}c_1(1 + \sqrt{1 + 8e^{2\lambda}})(1 - (1 - e^{r_1/V})(\nu_1(t) - [Vt])) \\
  + c_2(1 - \sqrt{1 + 8e^{2\lambda}})(1 - (1 - e^{r_2/V})(\nu_2(t) - [Vt])) \right\} e^{\lambda(n-[Vt])}, & n \leq [Vt] - 1 \\
  w_c + G + G_P + c_1(1 - (1 - e^{r_1/V})(\nu_1(t) - [Vt])) \\
  + c_2(1 - (1 - e^{r_2/V})(\nu_2(t) - [Vt])), & n = [Vt] \\
  w_c + G - 1/2 + \left\{ G_P + 1/2 + \frac{1}{4}c_1(1 + \sqrt{1 + 8e^{2\lambda}})(1 - (1 - e^{r_1/V})(\nu_1(t) - [Vt])) \\
  + c_2(1 - \sqrt{1 + 8e^{2\lambda}})(1 - (1 - e^{r_2/V})(\nu_2(t) - [Vt])) \right\} e^{-\lambda(n-[Vt])}, & n \geq [Vt] + 1.
\end{cases}
\]

The vector field \( \mathbf{v}(t) = (\nu_1(t), \nu_2(t)) \) satisfies

\[ \dot{\mathbf{v}} = -\mathbf{\alpha} \nabla \Phi(\mathbf{\nu}; G), \]

where the mobility matrix \( \mathbf{\alpha} = \text{diag}(\alpha_1, \alpha_2) \) is now diagonal (here \( \alpha_1 > 0 \) and \( \alpha_2 > 0 \) are constants). The potential \( \Phi(\nu_1, \nu_2; G) \) is piecewise quadratic; it depends on \( V \) and hence, through the kinetic relation \( V = \Gamma(G) \), on the driving force \( G \). Using (61) and (62), we obtain

\[
\Phi(\nu_1, \nu_2; G) = -\frac{r_1}{2\alpha_1} \left\{ (\nu_1 - [\nu_1])^2 - \frac{2}{1 - \exp(r_1/V(G))} \nu_1 + [\nu_1] \right\} \\
- \frac{r_2}{2\alpha_2} \left\{ (\nu_2 - [\nu_2])^2 - \frac{2}{1 - \exp(r_2/V(G))} \nu_2 + [\nu_2] \right\}.
\]

To determine the effective viscosities \( \alpha_1 \) and \( \alpha_2 \), we require that at \( G_P \) the DPN potential equals the relative Gibbs free energy of the system:

\[ \Phi(\mathbf{\nu}; G_P) = \mathcal{W}(\mathbf{\nu}; G_P) - \mathcal{W}(\mathbf{0}; G_P). \]

This yields

\[
\alpha_1 = -\frac{r_1 \sqrt{1 + 8e^{2\lambda}}}{(\sqrt{1 + 8e^{2\lambda}} + 3)G_P}, \quad \alpha_2 = -\frac{r_1 \sqrt{1 + 8e^{2\lambda}}}{(\sqrt{1 + 8e^{2\lambda}} - 3)G_P}
\]
and, finally,
\[
\Phi(\nu_1, \nu_2; G) = \left( \sqrt{1 + 8e^{2\lambda}} + 3 \right) G_P \left\{ \left( \nu_1 - [\nu_1] \right)^2 - \frac{2}{1 - \exp(r_1/V(G))} \nu_1 + [\nu_1] \right\} + \left( \frac{1}{2} \right) \left( \sqrt{1 + 8e^{2\lambda}} - 3 \right) G_P \left\{ \left( \nu_2 - [\nu_2] \right)^2 - \frac{2}{1 - \exp(r_2/V(G))} \nu_2 + [\nu_2] \right\}. \tag{66}
\]

The dynamic PN landscape (DPN) \( \Phi(\nu_1, \nu_2; G) \), along with the trajectory of the effective particle, is shown in Figure 7. The comparison of strain trajectories in the two-dimensional reduced theory with the exact result at \( G = \text{const} \) (see Appendix) shows the considerable improvement over the one-dimensional approximation. For instance, Figure 3b compares the evolution of strains near the phase boundary over the first three time periods at \( V = 0.1 \). While in the case \( K = 1 \) the evolution of only the transforming element is followed closely over each time period, in the \( K = 2 \) case the dynamics of the main nontransforming elements forming the core region of the defect is also captured extremely well. It is then natural to use the \( K = 2 \) approximation as the basis for the construction of the nonlocal rheological relation on the phase boundary.

8 Kinetic equations

In the previous section we saw that the traveling wave solution of the original infinite-dimensional system can be reproduced rather faithfully by the reduced two-dimensional system (52) and (53). This suggests that the \( K = 2 \) model may be extended to deal with the situation when the driving force is not constant but varies sufficiently slowly. In this more general setting we obtain the system
\[
\dot{x} = (-2D - 1)x + 2Dy + w_c + G(t) + 1/2 \\
\dot{y} = Dx + (-2D - 1 + e^{-\lambda}D)y + (w_c + G(t))(1 + D(1 - e^{-\lambda})). \tag{67}
\]

Equations (67) can be interpreted as the system of differential kinetic equations generalizing the kinetic relation (59). According to the description of kinetics implied by the system (67), the adjustment of the velocity \( V(t) \) to the dynamic configurational loading \( G(t) \) is not instantaneous and cannot be described by an algebraic relation if the function \( G(t) \) changes sufficiently fast. Instead, the relationship between the velocity and the driving force is expected to be history-dependent:
\[
V_*(t) = \mathcal{F}\{G(\tau), \tau \leq t\}. \tag{68}
\]

The goal of this section is to reconstruct the nonlocal relationship (68) from the system (67) and to illustrate the effect of nonlocality.
Suppose that the phase boundary is located at $n = i$ at time $t = t_i$, meaning that in this instance the $i$th spring has critical strain: $w_i(t_i) = w_c$. As before, we can define $x(t) = w_i(t)$ and $y(t) = (w_{i+1}(t) + w_{i-1}(t))/2$ when $t_i \leq t \leq t_{i+1}$. To obtain the average velocity $\bar{V}_i$ we need to solve the system of kinetic equations (67) in the interval $(t_i, t_{i+1})$, under the assumption that $G(t)$ is known.

Observe first that conditions
\begin{equation}
    x(t_i) = w_c 
    \tag{69}
\end{equation}
and
\begin{equation}
    y(t_{i+1}) = w_c + \frac{1 - e^{-\lambda}}{2},
    \tag{70}
\end{equation}
which are the extensions of (64) and (65) to the interval $[t_i, t_{i+1}]$, ensure that the system holds from $t = t_i$ until the time $t_{i+1}$ when the next spring reaches the critical strain: $w_{i+1}(t_{i+1}) = w_c$.

While for given $t_{i+1}$ conditions (69) and (70) are sufficient to find a unique solution of (67), the moment $t_{i+1}$ when the consecutive spring switches from one energy well to another remains unknown. If $G(t)$ varies sufficiently slowly, it is reasonable to assume that the motion is close to periodic in the sense that
\begin{equation}
    w_i(t_i) = w_{i+1}(t_{i+1}). 
    \tag{71}
\end{equation}
This condition allows us to close the system and find $t_{i+1}$ from
\begin{equation}
    y(t_i) = w_c + G(t_{i+1})(1 - e^{-\lambda}). 
    \tag{72}
\end{equation}
To this end, we solve (67) subject to (69) and (72), obtain for $t_i \leq t \leq t_{i+1}$,
\begin{align}
    x(t) &= g(t) + \int_{t_i}^{t} (e^{r_1(t-\tau)}f_1(\tau) + e^{r_2(t-\tau)}f_2(\tau)) \, d\tau \\
    y(t) &= h(t) + \frac{e^{-\lambda}}{4} \int_{t_i}^{t} \{ (1 + \sqrt{1 + 8e^{2\lambda}})e^{r_1(t-\tau)}f_1(\tau) \\ &+ (1 - \sqrt{1 + 8e^{2\lambda}})e^{r_2(t-\tau)}f_2(\tau) \} \, d\tau, \tag{73}
\end{align}

\footnote{This condition is obviously not exact because $G(t_i) \neq G(t_{i+1})$. By using the knowledge of the exact structure of the traveling waves at both $G(t_i)$ and $G(t_{i+1})$ this approximation can be in principle improved. However, in the interests of transparency, we do not pursue this more rigorous approach in this paper.}
where we defined
\[
g(t) = \frac{1}{\sqrt{1 + 8e^{2\lambda}}} \left\{ \frac{1}{2} \left( (\sqrt{1 + 8e^{2\lambda}} - 1)e^{r_1(t-t_i)} + (\sqrt{1 + 8e^{2\lambda}} + 1)e^{r_2(t-t_i)} \right)w_c + 2e^\lambda (e^{r_1(t-t_i)} - e^{r_2(t-t_i)})(w_c + G(t_{i+1})(1 - e^{-\lambda})) \right\}
\]
\[
h(t) = \frac{1}{\sqrt{1 + 8e^{2\lambda}}} \left\{ e^\lambda (e^{r_1(t-t_i)} - e^{r_2(t-t_i)})w_c + \frac{1}{2} \left( (\sqrt{1 + 8e^{2\lambda}} + 1)e^{r_1(t-t_i)} + (\sqrt{1 + 8e^{2\lambda}} - 1)e^{r_2(t-t_i)} \right)(w_c + G(t_{i+1})(1 - e^{-\lambda})) \right\}
\]
\[
f_1(t) = \frac{\sqrt{1 + 8e^{2\lambda}} - 1}{2\sqrt{1 + 8e^{2\lambda}}}(w_c + \frac{1}{2} + G(t)) + \frac{2e^\lambda}{\sqrt{1 + 8e^{2\lambda}}}(w_c + G(t))(1 + D(1 - e^{-\lambda}))
\]
\[
f_2(t) = \frac{\sqrt{1 + 8e^{2\lambda}} + 1}{2\sqrt{1 + 8e^{2\lambda}}}(w_c + \frac{1}{2} + G(t)) - \frac{2e^\lambda}{\sqrt{1 + 8e^{2\lambda}}}(w_c + G(t))(1 + D(1 - e^{-\lambda}).
\]

We can now determine the strains \(w_i(t) = x(t)\) and \(w_{i+1}(t) = y(t) \pm (1 - e^{-\lambda})/2\). The other strains can be recovered as before, from the constrained energy minimization:

\[
w_n(t) = \begin{cases} w_c + G(t) + 1/2 + (w_{i-1} - w_c - G(t) - 1/2)e^\lambda(n-i+1), & n \leq i - 2 \\
w_c + G(t) - 1/2 + (w_{i+1} - w_c - G(t) + 1/2)e^\lambda(1-n) & n \geq i + 2. \end{cases}
\]

Condition (70) applied to \(y(t)\) in (73) yields the nonlinear equation for \(t_{i+1}\):

\[
h(t_{i+1}) - w_c - \frac{1 - e^{-\lambda}}{2} + \frac{e^{-\lambda}}{4} \int_{t_i}^{t_{i+1}} \{ (1 + \sqrt{1 + 8e^{2\lambda}})e^{r_1(t_{i+1}-\tau)} f_1(\tau) \} + (1 - \sqrt{1 + 8e^{2\lambda}}) e^{r_2(t_{i+1}-\tau)} f_2(\tau) d\tau = 0.
\]

As we have seen in the previous section, at \(G = \text{const}\) this equation a unique solution and one can expect that at least for the case of slowly varying driving force \(G(t)\) the solution \(t_{i+1}\) also exists and is unique. Once it is found, we can obtain the average velocity corresponding to the time interval \([t_i, t_{i+1}]\) in the form

\[
\bar{V}_i = \frac{1}{t_{i+1} - t_i}
\]

Using this iterative process, one can generate the sequence of successive time intervals \([t_i, t_{i+1}]\) and find the average velocities associated with each of them. This gives a piecewise constant function \(\bar{V}(t_i)\), which appears at the macroscale as a continuous function \(V_\ast(t)\).
Figure 8: (a) Time-dependent driving force (77), with $\zeta = 0.1$ (dashed curve) and $\zeta = 10$ (solid curve). (b) The corresponding difference between the coordinate $s(t)$ of the phase boundary obtained using the instantaneous kinetic response $V(t) = \Gamma(G(t))$ and the coordinate $s_*(t)$ calculated using the kinetic equations (67). Here $G_0 = G(0.3) \approx 0.294$, $\Gamma = 0.001$ and $t_* = 20$.

To illustrate this procedure consider a specific time-dependent driving force of the form

$$G(t) = G_0 - \delta \tanh \frac{t - t_*}{\zeta}. \quad (77)$$

Here $G_0 = G(t_*)$ is the constant background driving force, $\delta$ is the amplitude of the diffuse jump in the driving force, and $\zeta$ is the characteristic time over which the driving force decreases by $2\delta$. Such perturbation of the driving force may represent an interaction of the phase boundary with an extended obstacle.

We now compare two responses of the steadily moving phase boundary to a perturbation (77). One is the instantaneous response governed by the kinetic relation (59). In this case we obtain $V(t) = \Gamma(G(t))$ and the location of the phase boundary assuming $s(0) = 0$ can be found by integration from

$$s(t) = \int_0^t \Gamma(G(\tau))d\tau.$$  

The second one is the history-dependent response governed by the kinetic equations (67). In this case the function $V_*(t)$ is obtained from the interpolation of the solution of the sequence of the discrete problems (67). The location of the phase boundary is given by

$$s_*(t_i) = \sum_{j=0}^i \bar{V}_j(t_j - t_{j-1}) = i.$$
The time-dependent separation between the two boundaries both located at the same point at time $t = 0$ but then driven by two different kinetic models is shown in Fig. 8. As $\zeta \to \infty$, the two kinetic models converge and the difference $s(t) - s^*(t)$ tends to zero. However, as Fig. 8 shows, at finite $\zeta$ the prediction of the model based on the kinetic relation may be markedly different from the one based on solving the kinetic equations.

9 Conclusions

In the classical macroscopic continuum description of lattice defects the core regions are represented by singularities, and the dynamics of these singularities is governed by algebraic kinetic relations. Such description is too coarse to capture the details of the dynamic response of the cores of the defects to relatively fast changes of the macroscopic driving forces. In particular, it averages out the details of the intricate interaction of the core regions with localized inhomogeneities which manifests itself through macroscopic velocity oscillations and a characteristic acoustic emission.

To describe the “breathing” of the core regions as well as other transient effects that are usually neglected, we proposed in this paper to replace the algebraic relations between the macroscopic velocity and the corresponding driving force, which imply internal steady state, by a system of differential kinetic equations. The explicit time dependence of the driving force makes these equations nonautonomous and allows them to represent a dependence between the current value of velocity and the history of the driving force. In the constitutive sense the proposed kinetic equations describe a relation between the thermodynamic force and the corresponding flux which is nonlocal in time. The ensuing rheological description of the moving defect can be qualified as a differential rate model.

The main idea of our construction is to follow the exact dynamics of only few discrete degrees of freedom. The adiabatic elimination of the infinite number of the remaining variables outside the core region serves as the matching condition with the classical continuum description outside the defect. The choice of the dimensionality of the reduced system remains heuristic and is based on the comparison of some special periodic solutions of the finite-dimensional system with the discrete traveling wave solutions of the microscopic infinite-dimensional model. We show that in contrast to the standard approach that involves only the center of mass of the defect, the minimally adequate approximation includes not only the location but also the internal configuration of the core. Such extension of the scope is necessary even if both the macroscopic driving force and the average velocity of the defect are constant because the core region may experience periodic configurational deformations instead of translating as a rigid body.

In this paper we presented only the contours of this approach and provided only the most elementary illustrations. More systematic study is needed to formulate the formal
mathematical structure of our center-manifold-type reduction procedure and to evaluate the errors of the approximation in mathematical terms. Other problems include transition from overdamped to underdamped dynamics and the generalization for higher dimensions. A specific development is also needed to move from a prototypical case of martensitic phase transitions to the cases of dislocations, cracks, and more complex singularities.

**Appendix: Traveling wave solution**

To construct a traveling wave solution of the system (22) with \( \sigma = \text{const} \), we assume that

\[
    w_n(t) = w(\eta), \quad \eta = n - Vt, \tag{78}
\]

where \( V \) is the dimensionless velocity of the front, which represents a moving phase boundary. Since we seek a description of an isolated phase boundary that leaves phase II behind, we require that

\[
    w(\eta) < w_c \quad \text{for} \quad \eta > 0, \quad w(\eta) > w_c \quad \text{for} \quad \eta < 0 \tag{79}
\]

Under these assumptions, \( (22) \) reduces to

\[
    Vw'(\eta) - D(w(\eta + 1) - 2w(\eta) + w(\eta - 1)) + w(\eta) = \theta(-\eta) + \sigma \tag{80}
\]

At infinity the solution must tend to uniform-strain equilibria of \( (19) \):

\[
    w(\eta) \to w_{\pm} \quad \text{as} \quad \eta \to \pm\infty. \tag{81}
\]

Finally, for consistency, we must also require that

\[
    w(0) = w_c. \tag{82}
\]

Since the equation \( (80) \) is linear, we can be solve it using Fourier transform (see [9, 11, 41] for details). We obtain

\[
    w(\eta) = \begin{cases} 
    \sigma + 1 + \sum_{k \in S^-(V)} \frac{e^{ik\eta}}{k\Lambda_k(k, V)} & \text{for} \ \eta < 0 \\
    \sigma - \sum_{k \in S^+(V)} \frac{e^{ik\eta}}{k\Lambda_k(k, V)} & \text{for} \ \eta > 0,
    \end{cases} \tag{83}
\]

where \( S^\pm(V) = \{k : \Lambda(k, V) = 0, \ \text{Im}k \geq 0\} \) are the sets of roots of the dispersion relation

\[
    \Lambda(k, V) \equiv 1 + 4D \sin^2(k/2) - V^2k = 0.
\]
Continuity of \( w(\eta) \) at \( \eta = 0 \) gives the relationship between the applied stress and velocity of the traveling wave:

\[
\sigma = \sigma_M + \frac{1}{2} + \sum_{k \in S^+(V)} \frac{1}{k \Lambda_k(k, V)} = \sigma_M - \frac{1}{2} - \sum_{k \in S^-(V)} \frac{1}{k \Lambda_k(k, V)}.
\]  

(84)

Since the difference between applied and Maxwell stresses is equal to the driving force \( G = \sigma - \sigma_M \) (see [40]), we obtain:

\[
G(V) = \frac{1}{2} + \sum_{k \in S^+(V)} \frac{1}{k \Lambda_k(k, V)}.
\]

(85)

The structure of the kinetic relation (85) is illustrated in Figure 9 for different values of \( D \). One can see that at \( D = 0 \) (no NNN interactions) the driving force must be constant and equal to the spinodal value \( G = G_S = 1/2 \); at \( V = 0 \) it can take any value between 0 and \( G_S \). In the limit \( D \to \infty \) the driving force becomes equal to zero at all values of \( V \). At large \( V \) complex roots in the set \( S^+(V) \) tend to infinity and the kinetic curves approach the common limit. For \( D > 1/12 \) the large-velocity discrete kinetics is well approximated by the formula [41]

\[
G(V) = \frac{V}{2\sqrt{V^2 + 4D} - 1/3},
\]

which describes the kinetics of the overdamped viscosity-capillarity model governed by the partial differential equation \( w_t = (D - 1/12)w_{xx} - \tilde{\sigma}(w) + \sigma \).

\[\text{Figure 9: Kinetic relation at different values of } D.\]

---

\(^6\)This semianalytic expression remains implicit until the exact locations of the roots \( k = k(V) \) of the dispersion equation are known [41].
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