Collective-variable dynamics and core-width variations of dislocations in a Peierls model

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The method of collective variables, reformulated by means of d’Alembert’s principle, is employed to set up a systematic perturbative approach to the solution of the dynamical Peierls equation for rectilinear screw and edge dislocations. In this nonlinear and dissipative integro-differential equation which includes radiation reaction, the slip function is a dynamically-evolving field. Its degrees of freedom are reshuffled by equating it to the sum of a “mean-field” arctangent ansatz, exact for steady motion, in which the collective variables are the time-dependent dislocation position and core width, and a residual term. Two constraints determine the collective variables. Equations for the latter and for the residual are obtained. To leading order, a known equation of motion for the dislocation position is retrieved, together with the yet unknown associated governing equation for the core width. The procedure systematizes Eshelby’s approach to dislocation dynamics, in a manner akin to treatments in soliton theory. The specificity of the present one however resides in the history-dependent character of the two governing equations. Both are combined into one single complex-valued equation for a complex coordinate, of real part the dislocation position and of imaginary part its half-width. The model allows for transient supersonic states inasmuch as they relax to subsonic ones. Numerical calculations show that a loading-dependent dynamical critical stress governs the forward subsonic-to-transonic transition of the edge dislocation. Its dependence with respect to the viscosity coefficient is investigated in the case of abrupt loading. The model reproduces the phenomenology of velocity and core width variations during the decay of transient transonic states to subsonic ones, previously observed in molecular-dynamics simulations by Gumbsch and Gao [P. Gumbsch and H. Gao, Dislocations faster than the speed of sound, Science 283, 965 (1999)].

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I. INTRODUCTION

In the last decade, high-velocity dislocation motion in crystals has been the subject of many two-dimensional studies by molecular dynamics,1–8 or via direct measurements in a complex plasma crystal9,10 which can be considered a two-dimensional experimental model of plasticity at high strain rates. Part of the difficulty of building a theory able to reproduce measurable data such as the dislocation velocity vs. time curve, resides in the drastic variations in shape and core width undergone by a moving rectilinear dislocation subjected to high-stress loading.11–15

In a recent paper,11 hereafter referred to as (I), that built on previous attempts to solve this problem,12–15 an equation of motion (EoM) for the dislocation position \( \xi(t) \) at time \( t \) was derived from a dynamical extension of the Peierls model16–19 called hereafter the dynamical Peierls equation (DPE).20 This non-linear and non-local field equation determines \( \eta(x,t) \), namely, the slip on the slip plane at abscissa \( x \) along the direction of motion. The EoM for \( \xi(t) \) followed from replacing in the DPE \( \eta(x,t) \) by a steady-state ansatz of the arctangent type12,20,22,23 centered on \( \xi(t) \) and with arbitrary time-dependence of its core width \( a(t) \). For lack of an independent governing equation for it, \( a(t) \) was simply assumed to depend on \( t \) via the instantaneous dislocation velocity, using its steady-state expression. The purpose of the present work is to relax this assumption, and to inscribe the arctangent ansatz within a perturbative approach to the solution of the DPE.

To this aim, we adapt to the DPE the method of collective variables (or collective coordinates)24–28 widely used in the soliton literature; for example, to study sine-Gordon (SG) or Frenkel-Kontorova (FK) models.29,30 Applied to these models, the method consists in representing the unknown field as the sum of a “mean-field” ansatz, of the same functional form as the exact steady-state solution of the model and depending on a small number of physically relevant parameters called collective variables (CV), and a residual term. In the context of the DPE, where the field \( \eta(x,t) \) is akin to a solitonic-wave solution, the mean-field part of the solution is the arctan ansatz with CVs \( \xi(t) \) and \( a(t) \). To preserve the overall number of degrees of freedom, the CVs must be related by functional constraints to the exact but unknown solution of the field equation. The problem then resides in determining governing dynamical equations for the CVs and for the residual. The set of equations must be such that the new representation of the solution is equivalent to the original one.24

From the outset, FK or SG models are one-dimensional, and admit a Hamiltonian.20 This circumstance allows one to address the constrained dynamics of the collective variables in these models by means of Dirac’s approach,21 in which Hamilton’s equations of motions for the CVs are obtained in terms of modified Poisson brackets that differ from usual ones by a term built from the constraints.25,28 Boesch et al. reformulated the method in terms of straightforward projections of the original field equation (to be identified with the DPE), onto suitable functions determined by the ansatz used. Their approach dramatically reduces the amount of work needed to obtain governing equations for collective variables.26,27 However, the proof of its equivalence with Dirac’s method, in which canonical momenta conjugate to the collective variables and to the residual term play a fundamental role, requires knowing the Hamiltonian (or a Lagrangian) of the system.

By contrast, the DPE arises from a reduction to one dimen-
sion of a two-dimensional problem involving wave emission and dynamic self-interactions during non-uniform dislocation motion — an approach that includes radiation reaction and belongs to the general category of boundary-integral-equation methods. As such, this equation is history-dependent and dissipative, which eludes standard Hamiltonian dynamics. Still, the problem of the moving dislocation resembles that of moving FK or SG kinks, so that the CV formalism in its projector-operator form is here again the right approach to use.

Prior to employing it, we must however establish its relevance when only the field equation is known, without appealing to Hamiltonian concepts such as canonical momenta. To this purpose, we invoke d’Alembert’s principle. It is operative whatever the type of dynamics (including dissipative situations) and can be employed whenever a field equation of motion is available. Calculations of a similar spirit have previously been carried out on a lattice dislocation model — but with fixed width, the residual being further decomposed into phonon-like degrees of freedom.

By this method, we derive the desired governing equations for the collective variables. Next, we discuss their numerical solution to lowest order, when the contribution with the residual term is ignored. We then examine some consequences as to the subsonic-to-transonic transition of edge dislocations.

Before going on, we point out the existence of a number of useful simplified approaches to dynamic dislocation motion that neglect radiation reaction. They underestimate dislocation inertia and do not allow one to investigate dynamical variations of the core. However, their dynamics can be summarized by a Lagrangian function. As our present interest lies in radiation-induced inertia and core-width variations, we do not consider them further hereafter.

II. THE DYNAMICAL PEIERLS EQUATION

In a two-dimensional set-up (plane or anti-plane strain), the dynamical Peierls equation describes a rectilinear dislocation with flat core that moves on its slip plane $y = 0$ by the slip $\eta(x, t) = \lim_{d \to 0} u(x, d/2, t) - u(x, -d/2, t)$ of the material displacement $u(x, y, t)$ between both sides of the slip plane. The in-plane and out-of-plane coordinates are $x$ and $y$, respectively, and $t$ is the time. The (signed) dislocation density is

$$\rho = \partial \eta / \partial x.$$  \hfill (1)

For one isolated dislocation boundary conditions are such that $\eta(x, t)$ has finite limits at infinity. Namely, $\eta(\pm \infty) = \eta(\mp \infty)$, which defines the asymptotic Burgers vector modulus $b = \eta(\infty) - \eta(\mp \infty)$. One imposes $\partial b / \partial t = 0$. The “no-dislocation” background slip $\eta(\infty)$, given by $\eta = \eta_{\infty}$, represents a nonlinear-elastic uniform relative displacement in the interplanar region induced by the applied stress. Then, the quantity

$$\tilde{\eta}(x, t) \equiv \eta(x, t) - \eta(\infty)$$  \hfill (2)

represents a local Burgers vector.

The field $\eta$ is determined as the solution of the nonlinear integro-differential equation

$$\mathcal{F}(x, t, [\eta]) = 0,$$  \hfill (3)

where

$$\mathcal{F}(x, t, [\eta]) = \sigma_q(x, t) + \sigma_D(x, t) + \sigma_a(t) - f'(\eta(x, t))$$  \hfill (4)

is the resultant of forces acting on the dislocation: $-f'(\eta)$ is the nonlinear, $b$-periodic, pull-back force of lattice origin that derives from the lattice potential $f$; $\sigma_D(x, t)$ is a phenomenologenl non-radiative drag force, and $\sigma_a(t)$ is the applied resolved shear stress. For consistency with boundary conditions, the present work is restricted to an applied stress 	extit{spatially uniform} on the slip plane, with arbitrary time dependence.

The term $\sigma_q(x, t)$ is the 	extit{self-stress}, a visco-inertial force of radiative origin. With $\Delta x = x - x'$ and $\Delta t = t - \tau$, it reads for screw and edge dislocations of the “glide” type

$$\sigma_q(x, t) = -\frac{\mu}{\pi} \int \frac{d\tau}{dx'} K(\Delta x, \Delta t) \rho(x', \tau) - \frac{2\mu}{2\varepsilon} \frac{\partial \tilde{\eta}}{\partial t}(x, t),$$  \hfill (5)

where $\mu$ is the shear modulus and $\varepsilon$ is the shear wave speed, the longitudinal wave speed being written $\varepsilon$ hereafter. The “local” term, proportional to $\partial \tilde{\eta} / \partial t$, accounts for out-of-plane radiative losses during motion. The kernel $K$ depends on the dislocation character and accounts for in-plane wave-propagation effects. As a functional of $\eta$, the above expression of $\sigma_q(x, t)$ is exactly the same as in the dynamic theory of self-healing cracks [except that in the latter $\eta(x, t)$ has compact support so that $\tilde{\eta}$ is written $\eta$]. For edge dislocations of the “climb” type the prefactor of the radiative loss term differs from the one in $\varepsilon$. Climb edge dislocations are not considered further hereafter.

The kernel $K$ is related to the velocity-dependent steady-state quasimomentum $p(v)$ of the dislocation, where $v$ is the velocity, by

$$K(x, t) = w_0^{-1} \theta(t) \lim_{\varepsilon \to 0} \frac{e^{-\varepsilon/t}}{t^2} p(x/t),$$  \hfill (6)

where

$$w_0 = \mu b^2 / (4\pi)$$  \hfill (7)

is a characteristic line energy density, and $\theta$ is the Heaviside function. A slight abuse of language, repeated hereafter, has been committed in writing this equation; see Note 44. For a screw dislocation, $p(x/t)$ is a locally-integrable function; for an edge, one of its terms contains a “finite part” prescription.

The phenomenological drag term reads

$$\sigma_D(x, t) = -\alpha \frac{\mu}{2\varepsilon} \frac{\partial \tilde{\eta}}{\partial t}(x, t).$$  \hfill (8)

The dimensionless friction parameter $\alpha$ embodies various drag mechanisms of non-radiative origin; see Ref. [18], p. 209. In order to simplify the writing of Eq. 5 below and like, $\alpha$
is defined here as twice the $\alpha$ coefficient of Refs. 11 and 23. The drag force $\sigma_D$ has the same form as the “local” term in the self-force, and is purely viscoplastic as its does not act on the background slip $\eta_{+\infty}(t)$. In the limit $x \to +\infty$, Eq. (3) reduces to

$$\sigma_a = f'(\eta_{+\infty}), \tag{9}$$

which determines $\eta_{+\infty}(t)$ as a function of $\sigma_a(t)$. For uniform motion at velocity $v$ under constant stress, writing Eq. (3) in a co-moving Galilean frame simplifies it as

$$-\frac{A(v)}{\pi} \int \frac{dx'}{x-x'} \frac{\partial \eta}{\partial x}(x') + B_\alpha(v) \frac{\partial \eta}{\partial x}(x') + \sigma_a = f'(\eta), \tag{10}$$

where $B_\alpha(v) = B(b) + \alpha(\mu/2)v/c_s$. This equation, first proposed by Weertman\textsuperscript{21} who determined the functions $A(v)$ and $B(v)$, has more recently [with Eq. (14)] been revisited by Rosakis under the name “Model I”\textsuperscript{24}.

### III. COLLECTIVE VARIABLES FROM D’ALEMBERT’S PRINCIPLE

By d’Alembert’s principle, a weak form of Eq. (3) is obtained by requiring the virtual work to vanish for instantaneous variations $\delta \eta(x, t)$:

$$\delta I(t, [\eta]) = \int dx F(x, t, [\eta]) \delta \eta(x, t) = 0. \tag{11}$$

Degrees of freedom are reshuffled by writing $\eta$ as

$$\eta(x, t) \equiv \eta_0(x, t) + \Delta \eta(x, t), \tag{12}$$

where $\eta_0$ is a single-dislocation “mean-field” ansatz, to be taken consistent with the steady-state solution of (3) and where $\Delta \eta$ is the residual term. Likewise, we write the dislocation density as

$$\rho(x, t) = \rho_0(x, t) + \Delta \rho(x, t), \tag{13}$$

where $\rho_0 = (\partial \eta_0/\partial x)$ and $\Delta \rho = (\partial \Delta \eta/\partial x)$.

Hereafter, we consider the usual Frenkel sine pullback force

$$f'(\eta) = \sigma_{th} \sin(2\pi \eta/b), \tag{14}$$

where $b$ is the Burgers vector and $\sigma_{th} = \max_\eta f'(\eta)$ is the theoretical shear stress, and confine ourselves to homogeneous applied stress conditions, $\sigma_a(x, t) = \sigma_a(t)$, such that $|\sigma_a| \leq \sigma_{th}$. We recall for further use the expression

$$\sigma_{th} = \frac{\mu b}{2 \pi d}, \tag{15}$$

where $d$ is the interplanar distance between the atom planes on both sides of the slip plane. The relevant one-dislocation ansatz, consistent with non-supersonic steady states, is\textsuperscript{11}

$$\eta_0(x, t) = \eta_{+\infty}(t) + \frac{b}{\pi} \left[ \frac{\pi}{2} - \arctan \frac{2(x - \xi(t))}{a(t)} \right]. \tag{16}$$

The dislocation position along the $x$-axis, $\xi(t)$, and width, $a(t)$, stand as CVs for which governing equations are sought. With Eqs. (14) and (9),

$$\eta_{+\infty} = \frac{b}{2\pi} \arcsin(\sigma_a/\sigma_{th}) \quad (|\sigma_a| \leq \sigma_{th}), \tag{17}$$

which saturates at $\pm b/4$ for $\sigma_a = \pm \sigma_{th}$.

Constraints to connect $a(t)$ and $\xi(t)$ to $\rho$ are deduced\textsuperscript{26,27} from minimizing over $\xi$ and $a$ the quadratic norm of the residual\textsuperscript{21},

$$N = \int dx \Delta \eta(x, t)^2 = \int dx \left[ \eta(x, t) - \eta_0(x, t; a, \xi) \right]^2, \tag{18}$$

where we have explicitly indicated the dependence of the ansatz with respect to the CVs. Setting

$$\rho_1(x, t) = [x - \xi(t)] \rho_0(x, t), \tag{19}$$

and differentiating $N$ with respect to the CVs leads to the following equations, to be obeyed at all times:

$$C_i = \int dx \Delta \eta(x, t) \rho_i(x, t) = 0, \quad i = 0, 1. \tag{20}$$

We shall assume that the initial state is either rest, or more generally a steady state at constant velocity $v$ [for which $\xi = vt$ and $a$ can be determined in terms of the functions $A(v)$ and $B_\alpha(v)$; see (55a)]. Then $\rho_0(x, t)$ is the exact solution at $t = 0$. Consequently, $\Delta \eta = 0$ and Eqs. (20) are trivially satisfied at $t = 0$. To enforce them at later times, it suffices to require their time-derivative (denoted with a dot) to vanish, namely, $\dot{C}_{0,1} \equiv 0$\textsuperscript{22}.

Suppose for a moment that the governing equation for $\eta$ could be obtained from a Lagrangian. Constrained governing equations for $\Delta \eta$, $\xi$, and $a$ would then be obtained by replacing $\eta$ by $\eta_0 + \Delta \eta$ in the Lagrangian, by adding to the latter the constraints $C_{0,1} = 0$ by means of Lagrange multipliers, before deducing by differentiation Euler-Lagrange-type equations of motion. However, one readily checks that the added constraints act as an ignorable null Lagrangian. Indeed one has first, for $z = \xi$ and $z = a$,

$$\frac{d}{dt} \frac{\partial \dot{C}_i}{\partial \dot{z}} - \frac{\partial \dot{C}_i}{\partial z} = 0, \quad i = 0, 1; \tag{21}$$

second, expressing $C_i$ in terms of Lagrangian densities $C_i$ as $C_i = \int dx C_i$, one shows that

$$\frac{d}{dt} \frac{\partial \dot{C}_i}{\partial \Delta \eta} + \frac{d}{dx} \frac{\partial \dot{C}_i}{\partial \Delta \eta_x} - \frac{\partial \dot{C}_i}{\partial \Delta \eta} = 0, \quad i = 0, 1. \tag{22}$$

Thus, considering constraints in the form of time derivatives allows equations of motion for the CVs to be derived without worrying about these constraints, and avoids in particular the introduction of Lagrange multipliers. In this setting, constraints are accounted for only in the next step of solving the equations. The constraints $C_{0,1} = 0$ imply vanishing higher-order time derivatives. In practice, identities $\dot{C}_{0,1} \equiv 0$ on the second time derivative can be used (see Ref.
Sec. III) as substitutes for the additional constraints involving the quasimomentum $\tau$ associated to $\Delta \eta$ [of the type $\int dx \pi(x, t)\rho_1(x, t) = 0$] that would be required in the Hamiltonian approach to CV theory.

In situations where no Lagrangian is available, but insofar as a Lagrangian might exist, the above justifies disregarding the constraints altogether in obtaining governing equations for $\Delta \eta$, $\zeta$, and $a$. However, a rigorous demonstration for proceeding likewise in presence of dissipation is still to be found. To make progress, we have to skip over this difficulty. The CV equations then simply follow from d’Alembert’s principle, by replacing in expression (11) of $\triangle$ the field $\eta$ by its parametrization $\eta_0 + \Delta \eta$ [see (16)], and by writing the variation $\delta \eta(x, t)$, $t$ in terms of the independent variations $\delta \Delta \eta(x, t)$, $\delta a(t)$ and $\delta \zeta(t)$. Thus,

$$\delta \eta = -\rho_0 \delta \zeta - \rho_1 \frac{\delta a}{a} + \delta \Delta \eta. \quad (23)$$

Zeroing the independent variations in the resulting expression of $\delta \triangle$ yields the following coupled equations of motion:

$$\int dx \frac{d}{dx} F(x, t; [\eta_0 + \Delta \eta])\rho_0(x, t) = 0, \quad (24a)$$

$$\int dx \frac{d}{dx} F(x, t; [\eta_0 + \Delta \eta])\rho_1(x, t) = 0, \quad (24b)$$

$$F(x, t; [\eta_0 + \Delta \eta]) = 0. \quad (24c)$$

The first two equations determine the collective coordinates given the residual $\Delta \eta$, while the third one determines $\Delta \eta$ given the collective coordinates. This Eq. (24b) is nothing but the DPE (3), in which $\eta$ has been substituted by $\eta_0 + \Delta \eta$. Introducing the bracket notation $\langle A|B \rangle = \int dx A(x)B(x)$, Eqs. (20), (24a) and (24b) can be written in the form of projections

$$\frac{d}{dt} \langle \rho_i | \Delta \eta \rangle \equiv 0, \quad \langle \rho_i | F(\eta_0 + \Delta \eta) \rangle \equiv 0, \quad i = 0, 1, \quad (25)$$

where $\rho_0 = \partial_x \bar{\eta}_0$ and $\rho_1 = (x-\zeta)\rho_0 \propto \partial_x \eta_0$. We notice in passing that definition (16) of $\eta_0$ implies (by construction) the orthogonality property $\langle \rho_0 | \rho_1 \rangle = 0$. Quite generally in the projector approach, the basis functions appear as derivatives of the ansatz with respect to the collective coordinates. The above derivation by means of d’Alembert’s principle makes this obvious.

While the above derivation is consistent with Boesch et al.’s systematic approach to CV theory, using alternatively a rather natural “ad-hoc” constraint such as, for instance,

$$\langle \rho | (x-\zeta)\rho \rangle = \int dx \frac{x-\zeta(t)^2}{2} x, t = 0 \quad (26)$$

to define $\zeta$ as an overall “center of mass”, would yield different results at order $O(\Delta \eta^2)$. Indeed, in the above theory Eq. (26) holds only (in the form $\langle \rho_0 | \rho_1 \rangle = 0$) if $\rho$ is substituted by $\rho_0$.

In the rest of the paper, we will consider only Eqs. (25) to leading order in $\Delta \eta$, leaving to further work the study of the residual and of its influence on the CVs. Thus, at first order, the constraints are irrelevant and the equations reduce to

$$\int dx \rho_0 F[\eta_0] = 0, \quad (27a)$$

$$\int dx \rho_1 F[\eta_0] = 0. \quad (27b)$$

Equation (27a) has been studied in (I) where, following Eshelby, it was postulated (rather than derived as we do here) as a projection onto $\rho_0$ of the equation $F(x, t; [\eta]) = 0$, in which $\eta$ was approximated as $\eta_0$. Equation (27b) has not previously been considered for dynamic dislocation motion.

IV. EQUATIONS OF MOTION

A. Governing equation for $\xi(t)$

We first briefly recall the equation for $\xi$, already obtained in (I), which we cast hereafter in a slightly different form. For notational consistency with (I) we drop from now on the subscript $0$ in $\eta_0(x, t)$ and $\rho_0(x, t)$ unless otherwise stated and denote these quantities by $\eta(x, t)$ and $\rho(x, t)$, keeping in mind that they refer to ansatz (16). Compatibility with the latter requires us to restrict ourselves to homogeneous stress conditions $\sigma_0(x, t) = \sigma(t)$. Indeed, $\eta_\infty(t)$ can be independent of $x$ only if $\sigma_0$ is. Introduce the complex position-width coordinate ($i = \sqrt{-1}$)

$$\zeta(t) = \xi(t) + \frac{a(t)}{2}, \quad (28)$$

and the mean complex “velocity” between instants $\tau$ and $t$

$$\Xi(t, \tau) = \frac{\zeta(t) - \zeta^*(\tau)}{t - \tau}, \quad (29)$$

where the star denotes the complex conjugate. In (I), Eq. (27b) was reduced to

$$-2 Re \int_0^t \frac{d\tau}{\Delta t^2} p(\Xi) + \kappa \frac{w_0}{c s(t)} \xi(t) - b \sigma_a(t) = 0, \quad (30)$$

where $\Delta t = t - \tau$, and $\kappa = 1 + \alpha$. The quantity $c_S$ is the shear wave velocity, $\Xi$ stands for $\Xi(t, \tau)$, and $p(v)$ is the quasimomentum function relevant to screw or edge dislocations introduced in Eq. (6). The equal-time limit of $p(\Xi)$ is purely imaginary if $a \neq 0$, of value

$$p(\Xi(t, t)) = \lim_{\tau \to t^-} p(\Xi(t, \tau)) = p(+i\infty) = \frac{i w_0}{c s}. \quad (31)$$

More precisely,

$$p(\Xi(t, \tau)) = p(\Xi(t, t)) + O(\Delta t^2). \quad (32)$$

To underline the connection with Eq. (41) below, it is appropriate to introduce the quasimomentum variation

$$\Delta p(t, \tau) = p(\Xi(t, t)) - p(\Xi(t, \tau)), \quad (33)$$
and write (30) as
\[ 2 \Re \int_{-\infty}^{t} dt \frac{\Delta p}{\Delta t^2} + \kappa \frac{w_0}{c_s} \frac{2 \dot{\zeta}}{a} - b \sigma_\alpha = 0, \] (34)
where \( \dot{\zeta}, a \), and \( \sigma_\alpha \) are evaluated at instant \( t \). Because of the Re operator, this modification is only a “cosmetic” one. Introducing next the mass function
\[ m(v) = \frac{dp}{dv}(v), \] (35)
and integrating by parts the first term of (34), the boundary contribution at \( \tau = -\infty \) vanishes trivially, while that at \( \tau = t \) vanishes owing to (32). One thus arrives at the governing equation for \( \zeta \) in “mass form”,
\[ 2 \Re \int_{-\infty}^{t} \frac{d\tau}{\Delta t} m(\tau) \frac{d\bar{\zeta}}{d\tau} + \kappa \frac{w_0}{c_s} \frac{2 \dot{\zeta}}{a} - b \sigma_\alpha = 0. \] (36)
Its most important component, the self-force, is the sum of the first two terms with \( \kappa = 1 \). It has been studied in (I).

B. Governing equation for \( a(t) \)

Turning to (27b), we evaluate in succession each contribution to \( \int dx \left( x - \xi(t) \right) \rho \, \mathcal{F} \), with \( \mathcal{F} \) read from Eqs. (4)–(5). Consider first (in the sense of a principal value at infinity)
\[ \lim_{M \to \infty} \int_{-M}^{M} dx \left[ x - \xi(t) \right] \rho(x,t) \sigma_a(t) - f'(\eta(x,t)) = b \frac{a(t)}{2} \sigma_\alpha \sqrt{1 - \sigma_\alpha^2 / \sigma_{\alpha t}^2}, \] (37)
where expression (17) has been used. Next,
\[ \int dx \left[ x - \xi(t) \right] \rho(x,t) \frac{\partial \rho}{\partial t}(x,t) = - \frac{b^2}{4\pi} \dot{a}(t). \] (38)
Finally, one finds that, for both screw and edge,
\[ -\frac{\mu}{\pi} \int dx dx' \left[ x - \xi(t) \right] \rho(x,t) K(x,t|x',\tau) \rho(x',\tau) = - a(t) \frac{2}{\Delta t^2} \Im \Delta p(t,\tau). \] (39)
The calculation leading to (39) closely follows the Fourier-transform approach of (I) and uses the integrals provided in that reference. Gathering terms yields the governing equation for \( a(t) \),
\[ -2 \frac{a}{2} \Im \int_{-\infty}^{t} d\tau \left( \frac{\Delta p}{\Delta t^2} + \kappa \frac{w_0}{c_s} \frac{\dot{\zeta}}{a} + b \frac{a}{2} \sigma_\alpha \sqrt{1 - \frac{\sigma_\alpha^2}{\sigma_{\alpha t}^2}} \right) = 0, \] (40)
or, in “mass form”, after integrating by parts, and multiplying by \( -2/a \) for further use
\[ 2 \Im \int_{-\infty}^{t} d\tau \frac{d\tau}{\Delta t} m(\tau) \frac{d\bar{\zeta}}{d\tau} - \kappa \frac{w_0}{c_s} \frac{\dot{\zeta}}{a} - b \sigma_\alpha \sqrt{1 - \frac{\sigma_\alpha^2}{\sigma_{\alpha t}^2}} = 0. \] (41)

C. Combined governing equation for \( \zeta(t) \)

Equations (36) and (41) are seen to constitute the real and imaginary parts of one single complex equation for \( \zeta(t) \), namely,
\[ 2 \int_{-\infty}^{t} d\tau \frac{d\tau}{\Delta t} m(\tau) \frac{d\bar{\zeta}}{d\tau} + \kappa \frac{w_0}{c_s} \frac{\dot{\zeta}}{a} - i b \sigma_{\alpha t} g \left( \frac{\sigma_\alpha}{\sigma_{\alpha t}} \right), \] (42a)
where
\[ g(x) = -\sqrt{1 - x^2} + ix \quad (|x| \leq 1) \] (42b)
The generalized (complex) self-force associated to \( \zeta(t) \) is
\[ F(\zeta)(t) = 2 \int_{-\infty}^{t} d\tau \frac{d\tau}{\Delta t} m(\tau) \frac{d\bar{\zeta}}{d\tau} + \kappa \frac{w_0}{c_s} \frac{\dot{\zeta}}{a} - \frac{b}{2} \sigma_{\alpha t} \] (43)
The dislocation position and half-width are deduced from \( \zeta(t) \) as \( \zeta(t) = \Re \zeta(t) \) and \( a(t)/2 = \Im \zeta(t) \). Equation (42a) is the main result of this paper. It is equivalent to
\[ \int dx \left( x - \xi \right) \rho_0 \mathcal{F}[\eta_0] = 0, \] (44)
which follows from combining (27a) and (27b).

D. Steady motion

We examine next the steady-state solution of (42a). It is obtained by assuming that \( \zeta(t) = vt + i(a/2) \), where the dislocation velocity \( v \) and the dislocation width \( a \) are constant. Then,
\[ \mathcal{F}(t,\tau) = v + i a \frac{\dot{a}}{\Delta t}, \] (45a)
\[ \frac{d\bar{\zeta}}{d\tau}(t,\tau) = i \frac{a}{\Delta t^2}. \] (45b)
The integral in (42a) can be carried out exactly by changing the integration variable into \( u = \mathcal{F}(t,\tau) \), and by remarking that
\[ m(v) = \frac{dp(v)}{dv} = \frac{d^2 L(v)}{dv^2}, \] (46)
where \( L(v) \) is the steady-state Lagrangian built from the elastic field of the dislocation.\textsuperscript{32} While obviously a related object, this quantity is not the Lagrangian function of the model in the sense of Hamiltonian dynamics. In terms of \( u \),
\[ \frac{1}{\Delta t} = \frac{1}{ia} (u - v), \] (47)
so that
\[ 2 \int_{-\infty}^{t} d\tau \frac{d\tau}{\Delta t} m(\tau) \frac{d\bar{\zeta}}{d\tau} = \frac{2}{ia} \int_{u+i0^+}^{u+i0^+} du (u - v) \frac{d^2 L}{du^2} \]
\[ = \frac{2}{ia} \left\{ \left[ (u - v) p(u) \right]_{u+i0^+}^{u+i0^+} - \int_{u+i0^+}^{u+i0^+} du \frac{dL}{du} \right\} \]
\[ = \frac{2}{ia} \left\{ \lim_{u \to +i\infty} \left[ (u - v) p(u) - L(u) \right] + L(v + i0^+) \right\}. \] (48)
The function $W(v) = v p(v) - L(v)$ is the steady-state line energy density and it has been shown in (I) that $W(\pm \infty) = 0$ for both screws and edges. Invoking moreover (31) leads to

$$2 \int_{-\infty}^{t} \frac{d\tau}{\Delta t} m(\tau) \frac{d\tau}{dt} = \frac{2}{ia} L(v + i0^+) - \frac{w_0}{cs} v. \quad (49)$$

The steady-state expression of the self-force (43) follows as

$$F_{\alpha}(v) = \frac{2}{ia}(v) L(v + i0^+). \quad (50)$$

The phenomenological drag term can be included in an augmented Lagrangian defined as

$$L_{\alpha}(v) = L(v + i0^+) + i\alpha \omega_0 \frac{v}{cs}. \quad (51)$$

The real-valued functions $A(v)$ and $B_{\alpha}(v)$ in Eq. (15) are related to the real and imaginary parts of $L_{\alpha}(v)$ by the identity

$$L_{\alpha}(v) = 2\omega_0 [-A(v) + iB_{\alpha}(v)]. \quad (52)$$

Non-zero values of $\text{Im} L(v + i0^+)$ stem from the prescription $+i0^+$, and arise for transonic ($cs < v < c_L$, for edges only) or supersonic ($v > c_L$ for screws; $v > c_k$ for edges) velocities in connection with dissipation in Mach fronts. Overall, steady-state dissipation processes are accounted for by $\text{Im} L_{\alpha}$. This quantity has the sign of $v$, equal to that of $\sigma_\alpha$ by (54).

Since $\kappa = 1 + \alpha$ the steady-state form of the left-hand side of (42a), namely, the sum of the generalized self-force (50) and the drag force, reads

$$F_{\alpha}(v) \equiv \frac{2L_{\alpha}(v)}{ia(v)}. \quad (53)$$

Combining (7) and (15) yields the identity $b\sigma_{th}/\omega_0 = 2/d$, which with Eq. (53) brings the EoM (42a) to

$$\frac{d}{w_0} L_{\alpha}(v) = a g \left( \frac{\alpha}{\sigma_{th}} \right) \quad (54)$$

in the steady state. Remarking that $|g(\alpha)| = 1$, see (42b), the width $a(v)$ follows from taking the modulus of (54).

$$a(v) = \frac{d}{w_0} |L_{\alpha}(v)|. \quad (55a)$$

Then, (54) reduces to a condition of equality between the complex arguments of both sides. It provides the stress-velocity relationship

$$\sigma_{\alpha} = \sigma_{th} \sin \text{Arg} L_{\alpha}(v). \quad (55b)$$

Derived in a way simpler than previously, Eqs. (55a) and (55b) are a reformulation, in complex Lagrangian form, of the steady-state kinetic relations of Rosakis’s Model I. The above shows that Eq. (42a) stands as a leading-order approximation to the fully dynamical extension of this model. In (I) for lack of the governing equation (41), an instantaneous relationship $a(t) \equiv a(\xi(t))$ with $a(v)$ given by (55a) was assumed in order to complement (36) – using different notations. Employing (42a) avoids this approximation, and produces Eqs. (55a) and (55b) as particular steady-state consequences.

As has already been emphasized, meaningful applications of these equations must be limited to situations where $|\sigma_{\alpha}| \leq \sigma_{th}$. Additional information regarding this restriction is provided in the Appendix.

**V. NUMERICAL METHOD**

The complex-valued EoM (42a) is solved numerically as follows. The dislocation is assumed to move initially with constant initial velocity $v_i$, and core width $a_i$. These values must consistently be related together and with the initially applied stress by Eqs. (55). The dislocation moves non-uniformly at times $t > 0$, due to a change of applied stress.

Motion is discretized as a series of velocity jumps. Effects of velocity jumps on the self-force have been widely studied in the past. In Eq. (42a), the position and core-width variables stand on the same footing and must therefore be of same order of regularity. Thus, any velocity jump must go along with a jump of the core-width *variation rate*. This new piece of information makes discretization straightforward, and avoids the complications of simultaneous velocity and core-width jumps.

Let velocity jumps occur at discrete times $t_k = k\delta t$, with $k$ a positive integer, and $\delta t > 0$ the time step. Let moreover $t_{-1} = -\infty$. The characteristic function of the time interval $I_k = (t_k, t_{k+1})$ for $k \geq -1$ is

$$\theta_k(t) = \theta(t - t_k) - \theta(t - t_{k+1}), \quad (56)$$

with $\theta_{-1}(t) = \theta(-t)$. The prescribed initial velocity is

$$\dot{\xi}_{-1} \equiv v_i. \quad (57)$$

The coordinate at $t = t_0 = 0$ is

$$\xi_0 \equiv \xi_0 + (i/2)a_i, \quad (58)$$

where $\xi_0$ is the reference position at which accelerated motion begins; and $a_i = a(v_i)$ by (55a). Then $\xi(t) = \xi_0 + v_i t$ for $t < 0$, and the piecewise-constant complex velocity reads

$$\dot{\xi}(t) = \sum_{k \geq -1} \dot{\xi}_k \theta_k(t), \quad (59)$$

where the $\dot{\xi}_k$ must be determined for $k \geq 0$. Likewise, the imposed time-dependent force in (42a) is sampled at intermediate times $t_{n+1/2}$ as

$$G_a(t) \equiv (t_{n+1} - t_n)^{-1} \int_{t_n}^{t_{n+1}} dt G_a(t), \quad (60)$$

where

$$G_a(t) \equiv -ib\sigma_{th} \left( \frac{\sigma_{\alpha}(t)}{\sigma_{th}} \right) = -2i\frac{w_0}{d} g \left( \frac{\sigma_{\alpha}(t)}{\sigma_{th}} \right). \quad (61)$$
Taking \( v_t \neq 0 \) requires by (54) that \( F_{un}(v_t) = G_a^{(-1)} \), the constant force force applied prior to non-uniform motion.

Let, for positive times, \( t = [t/\delta t] \) be the integer such that \( t \in I_n \) (brackets denote the integer part). Positions at times \( t = t_n \) are introduced as
\[
\zeta_n = \zeta_0 + \delta t \sum_{k=0}^{n-1} \zeta_k \quad (n \geq 0)
\]  
where the sum is zero if \( n = 0 \). Thus,
\[
\zeta(t) = \zeta_n + \zeta(t - t_n) \quad (t > 0).
\]  
The adopted discretization requires us to compute the self-force (63) at time \( t = t_{n+\frac{1}{2}} = t_n + \delta t/2 \). For \( \tau \in I_k \), we define the following quantities:
\[
\Delta \zeta_k = \zeta_k + \frac{\zeta^* (n + 1/2) \delta t}{2}, \quad \text{if } k = -1,
\]
\[
\zeta_k + \zeta^* (n - k + 1/2) \delta t, \quad \text{if } 0 \leq k \leq n.
\]  
We notice for further use that
\[
\Delta \zeta_n = 2 \text{Im}[\zeta_n + (\delta t/2) \zeta^*_n].
\]  
From (29) and (63) follows that
\[
\tau(t_{n+\frac{1}{2}}, \tau) = \zeta^*_k + \frac{\Delta \zeta_n}{\Delta t},
\]
\[
\frac{d \tau}{dt}(t_{n+\frac{1}{2}}, \tau) = \frac{-\Delta \zeta_n}{\Delta t^2},
\]  
where now \( \Delta t = t_{n+\frac{1}{2}} - \tau \). With (43) and (63), the self-force at time \( t_{n+1/2} \) is written as
\[
F_{\zeta}^{(n)} = 2 \sum_{k=-1}^{n-1} \left[ \int_{t_n}^{t_{n+1}} \frac{d \tau}{\Delta t} m(\tau) \frac{d \tau}{\Delta t} \right] + 2i \frac{u_0}{c_s} \frac{\zeta^*_n}{\Delta \zeta^*_n},
\]  
where the “local” term has been written by appealing to (65). Since velocity is constant over each time interval, integrals can be carried out as in Sec. [IV] Using (66a) and (66b), one obtains
\[
\int_{t_k}^{t_{k+1}} \frac{d \tau}{t_{n+\frac{1}{2}} - \tau} \frac{d \tau}{d \tau} = \frac{\Delta W_k - \zeta^* k \Delta p_k}{\Delta \zeta_k},
\]  
where we introduce the following intermediate quantities for \(-1 \leq k \leq n\):
\[
\Delta W_k = \begin{cases}
W(\tau_{k+1}) - W(\tau_k) & \text{if } k < n \smallskip
W(\tau_k) & \text{if } k = n,
\end{cases}
\]
\[
\Delta p_k = \begin{cases}
p(\tau_{k+1}) - p(\tau_k) & \text{if } k < n \smallskip
-p(\tau_k) & \text{if } k = n,
\end{cases}
\]
\[
\tau^*_k = \begin{cases}
\tau_k & \text{if } k = -1 \smallskip
\tau_k + \frac{\Delta \zeta_n}{(n - k + 1/2) \delta t} & \text{if } 0 \leq k \leq n,
\end{cases}
\]

\( \remark \text{that } \tau_{k+1}^* \neq \tau_{k+1}^* \). Since \( W(\infty) = 0 \) and \( p(\infty) = -\infty \), the rightmost integral in (67) reduces to
\[
\int_{t_k}^{t_{k+1}} \frac{d \tau}{t_{n+\frac{1}{2}} - \tau} = \frac{W(\infty) - W(\tau_k^*)}{\Delta \zeta_k} = \frac{\Delta W_k - \zeta^*_k \Delta p_k}{\Delta \zeta_k},
\]  
Substituting expressions (68) and (70) into Eq. (67) yields the following discretized expression of the self-force:
\[
F_{\zeta}^{(n)} = 2 \sum_{k=-1}^{n} \frac{\Delta W_k - \zeta^*_k \Delta p_k}{\Delta \zeta_k}.
\]

Accounting for the phenomenological drag, of same form as the last term in (67), the discretized EoM at time \( t_{n+1/2} \) finally reads
\[
E_n(\zeta_n, \zeta^*_n) \equiv F_{\zeta}^{(n)} + 2i \frac{u_0}{c_s} \frac{\zeta^*_n}{\Delta \zeta^*_n} - G_n^{(n)} = 0,
\]  
where \( F_{\zeta}^{(n)} \) is given by (71), and \( G_n^{(n)} \) is given by (60). Given \( \zeta_{n-1} = v_n \), and assuming that the velocities \( \zeta_k \) have been computed for \( 0 \leq k \leq n-1 \), each term of the sum (71) depends on \( \zeta_n \)—the unknown at time step \( n \)—for which (72) constitutes an implicit complex-valued equation.

This equation is solved by the Newton-Raphson method. Using the shorthand notation \( z = \zeta_n \), and since \( E_n \) is a function of the independent variables \( z \) and \( z^* \), iterations read
\[
z^{(0)} = \begin{cases}
\zeta_{n-1} & \text{if } n = 0 \smallskip
2 \zeta_{n-1} - \zeta_{n-2} & \text{if } n \geq 1,
\end{cases}
\]
\[
z^{(k+1)} = z^{(k)} + \frac{(\partial E_n/\partial z^*) z_n^{(k)} - (\partial E_n/\partial z) z_n^{(k)}}{|(\partial E_n/\partial z^*)|^2 - |(\partial E_n/\partial z^*)|^2},
\]  
where \( k \geq 0 \) is the iteration counter, \( z^{(0)} \) is an initial convenient guess, and \( E_n \) and its derivatives are evaluated at \( z^{(k)} \). The derivatives are readily obtained as sums involving the known functions \( W'(v) = v n(v) \) and \( p'(v) = m(v) \).

The natural time unit of the problem is \( \tau_0 = d/c_s \), namely, the characteristic propagation time of a shear wave across the interplane distance \( d \). In all cases examined in the next Section, we found the above algorithm stable, and reasonably well-converged results were produced with the time step \( \delta t = \tau_0/10 \).

VI. RESULTS

Simulations of an edge dislocation initially at rest, and instantaneously subjected to a constant stress \( \sigma_a \) for \( t > 0 \), were carried out to investigate inertial effects, and the transition to transonic states. The ratio between longitudinal and transverse wave speeds is \( c_l/c_s = 2 \) and \( c_k \simeq 0.93 c_s \) is the Rayleigh velocity.
Figure 1 represents velocity-time plots of a dislocation initially at rest, subjected to a sudden uniform stress $\sigma_a$, applied at $t = 0$, and kept constant thereafter. The group of plots (a) spanned by the arrow – which indicates the variation direction of the drag coefficient $\alpha$ – illustrates differences in the response for the same uniform stress $\sigma_a = 0.4 \sigma_0$, and seven different drag values (see caption). In all plots of this (a) set, the dislocation undergoes a fast acceleration during a time interval of order $\tau_0$, with a jump in the initial velocity at $t = 0^+$. For the highest drag $\alpha = 0.5$, the dislocation experiences strong (over)damping, and accelerates almost monotonically towards its steady-state velocity limit. As the drag is moderately lowered, damped oscillations take place in the velocity response but the whole motion remains subsonic. However, for drags $\alpha < 0.1$, the dislocation makes an incursion into the transonic domain (with no particular signal at the shear wave speed), followed by a rapid deceleration prior to resuming its subsonic motion.

Plots (b) and (c) in Fig. 1 are made with $\alpha = 10^{-4}$, and differ from the top curve of set (a) only by small modifications of the applied stress. They both involve sustained transonic motion. These two plots illustrate the existence of a dynamical critical stress that separates asymptotic subsonic states from transonic ones. Specifically, for $\sigma_a \approx 0.4148 \sigma_0$ [plot (b)], the dislocation remains transonic for quite a long time, before almost stopping, and quickly afterwards resumes its motion in the subsonic regime. Dislocation stopping is a physical consequence of the recoil due to the detachment of the shear Mach front during the transition. The model captures this effect, and produces in this respect a behavior in qualitative agreement with the one observed by Gumbsch and Gao on molecular-dynamics simulations for dislocations in tungsten. The asymptotic steady state lies close to $c_R$, which is the upper velocity bound for steady subsonic edge dislocations. For the slightly larger stress $\sigma_a \approx 0.4149 \sigma_0$ [plot (c)], the dislocation quits its transonic plateau before terminating in the steady transonic state predicted by Eq. (55b).

Figure 2. (Color online) Subsonic and transonic edge dislocation. Computed velocity-time response $\xi(t)$, for various applied stresses $\sigma_a$ and phenomenological drag coefficients $\alpha$. Solid (resp., dashed) horizontal line: shear wave (resp., Rayleigh) speed. (a) set of curves at same stress $\sigma_0/\sigma_0 = 0.4$ and drag coefficient $\alpha = 10^{-4}, 0.01, 0.1, 0.2, 0.3, 0.4,$ and $0.5$ (arrow direction). (b) and (c): response for same $\alpha$ and slightly different $\sigma_a$ (as indicated).
FIG. 4. Dynamical distribution of velocity \( v = \dot{\xi} \), and steady asymptotic states, vs. applied stress \( \sigma_a \), for the indicated three drag coefficients \( \alpha \). Solid black lines: stable steady states. Dashed white lines: unstable steady states. Grey tones, from background grey (zero) to white (threshold): distributions of velocities in non-uniform motion (spread along the vertical axis at each \( \sigma_a \)), normalized to 1 and thresholded at 0.005. Horizontal dashed lines: wave speeds \( c_S \), and \( c_L \). Vertical dashed line: critical stress \( \sigma_c \). Velocity distributions span the time window \( t/\tau \in [0, 100] \). The white arrow points towards the transient plateau state of Fig. 1. Plots (a1), (a2), and (a3) correspond to abrupt loading, while (b1), (b2), and (b3) correspond to same loads levels multiplied by the smoothing function \( [1 - \exp(-t/\tau_r)] \), with \( \tau_r = 2\tau_0 \).

The critical stress \( \sigma_c(\alpha) \), determined numerically by bisection on plots similar to Fig. 1 for one hundred values of \( \alpha \in (0, 4) \), is represented in Fig. 3. It is such that \( \sigma_c(0) \approx 0.4148(3)\sigma_h \) and approaches exponentially the theoretical shear stress as the drag is increased. It is well represented on the interval by the approximation \( \sigma_c(\alpha)/\sigma_h \approx 1 - 0.59 \exp(-1.00\alpha) \) (fit not shown). Note that the numbers given should slightly depend on the time step, and depends in general on the type of loading considered (see below).

The dynamical behavior of the model is conveniently surveyed in Fig. 4 where we compare dynamical data to the steady states of the model, for abrupt loadings (a1, a2, and a3). For comparison purposes, we also considered in this figure exponentially-relaxed smooth loadings (b1, b2, and b3). Calculations were made for three drag coefficients \( \alpha = 10^{-4} \) (a1 and b1), \( \alpha = 0.1 \) (a2 and b2), and \( \alpha = 0.01 \) (a3 and b3). Stable or unstable steady states follow curves in the \( (\sigma_a, v) \) plane. These curves are drawn as solid black (stable) or dashed white (unstable) lines. They represent the multibranch function \( v(\sigma_a) \), inverse of Eq. (55b). We superimposed them upon density maps of transient velocities, obtained as follows. Calculations for 76 stress values \( \sigma_a \) evenly spread in the interval \([0, \sigma_h]\), were run over a time span \( T = 100\tau_0 \) to generate time-velocity curves such as in Fig. 1. The velocity values \( v_i = v(t_i) \) produced during each run were distributed into 300 equispaced bins in the interval \( v/c_S \in [0, 2.3] \) (the range displayed) as a normalized frequency histogram. The numerical time step is \( \delta t = \tau_0/20 \) in these plots, to improve the sampling of velocities. Such distributions reveal which special velocities constitute temporary or permanent attractors for the dislocation. In the figures, one such distribution is plotted in shades of grey along the vertical for each \( \sigma_a \). The whole array of 76 distributions constitutes one density map.
Making meaningful comparisons with known steady-state velocity-stress curves supposes long-time runs when \( \alpha \) is small, because of the slow relaxation. However, such runs have the drawback of giving excessive weight to the vicinity of the asymptotic states. Consequently, to bring short-lived attractors into light, distributions are cut off at 0.005. This threshold is the value attributed to the white regions of the maps while the dominant grey tone represents 0.

The spread of the white zones in the subsonic region illustrates the slow relaxation towards asymptotic states. At low drag and low driving stress [Fig. 4(a1) and (b1)], the subsonic asymptotic state is far from being reached in the time window considered, consistently with the observations made by Jin, Gao and Gumbsch from molecular-dynamics simulations. The lower envelope of these zones bends downwards as the critical stress is approached, and represents minimal velocities of the time-response, such as observed in Fig. 1. However, the quasi-stopping point of plot (b) in Fig. 1 is too short-lived to be noticeable in Fig. 4(a1).

For abrupt loading, a line of marked transient states “connects” the subsonic and transonic stable branches in plots (a1–3), and corresponds to local plateau-like transients of the time-response. In particular, the white arrow in Fig. 4(a1) marks the plateaus observable in Fig. 1 [plots (b) and (c)]. For smooth loadings [Figs. 4(b1–3)] such transients are no more present in the transonic region, the dynamics being more concentrated around the line of transonic steady states. Thus, these features are strongly loading-dependent. In all cases, the unstable states of the steady-state model (white dashed lines) do no seem to influence the dynamical behaviour in a definite manner.

Comparing Figs. 4(a1–3) and Figs. 4(b1–3) illustrates the dependence of the critical stress on the loading. It is shifted upwards in the case of smoothly applied loads. This is not surprising, since for this type of loading \( \sigma_a \) on the horizontal axis represents the final load level, whereas the applied stress level at the instant of transition [exemplified by the instant of divergence of plots (b) and (c) in Fig. 1] must be lower. Establishing a more intrinsic definition of the critical stress than the one used in the plots is perhaps feasible, but has not been attempted.

Finally, we note that in all plots, stresses in the upper part of the range \([0, \sigma_a]\) produce transient supersonic states. Such states are allowed by theory inasmuch as they relax to subsonic ones (this rule being dictated by the choice of the ansatz and the principles of the CV approach). Figure 4 shows that passing over the “supersonic barrier” involves no special difficulty, partly because of the regularizing effect of the integral over past times in the EoM. Thus, in a fully-dynamical framework (and as far as regularity is concerned) employing a gradient theory to overcome the sound barrier is not indispensable.

### VII. SUMMARY

By applying the method of collective variables to the dynamical Peierls model, we obtained coupled equations of motion for the position and the core width of a dislocation, for which we described in detail an algorithm of resolution. We applied this model to the problem of an edge dislocation suddenly or smoothly accelerated, under the action of an applied stress. This revealed the existence of a drag-dependent dynamical critical applied stress \( \sigma_c(\alpha) \), absent from the steady-state theory, that separates subsonic asymptotic states from transonic ones. For low drag and low applied stress, slow (power-law) relaxation towards asymptotic subsonic states is observed. Both latter features are in qualitative agreement with results previously reported from molecular-dynamics simulations. The present model behaves smoothly during forward and reverse subsonic-transonic transitions, as well as during the forward and backwards transitions to transient supersonic states.

### Appendix A: The problem of high-stress supersonic motion

The calculations of Sec. IV can be formally adapted to allow high for applied stresses in spite of the poor physical relevance of the ansatz in this regime. To this purpose, one complements by continuity Eq. (17) by means of the saturation rule \( \eta_{\text{sat}} = \text{sign}(\sigma_a)b/4 \) for \( |\sigma_a| > \sigma_{th} \). One then finds that Eq. (56) remains unchanged, while integral (57) vanishes. It follows that the square-root term must be removed in (40) and (41) leading to \( g(x) = ix \) in (42b). Thus, (42a) can be generalized to all \( \sigma_a \) by simply multiplying the square root in (42b) by the Heaviside factor \( \theta(1 - |x|) \).

Consequences for steady motion are as follows. As the right-hand side of Eq. (55b) attains its maximum, \( L_\alpha \) vanishes (screw) or becomes purely imaginary (edge), which indicates supersonic motion. On the basis of (55b), it was incorrectly stated in (I) that supersonic motion occurs at saturated stress in this model. Rather, the complex arguments of both sides of (54) are identically equal for \( |\sigma_a| > \sigma_{th} \) and \( v \) supersonic, since now \( g(x) = ix \). Thus, a stress–velocity relationship such as (55b) no more exists, and the model instead admits a degenerate continuum of supersonic states with velocity- and stress-dependent core width

\[
\alpha(v, \sigma_a) = \frac{d}{w_0} \frac{\sigma_{th}}{|\sigma_a|} |L_\alpha(v)| \quad (|\sigma_a| \geq \sigma_{th}, v \text{ supersonic}).
\]

(A1)

This degeneracy indicates that the arctangent ansatz is not consistent with stable supersonic motion. In other words, in the equations for \( \xi \) and \( a \) the phenomenological friction term cannot equilibrate a supersonic dislocation subjected to constant stress, which always accelerates. Indeed, numerical experiments carried out with the above modification of the theory, using the implementation of Sec. IV show that the velocity grows asymptotically as \( \log t \) in the supersonic regime. In spite of its dubious physical character, the modification is nonetheless useful to extend the working domain of the numerical implementation in order to preserve continuity and prevent code crashes at high stress (e.g., for short loading pulses).

In essence, the theoretical problem we face is that Weertman’s equation (10), in which \( A(v) = 0 \) in the supersonic
regime, produces no supersonic solution of Burgers vector \( b \) that could be used as an alternative ansatz. Indeed, the three truly supersonic steady-state solutions of Weertman’s equation (two independent solutions representing isolated partial dislocations with Burgers vector less than \( b \) that build or relax a stacking fault, and one solution representing a supersonic train of dislocations) seem inappropriate to the present single-dislocation problem. A known way of producing steady supersonic states is to use a gradient extension of the theory, which goes along with steady-state solutions of a more complex analytical form. This option has not been considered to keep the present theory at a manageable level.

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