Phase-field-crystal and Swift-Hohenberg equations with fast dynamics

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A phenomenological description of transition from an unstable to a (meta)stable phase state, including microscopic and mesoscopic scales, is presented. It is based on the introduction of specific memory functions which take into account contributions to the driving force of transformation from the past. A region of applicability for phase-field crystals and Swift-Hohenberg-type models is extended by inclusion of inertia effects into the equations of motion through a memory function of an exponential form. The inertia allows us to predict fast degrees of freedom in the form of damping perturbations with finite relaxation time in the instability of homogeneous and periodic model solutions.

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I. INTRODUCTION

Considerable study has been given recently in various phenomena of materials physics using phase-field theory and modeling. Coming from the Landau theory of phase transitions [1] and Ginzburg-Landau form of free-energy functional [2], the phase-field methodology has lead to successful description of various phenomena on the mesoscopic scale such as solidification patterns, nucleation, grain growth, coarsening, fluid convection, and multiphase and multiscale transformations (see overviews [3]).

One of the new directions in phase-field theory has been proposed as phase-field crystals (PFCs) [4] being a tool to simulate materials on the microscopic scale. It is based on the free energy of the Brazovskii form [5] which can also be considered as a transposition of the Swift-Hohenberg (SH) model of pattern formation [6] to crystalline solids. As a result, the PFC model provides efficient simulation of the liquid-solid transition [7], diffusion defects [8], and glass formation [9].

A main focus of the current investigation is to extend a region of applicability of the PFC- and SH-type models. Indeed, as it urged [9], the PFC-type models allow for essentially speed up computations of microstructure formation in comparison with results of density functional studies and molecular dynamic (MD) simulations. High-speed simulations are possible because fast degrees of freedom are not present in the PFC-type models, e.g., in comparison with MD [10]. Consequently, one may distinguish between the PFC/SH models with slow dynamics (which ignoring fast degrees of freedom) from their extensions that cover also other degrees of freedom with a fast dynamics.

Generally, both cases can be characterized as follows. Slow dynamics can be observed in systems whose current state just slightly deviates from its thermodynamic equilibrium. Such systems have an instant response for the change in the order parameter in time and the action of driving force of phase transition, which is in fact close to local equilibrium [11].

In far-from-equilibrium systems, slow dynamics can be found as well if the characteristic time scale of an observed phenomenon is larger than the transient period or period of intense forced oscillations. In these cases, one would characterize, as a first approximation, the slow dynamics through pure dissipative or simple harmonic behavior of the system [12].

Fast dynamics of relaxation processes is observed, first of all, in systems far beyond the equilibrium. Studying rapidly changing dynamical systems, transient phenomena should be taken into account. Among these phenomena one can mention propagation of disturbances with finite speeds and damping perturbations during finite period of relaxation to the local equilibrium state. The transient phenomena may also affect the way of relaxation to steady states in strongly nonequilibrium systems. Therefore, fast dynamics can be predicted on the scale of the order of (or even smaller than) the time of inertial behavior or local relaxation time.

The main purpose of the present paper is to describe an approach to slow and fast transitions in periodic systems described by PFC and SH equations. We derive and analyze governing equations compatible with the thermodynamic formalism that gives a robust basis for description of periodic systems on the microscopic and mesoscopic scales of their evolution.

The paper is organized as follows. A general constructive formalism for systems with fast and slow phase transitions is introduced in Sec. II. Using this formalism, a particular case of fast phase transitions in periodic systems described by hyperbolic PFC and SH equations is presented in Sec. III. Linear stability analysis for homogeneous and periodic solutions in nonconserved dynamics is executed in Sec. IV. We

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discuss the obtained results and a new behavior of damping perturbations predicted by hyperbolic dynamics in comparison with the parabolic dynamics in Sec. V. Finally, Sec. VI presents a summary of our conclusions.

II. SLOW AND FAST DYNAMICS IN PHASE TRANSITIONS

Assume a system whose evolution is characterized by the order parameter $\phi(\vec{r},t)$ with the radius vector $\vec{r}$ of a point in the bulk system and the time t. Our goal is to describe all the stages of the transition from an unstable to a metastable or stable phase state on a phenomenological level, including both short time periods (comparable with a collision time) and macroscopic time (comparable with the time evolution of the whole system). This can be done using the prehistory of response between the driving force $\delta\mathcal{F}/\delta\phi$ [given by the change in the free energy $\mathcal{F}(\phi)$ with respect to the order parameter ϕ] and the order parameter evolution [13].

For the conserved dynamics of phase transition, one may write the flux

$$\vec{j} = -\int_{-\infty}^{t} M(t-t^*)\vec{\nabla}\left(\frac{\delta\mathcal{F}(t^*,\vec{r})}{\delta\phi}\right)dt^*, \tag{1}$$

with $M(t-t^*)$ as the memory function which adopts the correlation between the system's dynamics at the past moment of time t^* and the current dynamics at time t. Together with the balance law $\partial\phi/\partial t=-\vec{\nabla}\cdot\vec{j}$, Eq. (1) gives the following equation for the arbitrary slow or fast dynamics:

$$\frac{\partial\phi}{\partial t} = \vec{\nabla}\cdot\int_{-\infty}^{t} M(t-t^*)\vec{\nabla}\left(\frac{\delta\mathcal{F}(t^*,\vec{r})}{\delta\phi}\right)dt^*. \tag{2}$$

In addition, the nonconserved dynamics of the order parameter ϕ is written through the relaxation with memory as

$$\frac{\partial\phi}{\partial t} = -\int_{-\infty}^{t} M(t-t^*)\frac{\delta\mathcal{F}(t^*,\vec{r})}{\delta\phi}dt^*. \tag{3}$$

Both Eqs. (2) and (3) represent the causality for the order parameter evolution: the present distribution of ϕ depends on the evolution of the flux $\vec{j}$ and the rate of change $\partial\phi/\partial t$, respectively, in their own past. Therefore, as it follows from Eqs. (2) and (3), the concrete dynamics of the system is defined by the memory function $M(t-t^*)$.

Now we consider a memory function $M(t-t^*)=M^{(1)}(0)\delta(t-t^*)$ with the constant $M^{(1)}(0)$ at $t=t^*$ and $\delta(t-t^*)$ as the Dirac delta function. Substituting this expression into Eqs. (2) and (3), one obtains the following equations of motion for conserved order parameter,

$$\frac{\partial\phi}{\partial t} = \vec{\nabla}\cdot\left[M^{(1)}(0)\vec{\nabla}\left(\frac{\delta\mathcal{F}}{\delta\phi}\right)\right], \tag{4}$$

and nonconserved order parameter,

$$\frac{\partial\phi}{\partial t} = -M^{(1)}(0)\frac{\delta\mathcal{F}}{\delta\phi}. \tag{5}$$

The equation in Eq. (4) for conserved order parameter gives a standard equation of the parabolic type which describes the pure dissipative regime of phase transition. It is characterized by an infinite speed of propagation of ϕ within phases due to instantaneous local relaxation given by the function $\delta(t-t^*)$ in the memory function $M(t-t^*)$. Therefore, for the fast transitions, proceeding with the characteristic speed of disturbance propagation, it fails due to the assumption of an immediate response to a disturbance at a distant point.

The equation for nonconserved order parameter in Eq. (5) gives an instantaneous response of $\partial\phi/\partial t\sim\delta\mathcal{F}/\delta\phi$. This equation was first introduced and justified by Mandel'shtam and Leontovich [11] for a problem of sound adsorption by liquids. It is also well known as the time-dependent Ginzburg-Landau equation. As often noted [11,14,15], this equation can be applied to near equilibrium systems, i.e., for systems just slightly disturbed from their thermodynamic equilibrium. Therefore, Eqs. (4) and (5) describe the slow dynamics of phase transitions under local thermodynamic equilibrium.

The second case presents by a constant memory function $M(t-t^*)\equiv$const whose substituting into Eqs. (2) and (3) gives the equations for conserved order parameter

$$\frac{\partial^2\phi}{\partial t^2} = \vec{\nabla}\cdot\left[M(0)\vec{\nabla}\left(\frac{\delta\mathcal{F}}{\delta\phi}\right)\right] \tag{6}$$

and nonconserved order parameter

$$\frac{\partial^2\phi}{\partial t^2} = -M(0)\frac{\delta\mathcal{F}}{\delta\phi}, \tag{7}$$

where $M(0)$ is the mobility at $t=t^*$. As a simplest example, one can assume that $\delta\mathcal{F}/\delta\phi\propto\phi$. In this case, the nonconserved case in Eq. (7) is given by the equation

$$d^2\phi/dt^2 + \omega_*^2\phi = 0, \tag{8}$$

which describes undamped homogeneous relaxation of the order parameter ϕ. For second-order transitions, the coefficient ω_* in Eq. (8) characterizes a small energy gap for a new optical branch of vibrations below the transition point to a new crystalline modification (see p. 168 in Ref. [15]). Oscillatory dynamics (8) never reaches nonconserved "dissipative" dynamics (5) due to its own undamped character. In this case, the system oscillates around equilibrium state infinitely long time due to its own constant memory. However, if the system has essential interaction of the new branch given by $d^2\phi/dt^2$ with the other thermal motions, Eq. (8) should be extended by the term proportional to $d\phi/dt$ that assumes dissipation (i.e., "the system friction" by the terminology of Patashinskii and Pokrovskii [15] for the second-order phase transitions).

The third case deals with the exponential relaxation of the Maxwell type—$M(t-t^*)=\tau_R^{-1}M^{(2)}(0)\exp[-(t-t^*)/\tau_R]$ with τ_R as the characteristic relaxation time for changing regime of motion—from inertial (ballistic) to diffusion regime. It characterizes the time to reach pure dissipative dynamics predicted by Eqs. (4) and (5) for a motion without inertia.

Substituting the Maxwell memory function into Eqs. (2) and (3) gives the equations for conserved order parameter,

$$\tau_R \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = \vec{\nabla} \cdot \left[M^{(2)}(0) \vec{\nabla} \left(\frac{\delta \mathcal{F}}{\delta \phi} \right) \right], \tag{9}$$

and nonconserved order parameter,

$$\tau_R \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = - M^{(2)}(0) \frac{\delta \mathcal{F}}{\delta \phi}. \tag{10}$$

These equations were previously derived from entropy functional within the phase-field methodology applied to fast phase transitions [13]: the positiveness of the entropy production for Eq. (9) demands that $M^{(2)}(0) > 0$, and the stability condition $\delta^2 \mathcal{F} > 0$ implies that $\tau_R > 0$.

Conservation dynamics given by the second equation from Eq. (9) has been introduced also into the phase-field crystal model [16] to describe density modes in elastic displacement fields and defect current. It directly follows from the dynamical density functional theory (Ref. [17] and references therein) or uses the Poisson bracket relationships [18]. Thus, Eqs. (9) and (10) describe the intermediate regime of phase transition between oscillatory dynamics (6) and (7) and dynamics (4) and (5) with dissipation.

Finally, a mixed case of the system memory is obtained using the Jeffreys-type function: $M(t-t^*) = M^{(1)}(0) \delta(t-t^*) + \tau_R^{-1} M^{(2)}(0) \exp[-(t-t^*)/\tau_R]$. For every point of the system, it represents both dynamics with instant relaxation of an "effective transport conductivity" [given by the term $M^{(1)}(0) \delta(t-t^*)$] and exponential relaxation of an "elastic conductivity" (given by the term $\tau_R^{-1} M^{(2)}(0) \exp[-(t-t^*)/\tau_R]$) [19]. Substituting the Jeffreys-type memory function into Eqs. (2) and (3) gives the equations for conserved order parameter,

$$\tau_R \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = \vec{\nabla} \cdot \left\{ [M^{(1)}(0) + M^{(2)}(0)] \vec{\nabla} \left(\frac{\delta \mathcal{F}}{\delta \phi} \right) + \tau_R M^{(1)}(0) \frac{\partial}{\partial t} \vec{\nabla} \left(\frac{\delta \mathcal{F}}{\delta \phi} \right) \right\}, \tag{11}$$

and nonconserved order parameter,

$$\tau_R \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = - [M^{(1)}(0) + M^{(2)}(0)] \frac{\delta \mathcal{F}}{\delta \phi} - \tau_R M^{(1)}(0) \frac{\partial}{\partial t} \frac{\delta \mathcal{F}}{\delta \phi}. \tag{12}$$

Similarly to Eqs. (9) and (10), both Eqs. (11) and (12) have the inertial term $\tau_R \partial^2 \phi / \partial t^2$ due to the exponential relaxation of the Maxwell type. Additionally, including the delta function into the memory, the additional terms in right-hand side (RHS) of Eqs. (11) and (12) appear as well. These describe the change in time of the ϕ inhomogeneity by the term $\partial \vec{\nabla} (\delta \mathcal{F} / \delta \phi) / \partial t$ in Eq. (11) and change in time of the variational derivative from the free energy by the term $\partial (\delta \mathcal{F} / \delta \phi) / \partial t$ in Eq. (12).

In Eq. (11), the factor $M^{(1)}(0) + M^{(2)}(0)$ has the meaning of the mobility coefficient. The factor $\tau_R M^{(1)}(0) = \ell_{inhom}^2$ gives a square of the spatial length ℓ_{inhom} for the inhomogeneity described by the gradient $\vec{\nabla} (\delta \mathcal{F} / \delta \phi)$. The quantity $[M^{(1)}(0) + M^{(2)}(0)]^{-1}$ in Eq. (12) plays the role of the characteristic time for relaxation of the order parameter ϕ (which is different from the time τ_R responsible for relaxation of the fast variable $\partial \phi / \partial t$). The factor $\tau_R M^{(1)}(0)$ is the proportionality constant between rate of change in the order parameter ϕ and variational derivative $\delta \mathcal{F} / \delta \phi$.

Hence, if the free energy $\mathcal{F}$ depends on spatial inhomogeneity of ϕ, Eqs. (11) and (12) for the fast and slow dynamics have the common feature. These equations describe temporal nonlocality by the term $\partial^2 \phi / \partial t^2$ as well as they take into account the spatial nonlocality by assuming terms $\partial \vec{\nabla} (\delta \mathcal{F} / \delta \phi) / \partial t$ and $\partial (\delta \mathcal{F} / \delta \phi) / \partial t$ for conserved and nonconserved dynamics, respectively. Within the limit $\tau_R \to 0$, Eqs. (11) and (12) are reduced to the pure dissipative dynamics given by Eqs. (4) and (5) so that each local volume is in local equilibrium.

With finite time τ_R and specific form of $\mathcal{F}$, the stability and bifurcation of stationary states predicted by the equation of type (11) was investigated for conserved dynamics in a viscoelastic fluid flow and diffusion process [20]. The conserved dynamics given by Eq. (11) has also been derived from the Poisson bracket formalism which was attributed for the phase-field crystal model (see Eq. (73) in Ref. [18]).

III. FAST PHASE TRANSITIONS IN PERIODIC SYSTEMS

A simplest form of the free-energy functional $\mathcal{F}$, which is minimized by a spatial periodic structure of the order parameter ϕ, is

$$\mathcal{F}(\phi) = \int dv \left\{ - a \Delta_0 \frac{\phi^2}{2} + u \frac{\phi^4}{4} + \frac{\lambda}{2} \phi (q_0^2 + \nabla^2)^2 \phi \right\}, \tag{13}$$

where v is a subvolume of the system, $a > 0$ is the parameter of the system periodicity, q_0 is the wave number giving the minimum of $\mathcal{F}$, $u > 0$ and λ are the system parameters, and $\Delta_0 = T_c - T$ is the quench depth representing the control parameter with the critical temperature T_c and actual temperature T. With $\Delta_0 > 0$ the homogeneous ϕ must be unstable to the formation of a periodic structure for some values of the wave vector $\vec{q}$.

Both SH and PFC equations are based on functional (13). The SH equation describes a minimization of the free-energy functional by a nonconserved evolution of the order parameter [6] and PFC equation deals with conserved fields such as density [7]. Free-energy (13) is limited by the minimization, e.g., in two-dimensional space, by a periodic hexagonal pattern (or by triangular lattice) [5]. The peculiarity of the transition based on minimization of Eq. (13) shows up in elasticity: it has been used to model elasticity in growing crystals [4], to describe a stripe-bubble transition [21], and for crystalline or copolymeric chains [22].

An important and practically applicable case of fast and slow dynamics in transient states is obtained by the simplest case described by the equation of a hyperbolic type [13]. This case gives intermediate dynamics between propagative (wave) regime and dissipative (diffusive) regime of phase transitions and, for the case of periodic patterns, it is given by the system of Eqs. (9) and (10) together with free-energy (13).

Considering the latter case of the "hyperbolic" dynamics, we introduce the following dimensionless variables

$$\tilde{t} = tM^{(2)}(0)\lambda q_0^k, \quad \tilde{\nabla} = q_0\vec{\nabla}, \quad \tilde{\phi} = \phi\sqrt{\frac{u}{\lambda q_0^4}} \tag{14}$$

and parameters

$$\tau = \tau_R M^{(2)}(0)\lambda q_0^k, \quad \epsilon = \frac{a\Delta_0}{\lambda q_0^4} \tag{15}$$

into Eqs. (9) and (13). Then, omitting "tilde" from the equations, one gets conserved dynamics for the hyperbolic PFC [with $k=6$ in Eqs. (14) and (15)],

$$\tau\frac{\partial^2\phi}{\partial t^2} + \frac{\partial\phi}{\partial t} = \nabla^2\{[-\epsilon + (1+\nabla^2)^2]\phi + \phi^3\}, \tag{16}$$

and nonconserved dynamics given by the hyperbolic SH equation [with $k=4$ in Eqs. (14) and (15)],

$$\tau\frac{\partial^2\phi}{\partial t^2} + \frac{\partial\phi}{\partial t} = [\epsilon - (1+\nabla^2)^2]\phi - \phi^3. \tag{17}$$

For conserved dynamics (16), the relaxation time τ gives the delay which the flux $\vec{j}$ by Eq. (1) reduces to its previously suggested form of Elder and Grant [7]. This delay indicates a loss of inertia in the transitive dynamics. The relaxation term $\tau\partial^2\phi/\partial t^2$ may be neglected in many circumstances but becomes crucial in some important situations. For instance, it leads to a maximum possible value for the speed of the front of the ϕ profile. Moreover, the relaxation term leads to the possibility of oscillatory phenomena at least at the initial stages of transition. Under a large driving force for the change in the order parameter a pair of Eq. (16) might present a reasonable analysis of a transition from the diffusion-limited to diffusionless transformation. It can be done in a manner of analysis of dendritic growth at deep supercoolings as described within a hyperbolic sharp interface model [23]. Additionally, for nonconserved dynamics (17), the acceleration $\partial^2\phi/\partial t^2$ presents inertia effects within the rapidly transforming domain. From the thermodynamic view point [13], this acceleration appears due to the introduction of both slow variable ϕ and fast variable $\partial\phi/\partial t$ as independent variables in a basic space of thermodynamic variables. With the neglecting inertia, $\tau\to 0$, the dynamics reduces to the parabolic SH equation [6].

Now we prove the consistency of Eq. (17) with the thermodynamic (macroscopic) theory which should satisfy three main conditions. (i) The free energy must be at a minimum in the equilibrium state. (ii) The free energy (as a dissipative function) does not increase in time, i.e., $\partial\mathcal{F}/\partial t \le 0$. (iii) The second differential of the free energy with respect to its basic variables must be positive, $\delta^2\mathcal{F} > 0$, in order to lead to dynamically stable solutions. To check the internal thermodynamic consistency by conditions (i)–(iii), we modify free-energy (13) in the following dimensionless form [by normalization given by Eqs. (14) and (15) with $k=4$]:

$$\mathcal{F}(\phi,\partial\phi/\partial t) = \int dv\left\{g(\phi) - |\vec{\nabla}\phi|^2 + \frac{1}{2}|\nabla^2\phi|^2 + \frac{\tau}{2}\left(\frac{\partial\phi}{\partial t}\right)^2\right\}, \tag{18}$$

where

$$g(\phi) = -\frac{\epsilon-1}{2}\phi^2 + \frac{1}{4}\phi^4 \tag{19}$$

is the standard double-well potential.

Free-energy (18) depends on the slow variable such as the order parameter ϕ and the fast variable $\partial\phi/\partial t$ which is chosen as a rate of change in the order parameter. Such structure of the free energy (or entropy) allows us to describe local nonequilibrium systems by extended thermodynamics [24,25] and it has been used in derivation of equations for fast phase transitions [13]. Following this idea, the first three terms in the integrand of Eq. (18) represent the local equilibrium part of energy (13) (in its dimensionless form). The last term in the integrand of Eq. (18) has the meaning of the kinetic contribution proved for the case of fast spinodal decomposition [26] that may also be applied to the present case of fast transition in periodic systems.

It can be seen immediately that the condition (i) is satisfied in the present proposal. Indeed, form (18) of the free energy guarantees that, in the stationary situation, spatially homogeneous equilibrium takes place within minima states given by double-well function (19) as compared to nonequilibrium states with the same local value of ϕ.

To check the second condition (ii), we describe the evolution of $\mathcal{F}$ as $\partial\mathcal{F}/\partial t = (\partial\mathcal{F}/\partial t)_{ex} + (\partial\mathcal{F}/\partial t)_{in}$, where $(\partial\mathcal{F}/\partial t)_{ex}$ is the external exchange of the free energy and $(\partial\mathcal{F}/\partial t)_{in}$ is the internal change in the free energy inside of the system. Then, from the procedure described in Ref. [13] and applied to Eq. (18), one finds

$$\left(\frac{\partial\mathcal{F}}{\partial t}\right)_{ex} = \oint_s ds\left\{\left(\vec{\nabla}_n\frac{\partial\phi}{\partial t}\right)\nabla^2\phi - \frac{\partial\phi}{\partial t}\vec{\nabla}_n(\nabla^2\phi) - 2\frac{\partial\phi}{\partial t}\vec{\nabla}_n\phi\right\}, \tag{20}$$

$$\left(\frac{\partial\mathcal{F}}{\partial t}\right)_{in} = \int_v dv\left\{\frac{dg(\phi)}{d\phi} + 2\nabla^2\phi + \nabla^4\phi + \tau\frac{\partial^2\phi}{\partial t^2}\right\}\frac{\partial\phi}{\partial t}, \tag{21}$$

where $\vec{\nabla}_n$ is the vector of gradient pointed by the normal vector $\vec{n}$ to the surface s. Obviously, simple boundary conditions which give absence of free-energy exchange by Eq. (20) are described by

$$\phi \equiv \text{const}, \quad \vec{\nabla}_n\phi = 0. \tag{22}$$

These conditions must hold at any point on s.

Around a steady state, dissipative function (21) must decrease in time, so that the free energy of the entire system decreases. This condition implies a relation between thermodynamic fluxes J_i and their respective conjugated forces X_i which, in the simplest case, is assumed to be linear $J_i \sim X_i$ [25]. For Eq. (21), it gives

$$J_i \equiv \frac{\partial \phi}{\partial t} = -MX_i \equiv -M\left(\frac{dg(\phi)}{d\phi} + 2\nabla^2\phi + \nabla^4\phi + \tau\frac{\partial^2\phi}{\partial t^2}\right), \tag{23}$$

with M as the coefficient which is the dimensionless unit to satisfy to Eq. (17). Then, using the bilinear form $(\partial\mathcal{F}/\partial t)_{in} = \int_v (J_i X_i) dv$, condition (22), contributions (20) and (21), and Eq. (23), one gets

$$\frac{\partial \mathcal{F}}{\partial t} = \left(\frac{\partial \mathcal{F}}{\partial t}\right)_{in} = -\int_v dv\left(\frac{dg(\phi)}{d\phi} + 2\nabla^2\phi + \nabla^4\phi + \tau\frac{\partial^2\phi}{\partial t^2}\right)^2 \leq 0. \tag{24}$$

Thus, $\mathcal{F}$ given by Eq. (18) serves a Lyapunov functional for the hyperbolic SH equation [Eq. (17)].

Now we check thermodynamic consistency along the above condition (iii). The second variation in free-energy (18) is

$$\delta^2\mathcal{F} = \int dv\left\{\delta\left(\frac{\partial f}{\partial \phi}\right)\delta\phi + \delta\left(\frac{\partial f}{\partial(\partial\phi/\partial t)}\right)\delta\frac{\partial\phi}{\partial t}\right\}, \tag{25}$$

with

$$f(\phi, \partial\phi/\partial t) = g(\phi) - |\vec{\nabla}\phi|^2 + \frac{1}{2}|\nabla^2\phi|^2 + \frac{\tau}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 \tag{26}$$

as the free-energy density and it is assumed that $\delta^2\phi = 0$ and $\delta^2(\partial\phi/\partial t) = 0$ due to independency of variables ϕ and $\partial\phi/\partial t$. Then, using Eqs. (25) and (26), one obtains

$$\delta^2\mathcal{F} = \int dv\left\{\mathcal{L}(\phi, \vec{\nabla})(\delta\phi)^2 + \tau\left(\delta\frac{\partial\phi}{\partial t}\right)^2\right\}, \tag{27}$$

with the operator

$$\mathcal{L}(\phi, \vec{\nabla}) = \frac{d^2 g}{d\phi^2} + \nabla^2 + \frac{1}{2}\nabla^4. \tag{28}$$

The second variation $\delta^2\mathcal{F}$ should define the dynamic stability of solution in some specific cases. In our case (27), although a sign of the operators ∇^2 and ∇^4 might be specified (due to the nonpositive spectrum of ∇^2 and the non-negative spectrum of ∇^4), whole operator (28) has no fixed sign. From this it follows that the SH equation may give instability of its solutions in some ranges of wave vectors. Direct definition of the dynamic stability by criterion (27), consequently, is actually absent for it. Therefore, in Sec. IV we provide linear stability analysis of the hyperbolic SH-equation solutions.

IV. EVALUATION OF THE FAST DYNAMICS BY THE SH EQUATION

For stationary states with $\partial\phi/\partial t = 0$, Eq. (17) exhibits various periodic solutions [27]. Solutions of Eq. (17) were analyzed for nonstationary cases $\partial\phi/\partial t \neq 0$ with $\tau \to 0$ and small values of the governing parameter ϵ [28]. The statics and dynamics of periodic states described by the parabolic SH equation are the subjects of special attention in description of emerging patterns [7,29]. Therefore, in this section, general features of hyperbolic SH equation are analyzed with regard to advancements [7,27–29] for the parabolic SH equation.

A. Stability of homogeneous solution

Equation (17) has the trivial solution $\phi_0 \equiv 0$. This solution undergoes a supercritical stationary bifurcation at $\epsilon = 0$ leading to a small-amplitude periodic pattern at $\epsilon > 0$. To analyze this bifurcation we consider the perturbation $\delta\phi = \phi - \phi_0$ of the trivial solution $\phi_0 = 0$ with $|\delta\phi| \ll 1$. Then, from Eq. (17), one obtains

$$\tau\frac{\partial^2\delta\phi}{\partial t^2} + \frac{\partial\delta\phi}{\partial t} = [\epsilon - (1+\nabla^2)^2]\delta\phi, \tag{29}$$

where the high-order term $\delta\phi^3$ was dropped.

Using the Fourier transform $\delta\hat{\phi}_q$, Eq. (29) can be rewritten as

$$\tau\frac{d^2\delta\hat{\phi}_q}{dt^2} + \frac{d\delta\hat{\phi}_q}{dt} = [\epsilon - (1-q^2)^2]\delta\hat{\phi}_q. \tag{30}$$

The solution of Eq. (30) has the form

$$\delta\hat{\phi}_q(t) = e^{\gamma_q t}\delta\hat{\phi}_q(0), \tag{31}$$

where the amplification rate γ_q is determined by the equation

$$\tau\gamma_q^2 + \gamma_q - \epsilon + (1-q^2)^2 = 0, \tag{32}$$

having following roots:

$$\gamma_q^{(\pm)} = \frac{-1 \pm \sqrt{1 + 4\tau[\epsilon - (1-q^2)^2]}}{2\tau}. \tag{33}$$

The maximum rate $\gamma_q^{(+)}$ (a rapidly growing harmonics) corresponds to the value of $q = 1$. It is given by

$$\gamma_{\max}^{(+)} = \frac{1}{2\tau}(-1 + \sqrt{1 + 4\tau\epsilon}). \tag{34}$$

Analyzing the maximum amplification rate $\gamma_{\max}^{(+)}$ in Eq. (34), three various regimes can be outlined. *First*, with $\epsilon > 0$ one has $\gamma_{\max}^{(+)} > 0$ and the homogeneous trivial solution $\phi_0 = 0$ is unstable to small perturbations $\delta\phi$. *Second*, within the region of governing parameter ϵ given by $-1/(4\tau) < \epsilon < 0$ the maximum amplification rate is a real number and takes negative values $\gamma_{\max}^{(+)} < 0$. The solution $\phi_0 = 0$ becomes stable with a monotonic damping of the small perturbations $\delta\phi$ in time. *Third*, with $\epsilon < -1/(4\tau)$, the value of $\gamma_{\max}^{(+)}$ becomes complex. Using the denotation $\alpha = \sqrt{-4\tau\epsilon - 1} > 0$, we write Eq. (34) as

$$\gamma_{\max}^{(+)} = \frac{1}{2\tau}(-1 + i\alpha), \tag{35}$$

and solution (31) is given by

$$\delta\hat{\phi}_q(t) = \exp\left(\frac{i\alpha t}{2\tau}\right)\exp\left(-\frac{t}{2\tau}\right)\delta\hat{\phi}_q(0). \tag{36}$$

This solution describes an oscillating behavior of the perturbations with the exponential decay of their amplitudes during the time of the order of 2τ. Such behavior with damping

oscillations is absent in the model given by the parabolic SH equation [Eq. (17) with $\tau=0$].

B. Stability of periodic solution

Let us consider a perturbed solution

$$\phi(x,t) = \phi_0(x) + \delta\phi(x,t), \quad |\delta\phi| \ll 1, \tag{37}$$

with the perturbation $\delta\phi$ imposed on an initially periodic solution $\phi_0(x)$ of Eq. (17). The linearized up to first order of $\delta\phi$ last nonlinear term in Eq. (17) reads

$$\phi^3 = (\phi_0 + \delta\phi)^3 = \phi_0^3 + 3\phi_0^2\delta\phi + O(\delta\phi^2). \tag{38}$$

Substituting solution (37) into Eq. (17) and taking from Eq. (38) only the first order in $\delta\phi$, one can get

$$\tau\frac{\partial^2\delta\phi}{\partial t^2} + \frac{\partial\delta\phi}{\partial t} = (\epsilon - (1+\nabla^2)^2 - 3\phi_0^2)\delta\phi. \tag{39}$$

Equation (39) describes the evolution of the perturbation $\delta\phi$ around the periodic solution ϕ_0. Consequently, solutions of Eq. (39) might be expanded in series by basic functions of irreducible representations of the translation group. This should be the Abelian group. Therefore, the result can be expressed using the Bloch-Mathieu-Floquet theorem: the basis is generated by periodic functions multiplied on a plane wave with the wave vector from the first Brillouin zone. The latter one can be chosen as an elementary cell of the reciprocal space. In one-dimensional case, Eq. (39) is symmetric with regard to coordinate translation $x\rightarrow -x$. Therefore, the cell symmetry should correspond to the equation symmetry in the coordinate space, i.e., it should have a parity symmetry. Because the interval L of periodicity corresponds to the wave vector $q=2\pi/L$, the boundary for the Brillouin zone is defined as $Q_{gr}=\pm\pi/L=\pm q/2$. For the first Brillouin zone, one gets $-\pi/L\leq Q\leq\pi/L$. All physical characteristics can be obtained by the periodic continuation from the first Brillouin zone with the other values of Q.

Taking the above arguments into account, one can chose a linear stability Bloch-Floquet analysis used for the phase-field crystal type models by Elder and Grant [7]. We set unperturbed solution ϕ_0 and the imposed perturbation $\delta\phi(x,t)$ as

$$\phi_0(x) = \sum_n a_n e^{iqnx} \quad \text{with} \quad a_n^* = a_{-n}, \tag{40}$$

$$\delta\phi(x,t) = \sum_n b_n(t) e^{[i(qn+Q)x]}. \tag{41}$$

Substituting Eqs. (40) and (41) into Eq. (39), with the reduced term e^{iQx}, gives

$$\tau\sum_n \frac{\partial^2 b_n}{\partial t^2}e^{iqnx} + \sum_n \frac{\partial b_n}{\partial t}e^{iqnx} = \sum_n \{\epsilon - [1-(nq+Q)^2]^2\}b_n e^{iqnx} - 3\sum_{n,m,p} b_n a_m a_p e^{i(n+m+p)qx}. \tag{42}$$

Obviously, every j harmonics from Eq. (42) is given by

$$\tau\frac{\partial^2 b_j}{\partial t^2} + \frac{\partial b_j}{\partial t} = \{\epsilon - [1-(jq+Q)^2]^2\}b_j - 3\sum_{m,p} b_{j-m-p}a_m a_p. \tag{43}$$

Let us assume the one mode approximation for the undisturbed solution (40): $\phi_0(x)\sim\sin(qx)$, $a_{\pm1}\neq 0$, and $a_i=0$ for $i\neq\pm1$. Then, from Eq. (43), one gets

$$\tau\frac{\partial^2 b_j}{\partial t^2} + \frac{\partial b_j}{\partial t} = \{\epsilon - [1-(jq+Q)^2]^2\}b_j - 3(b_{j+2}a_{-1}^2 + 2b_j a_1 a_{-1} + b_{j-2}a_1^2). \tag{44}$$

Taking the one mode approximation also for perturbation (41), only two equations for $b_{\pm1}$ remain for the further analysis. These are

$$\tau\frac{\partial^2 b_{-1}}{\partial t^2} + \frac{\partial b_{-1}}{\partial t} = \{\epsilon - [1-(-q+Q)^2]^2\}b_{-1} - 3(b_{+1}a_{-1}^2 + 2b_{-1}a_{+1}a_{-1}), \tag{45}$$

$$\tau\frac{\partial^2 b_{+1}}{\partial t^2} + \frac{\partial b_{+1}}{\partial t} = \{\epsilon - [1-(q+Q)^2]^2\}b_{+1} - 3(2b_{+1}a_{+1}a_{-1} + b_{-1}a_{+1}^2). \tag{46}$$

Using relationship $a_n^*=a_{-n}$ for the a coefficients, one has $a_{+1}a_{-1}=|a|^2$. Then, introducing denotations

$$\bar{\gamma}_{-1} = \epsilon - [1-(-q+Q)^2]^2, \quad \bar{\gamma}_{+1} = \epsilon - [1-(q+Q)^2]^2, \tag{47}$$

we search for solution of Eq. (39) in the following form: $b_i = B_i\exp(\omega t)$. Substituting Eq. (45) into Eq. (46) gives

$$(\tau\omega^2+\omega)B_{-1} = (\bar{\gamma}_{-1} - 6|a|^2)B_{-1} - 3a_{-1}^2 B_{+1}, \tag{48}$$

$$(\tau\omega^2+\omega)B_{+1} = (\bar{\gamma}_{+1} - 6|a|^2)B_{+1} - 3a_{+1}^2 B_{-1}. \tag{49}$$

In a matrix form, Eqs. (48) and (49) are

$$\begin{bmatrix} \tau\omega^2+\omega-\bar{\gamma}_{-1}+6|a|^2 & 3a_{-1}^2 \\ 3a_{+1}^2 & \tau\omega^2+\omega-\bar{\gamma}_{+1}+6|a|^2 \end{bmatrix}\begin{bmatrix} B_{-1} \\ B_{+1} \end{bmatrix} = 0. \tag{50}$$

Nontrivial solution of Eq. (50) exists for the following condition:

$$\det\begin{bmatrix} \tau\omega^2+\omega-\bar{\gamma}_{-1}+6|a|^2 & 3a_{-1}^2 \\ 3a_{+1}^2 & \tau\omega^2+\omega-\bar{\gamma}_{+1}+6|a|^2 \end{bmatrix} = 0, \tag{51}$$

which is equivalent to

$$(\tau\omega^2+\omega-\bar{\gamma}_{-1}+6|a|^2)(\tau\omega^2+\omega-\bar{\gamma}_{+1}+6|a|^2) - 9|a|^4 = 0. \tag{52}$$

Denoting

$$X = \tau\omega^2+\omega+6|a|^2, \tag{53}$$

Eq. (52) can be rewritten as follows:

$$X^2 - (\bar{\gamma}_{-1} + \bar{\gamma}_{+1})X + \bar{\gamma}_{-1}\bar{\gamma}_{+1} - 9|a|^4 = 0. \tag{54}$$

The roots of Eq. (54) are described by

$$X_{\pm} = \tfrac{1}{2}(\bar{\gamma}_{-1} + \bar{\gamma}_{+1} \pm \sqrt{(\bar{\gamma}_{-1} - \bar{\gamma}_{+1})^2 + 36|a|^4}). \tag{55}$$

1. Parabolic case (τ=0)

In analysis of stability an amplitude of a faster growing perturbation is important. Therefore, in the following analysis of the unperturbed periodic solution (40), only the largest root for frequency ω is considered.

From Eqs. (53) and (55), one can find the maximum frequency with the zero relaxation time

$$\omega_0^+ = \omega^+|_{\tau=0} = X_+ - 6|a|^2 \tag{56}$$

as follows:

$$\omega_0^+ = \tfrac{1}{2}(\bar{\gamma}_{-1} + \bar{\gamma}_{+1} - 12|a|^2 + \sqrt{(\bar{\gamma}_{-1} - \bar{\gamma}_{+1})^2 + 36|a|^4}), \tag{57}$$

with $\bar{\gamma}_{\pm 1}$ given by Eq. (47). In the one mode approximation, the free-energy functional $\mathcal{F}$ is minimized by solution (40) in the form

$$\phi_0(x) = 2\sqrt{\frac{\epsilon - (1-q^2)^2}{3}}\sin(qx) = i\sqrt{\frac{\epsilon - (1-q^2)^2}{3}}e^{-iqx} - i\sqrt{\frac{\epsilon - (1-q^2)^2}{3}}e^{iqx}, \tag{58}$$

and, respectively, we have

$$a_{+1} = -i\sqrt{\frac{\epsilon - (1-q^2)^2}{3}}, \quad a_{-1} = i\sqrt{\frac{\epsilon - (1-q^2)^2}{3}}, \tag{59}$$

$$|a|^2 \equiv a_{+1}a_{-1} = \frac{\epsilon - (1-q^2)^2}{3}. \tag{60}$$

Finally, from Eq. (33) it follows that the treatment of γ_q^+ into zero corresponds to the supercritical bifurcation at which the homogeneous solution loses its stability following the inequality

$$\epsilon > (1-q^2)^2. \tag{61}$$

This condition coincides with that one directly following from the parabolic SH equation [29]. The range of existence of solution (58) is limited by inequality (61).

Substituting Eq. (60) into Eq. (57) gives the equation

$$\omega_0^+ = \tfrac{1}{2}\{\bar{\gamma}_{-1} + \bar{\gamma}_{+1} - 4[\epsilon - (1-q^2)^2] + \sqrt{(\bar{\gamma}_{-1} - \bar{\gamma}_{+1})^2 + 4[\epsilon - (1-q^2)^2]^2}\}, \tag{62}$$

where $\bar{\gamma}_{\pm 1}$ depend on Q as given by Eq. (47). Note that Eq. (62) is previously found from the parabolic SH equation (see Eq. (231) in Ref. [29]).

The frequency $\omega_0(Q)$ computed by Eq. (62) is shown by the dashed lines in Fig. 1(a) at ϵ=0.3 and for three various values of the wave number q. It is seen that the value q=1 gives nonpositive frequencies, $\omega(Q) \le 0$, for all wave numbers Q of the imposed perturbation. In this case, the initial periodic solution (40) is stable against the imposed perturbation $\sim\exp(iQx)$ given by Eq. (41). Contrary to that, instability of solution (40) occurs for some values of q; however, the scenario of the new mode selection can be more complicated. This scenario is governed by the quench depth $\epsilon(q)$ and occurs due to the Eckhaus instability [30]. In this context, the effect of $\epsilon(q)$ on the transition to the new state is evaluated as follows.

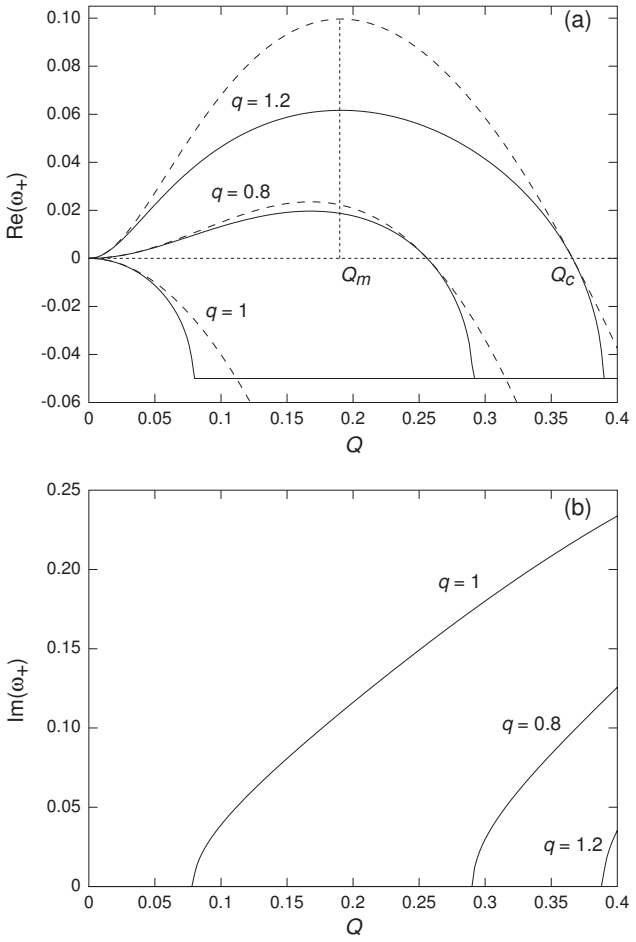

FIG. 1. Dispersion relationship $\omega(Q)$ for ϵ=0.3 and various values of q. Dashed lines are computed by Eq. (62) predicted by the SH equation [Eq. (17)] at τ=0. Solid lines are computed by Eq. (66) predicted by the SH equation [Eq. (17)] at τ=10. (a) Real part of $\omega(Q)$. For curves with q=1.2 the system becomes unstable at $Q < Q_c$ and the maximum $\omega(Q_m)$ is selected at $Q=Q_m$. (b) Imagine part of $\omega(Q)$ exist only with $\omega_0 > -1/(2\tau)$ for the hyperbolic dynamics by SH equation [Eq. (17)].

From ω_0^+ defined by Eq. (62) one can find the quench depth ϵ which governs the transition to the new state. At small values of Q, expansion of ω_0^+ from Eq. (62) yields

$$\omega_0^+ = -2\frac{1 - \epsilon(1-3q^2) - 9q^2 + 15q^4 - 7q^6}{\epsilon - (1-q^2)^2}Q^2 + \cdots. \tag{63}$$

Obviously, with the quench depth equals [29]

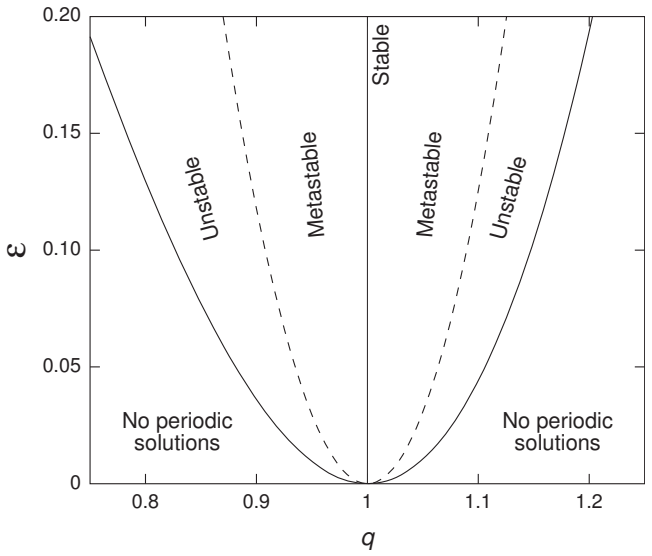

FIG. 2. Stability diagram defined by the function $\epsilon(q)$ from Eq. (64) for parabolic dynamics and Eqs. (67) and (68) for hyperbolic dynamics.

$$\epsilon(q) = \frac{1 - 9q^2 + 15q^4 - 7q^6}{1 - 3q^2}, \tag{64}$$

the coefficient with Q^2 in expansion (63) becomes zero. The negative coefficient with Q^2 in expansion (63) leads to nonpositive values of the function ω_0^+ and therefore to stable initial solution. In the opposite case, the function ω_0^+ takes positive values in an interval $0<Q<Q_c$ and the perturbation $\delta\phi$ grows in time making the initial solution unstable. In this meaning, the function $\epsilon(q)$ defines a subcritical bifurcation under which a metastable state appears (in the one mode approximation). This is shown in Fig. 2.

In the region "no periodic solutions" of Fig. 2 the homogeneous solution may exist. Therefore, the solid curve defines a bifurcation boundary $\epsilon=(1-q^2)^2$ above which the homogeneous solution loses its stability. Hence, in the region "unstable" of Fig. 2, both homogeneous solution and periodic (one mode) solution are unstable. Finally, in the region "metastable" of Fig. 2, the periodic solution is stable only at $q=1$, and with $q\neq 1$ it has a finite lifetime before losing its stability. The homogeneous solution is always unstable in the metastable region.

2. *Hyperbolic case* ($\tau\neq 0$)

Now we analyze the hyperbolic SH equation [Eq. (17)] in which $\tau\neq 0$ in order to compare its qualitative predictions with the parabolic SH equation. From Eqs. (53) and (55) one gets

$$\tau\omega_\pm^2 + \omega_\pm = \omega_0, \tag{65}$$

where $\omega_0 \equiv \omega_0^+$ is the maximum frequency from the parabolic case $\tau=0$ obtained by solution (62). Equation (65) has two roots but only the maximum root ω_+ corresponding to the faster growing amplitude of perturbation is important.

From Eq. (65) one finds the maximum root for frequency as

$$\omega_+ = \frac{-1 + \sqrt{1 + 4\tau\omega_0}}{2\tau}. \tag{66}$$

It is expressed through the frequency ω_0 obtained from the parabolic SH equation [Eq. (17)] with $\tau\to 0$.

In the same way as for the parabolic case, the boundary between stable and metastable states is determined by the condition

$$\left.\frac{\partial^2\omega_+}{\partial Q^2}\right|_{Q\to 0} = 0. \tag{67}$$

From Eq. (66) it follows that

$$\frac{\partial^2\omega_+}{\partial Q^2} = \frac{1}{(1+4\tau\omega_0)^{1/2}}\frac{\partial^2\omega_0}{\partial Q^2} - \frac{2\tau}{(1+4\tau\omega_0)^{3/2}}\left(\frac{\partial\omega_0}{\partial Q}\right)^2. \tag{68}$$

Therefore, at $Q\to 0$, condition (67) is equivalent to expression (64) for the function $\epsilon(q)$ because $\partial\omega_0/\partial Q=0$. Section V gives a discussion about stability of the homogeneous and periodic solutions in parabolic and hyperbolic SH equations.

V. DISCUSSION

A. Homogeneous solution

The results of Sec. IV A demonstrate the effect of the second time derivative in Eq. (17). It reflects the effect of memory through a finite relaxation of flux (1). Obviously, in case $\epsilon<0$, the homogeneous solution $\varphi_0=0$ is stable and any small perturbation $\delta\phi$ decays with characteristic rate $\gamma_q<0$ [see Eqs. (31) and (34)]. However, parabolic and hyperbolic dynamics exhibit principally different behavior in damping perturbations.

In the parabolic case of $\tau\to 0$, Eq. (34) reduces to the simple relation $\gamma_{\max}^{(+)}=\epsilon$ for the perturbation with wave vector $q=1$. The decay rate increases with increasing in the quench depth $|\epsilon|$. Therefore, for high values of $|\epsilon|$, the perturbations disappear "instantaneously" in the parabolic dynamics.

Introduction of the relaxation time $\tau>0$ leads to appearance of an upper limit for the absolute value of the real part $|\mathrm{Re}(\gamma_{\max}^{(+)})|$ of the decay rate in contrast to unlimited decay rates in parabolic case with $\tau=0$. According to Eq. (35), the memory effect in the system limits the maximal exponential decay by $-1/(2\tau)$. For values $\epsilon<-1/(4\tau)$, the exponential relaxation of the perturbations is accompanied by the time oscillation of the perturbation amplitude [Eq. (36)].

B. Periodic solution

From Eq. (66) it can be seen that the faster growth mode with frequency ω_+ can take both positive values (with $\sqrt{1+4\tau\omega_0}>1$) and negative values (with $\sqrt{1+4\tau\omega_0}<1$). Solid lines in Fig. 1(a) demonstrate the real part of the frequency ω_+ computed by Eq. (66). One can show that the root $Q>0$ of equation $\omega(Q)=0$ does not depend on the relaxation time τ. Therefore, as is presented in Fig. 1(a), the values of function $\omega(Q)$ merge for hyperbolic and parabolic cases at $Q=Q_c$. One can also see that ω_+, obtained from the analysis of the hyperbolic equation and computed by Eq. (66), essen-

tially differs from ω_+ found from the analysis of the parabolic equation and computed by Eq. (62), particularly, at $Q > Q_c$.

Both parabolic and hyperbolic functions $\omega_+(Q)$ reach a maximum value at the same point Q_m. The maximum of ω_+ obtained from the analysis of the hyperbolic equation is always lower than the same value given by the parabolic SH equation. Hence, the new selected pattern predicted from the hyperbolic SH equation is selected slower than in the parabolic case.

Another feature of the hyperbolic SH equation [Eq. (17)] can be seen in predicting complex values of ω which additionally contribute into the frequency ω_+. Indeed, the square root in Eq. (66) can give the complex values for ω_+ with $1+4\tau\omega_0<0$. Therefore, with $\omega_0<-1/(4\tau)$, the frequency ω_+ gives nonzero imaginary part [see Fig. 1(b)] and the real part of the frequency is equal to the constant value of $\omega_+=-1/(2\tau)$ [see Fig. 1(a)]. In any case, however, the imaginary part of ω_+ gives degenerating modes with $\omega_+<0$ and it has no influence on instability.

The periodic solution has analog peculiarity with the result of stability analysis of homogeneous solution discussed in Sec. V A. Indeed, the relaxation of perturbation $\delta\phi$ of the stable periodic solution ϕ_0 in Eq. (40) has the upper limit for the decay rate ω. This limit has the same value $-1/(2\tau)$ [see also Fig. 1(a)] and exhibits the general attribute of the system with memory: the damping of perturbation occurs during finite time and the perturbation does not disappear instantaneously.

C. Difference in parabolic and hyperbolic dynamics

Suggested in Secs. II and III a phenomenological method for constructing various extended equations of motion in PFC and SH models has been demonstrated through the application of exponentially decaying memory function which leads to the system of hyperbolic equations [Eqs. (16) and (17)]. The inertia term $\tau\partial^2\phi/\partial t^2$ distinguishes the hyperbolic dynamics from the parabolic one (with $\tau\to 0$) in the evolution delay of the system. Such delay is the result of adopting the additional fast degree of motion in hyperbolic equations using the fast variable $\partial\phi/\partial t$ in free-energy (18).

Two characteristic time scales appear in the evolving hyperbolic system: the time τ for vanishing of the fast variable $\partial\phi/\partial t$ by exponential relaxation and the dissipative time $\tau_{dif}\equiv 1/\gamma_{\max}^{(+)}=-1/(2\epsilon)$ for structural relaxation given by Eq. (34) at $\tau\to 0$. At small driving force of phase transition (small ϵ), the dissipative relaxation time τ_{dif} is large enough to neglect the inertia motion in the system evolution (or to neglect the memory function of any other kind to construct the extended mode). In this case the system is described by usual dissipative model based on a parabolic equation. In contrast, at large driving force of phase transition, the parameter ϵ can be large enough to consider the dissipation time $\tau_{dif}\sim\epsilon^{-1}$ in fast time scale. In this case, inertia motion cannot be neglected; it is considered as a fast process comparable with structural relaxation process, and it may play an essential role in dynamics of the system with memory.

As the first example, the dynamics predicted by parabolic and hyperbolic SH equations differs in transition from unstable homogeneous solution to metastable periodic solution. This difference can be visible from the direct numeric modeling of the transition. Using an explicit numerical scheme, the one-dimensional discrete equation [Eq. (17)] is

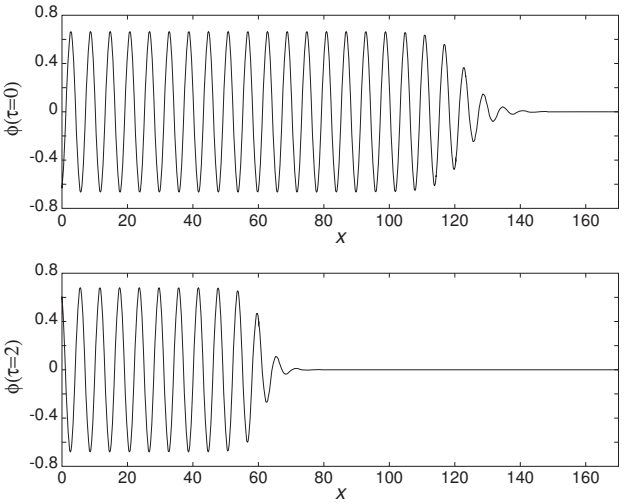

FIG. 3. Dynamics of the transition from homogeneous unstable to periodic metastable pattern predicted by solution of Eq. (69). Predictions are given for parabolic system (upper figure) and hyperbolic system (below figure).

$$\phi_i^n = [c_1 + c_3(\epsilon - 1)]\phi_i^{n-1} - c_2\phi_i^{n-2} - c_3[(\phi_i^{n-1})^3 + 2\Delta\phi_i^{n-1} + \Delta^2\phi_i^{n-1}] \quad (69)$$

with $c_1=(2\tau+\delta t)/(\tau+\delta t)$, $c_2=\tau/(\tau+\delta t)$, and $c_3=(\delta t)^2/[\tau(1+\delta t/\tau)]$ as the coefficients of the numerical scheme, Δ as the numerical approximation of the Laplace operator which in the present scheme is given by the three-point approximation with the accuracy of $(\delta x)^2$, δt as the time step, δx as the spatial grid size, and n as the number of time steps. Initial conditions are taken as $\partial\phi/\partial t=0$, one fluctuation of ϕ at the first node of the grid and $\phi=0$ at the other grid nodes. The constant values $\phi=0$ are taken at both boundaries of the grid. Figure 3 demonstrates results of solution of Eq. (69) at the following parameters: $\epsilon=0.35$, $n=18\,000$, and $\delta t=0.01$ and $\delta x=0.85$ for parabolic evolution ($\tau=0$) and hyperbolic evolution ($\tau=2$). It is clearly seen that the front of the periodic pattern invades the unstable homogeneous state more slowly in hyperbolic dynamics (below figure) in comparison with the parabolic dynamics of the same transition (upper figure).

As the second example, one can finally consider the transition within the periodic structure itself. Results of the analysis demonstrate that the transition from unstable periodic state to the new (meta)stable periodic state proceeds more slowly in hyperbolic dynamical system than in the parabolic one. Indeed, the quench depth $\epsilon(q)$ given by Eq. (62) and Eqs. (67) and (68) for parabolic and hyperbolic cases, respectively, predicts the same boundaries between regions of metastability or instability, as is shown in Fig. 2. It means that the final critical points for metastability or instability in the evolution are the same but the dynamics between these metastable and unstable states is different for the parabolic and hyperbolic cases. It can be clearly seen in selection

of maximum ω_+ shown by Fig. 1(a): every solid curve gives lower maximum than the corresponding dashed curve at $Q = Q_m$.

In both cases, demonstrated by Figs. 1 and 3, the slower hyperbolic dynamics is the result of introducing fast degrees of freedom through the memory which is phenomenologically described by the delay given by the inertia term $\tau\partial^2\phi/\partial t^2$ in Eq. (17).

D. Attribution to experiment

Several comments on experimental verification of the analyzed effects in hyperbolic system described by Eqs. (16) and (17) can be outlined. First, an experimentally tested system must be nonequilibrium under applied large quench depth ϵ (undercooling) into the unstable (metastable) region of phase diagram. In this case, the system evolves with short periods of its relaxation on the order of the characteristic time τ. Due to appearing of such "fast" time scale measured in units of relaxation time τ, the observable time for experimental measurement should be on the order of τ. Second, considering nonconserved dynamics, the time for measurements might be essentially increased to observe effects from damped oscillations in hyperbolic SH system (discussed in Secs. V A and V B). This increases becomes possible if the periodic pattern is formed under additional governing parameter which can be seen as anisotropy amplifying the growth of perturbations and prolonging damped oscillations. A well-known example from the nonconserved dynamics of periodic pattern is the crystalline anisotropy which amplifies action of perturbations along the needlelike shape of a dendritic crystal [31]. In this analogy, one may expect amplifying and prolongation of damped oscillations in nonconserved dynamics of strongly nonequilibrium system with anisotropic interfaces (surfaces with edges and faces with preferable crystalline directions). Third, considering conserved dynamics, the influence of inertia motion in a system described by hyperbolic PFC equation(s) can be verified, e.g., in a fast solidifying system. In this system, nonequilibrium effects, such as disorder trapping or solute trapping, are investigated using modern experimental techniques [32] including *in situ* high-speed-diagnostic methods [33]. Particularly, as a result of complete solute trapping, the diffusionless regime of solidification occurs at a finite solidification velocity as obtained in experiments. A transition from chemically partition regime to the diffusionless regime of solidification with complete solute trapping is reasonably predicted in a system with hyperbolic dynamics [34]. The details of the mechanism of solute trapping and the transition to diffusionless solidification in experimental findings can be clarified using hyperbolic PFC-type model(s).

VI. CONCLUSIONS

Slow and fast dynamics in phase transitions are described using memory functions of various forms. The present extended version of PFC- and SH-type models is analyzed by the second-order approximation of the fast variable [see the last term in the integrand of Eq. (18)]. This approximation though is sufficient to deal with a wide range of physical problems having inertia and fast degrees of freedom. The procedure of finding thermodynamic consistency used for nonconserved dynamics by the hyperbolic SH equation can be applied to the analysis of the hyperbolic PFC equation [Eq. (16)] as well as to other models described by Eqs. (4)–(12).

The present analysis of solutions in nonconserved dynamics predicts oscillations during finite time in damping perturbations which is neglected in the solution of the problem with pure parabolic dissipative dynamics. Thus, including memory into analysis leads to prediction of fast degrees of freedom in phase transitions that is demonstrated in examples of PFC and SH equations with inertia.

Introducing inertia into equations of motion gives two-stage relaxation in the system. The first stage is represented by local relaxation of the fast variable (rate of change in the order parameter $\partial\phi/\partial t$) to its steady state. This type of relaxation has characteristic relaxation time τ. The second stage is considered as a structural relaxation of the periodic pattern with the diffusive time τ_{dif}. At large quenching depth ϵ (undercooling) into the unstable (metastable) region of the phase diagram, these quantities, τ and τ_{dif}, become comparable by the order of magnitude and inertia plays a crucial role in evolution of the system. This two-stage relaxation process can be considered as one of the principally important qualitative features of the nonequilibrium formation of periodic patterns.

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