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Physical analogy between continuum thermodynamics and classical mechanics

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The main focus of this paper is the profound physical analogy between a continuum thermodynamical system, which evolves with relaxation under (possibly) nonisothermal conditions, and a classical mechanical system of a few interacting particles moving with dissipation in (possibly), time-dependent nonconservative fields. This analogy is applied to the problem of phase transitions in a one-dimensional thermodynamic system. The thermomechanical analogy stems from the validity of variational methods in mechanics and thermodynamics and allows for a different interpretation of the dynamical selection principle in the theory of pattern formation. This physical analogy is very helpful for understanding different nonlinear thermodynamic phenomena and for developing intuition in numerical simulations.

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I. INTRODUCTION

Equilibrium and dynamical analysis of heterogeneous thermodynamic systems has been taking a stride forward in the past few years. Much of the credit for this progress should be given to the introduction and development of the continuum methods in the thermodynamics of heterogeneous systems. Conceived in different scientific communities, these methods received different names: Ginzburg-Landau in physics [1], Cahn-Hilliard in materials science [2], phase field in applied mathematics [3], although the underlying idea of all these methods is the same. In order to characterize different thermodynamic states of the system, one attempts to introduce a set of continuum variables with distinctly different values at different states. Such variables obey dynamic equations that describe evolution of the thermodynamic system. This method represents a whole paradigm, which has spread to many different branches of science beyond thermodynamics.

The success of the continuum method is mainly due to two reasons. It opens the door for a broad range of variational methods to be used in thermodynamics [4] and, on the other hand, proves to be extremely convenient in numerical realization for computer simulation of different sorts of transformations in thermodynamic systems [5,6].

In the course of the development of these ideas, a profound physical analogy has been found between the steady motion of a scalar thermodynamic field and the classical (nonrelativistic) mechanical motion of a particle [7–9,4]. The thermomechanical analogy stems from the validity of variational methods in both mechanics and thermodynamics and is the main focus of the present paper. Although the subject of a thermomechanical analogy is not completely original (it suffices to recall the usage of the Legendre transformation in mechanics and thermodynamics [10]), the particular one discussed here has not received sufficient attention in the literature. Analogies helpfully link what is being studied to what is already understood and allow for developing intuition, which is very useful in numerical simulations. In this article we intend to generalize this analogy to the case of thermodynamic systems with many internal parameters undergoing different phase transitions, and elucidate the connection of this analogy to a dynamical selection principle in the theory of pattern formation. Another goal is to show how mechanical intuition can be used for computer simulations of phase transitions.

II. EQUILIBRIUM IN A MULTICOMPONENT SYSTEM

A. Continuum thermodynamics of one-dimensional heterogeneous systems

The first step in any theoretical description of a thermodynamic system is the selection of a set of independent variables that specify the system and conjugate-dependent functions that characterize the state of thermodynamic equilibrium. One may argue that temperature and pressure is a better choice of independent variables than energy density and specific volume because, regardless of the outer constraints of open or closed systems, conditions of equilibrium include constant temperature and pressure throughout, but not constant energy density or specific volume. In addition to temperature T and pressure P, a thermodynamic system is characterized by the densities of n different components, $\rho_1, \rho_2, \rho_3, \ldots, \rho_n$, which specify the overall composition of a system and obey the conservation of particles condition:

$$\frac{d}{dt}\int \rho_i d^3x = 0. \qquad (1)$$

Another set of internal variables $\{\eta_j\}$ is associated with the underlying physical differences between the states. In the framework of the Ginzburg-Landau theory of phase transitions [1], the internal variables $\{\eta_j\}$ are associated with symmetries of the states and are usually called order parameters (OP's). The thermodynamic potentials of the system become

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continuous functions of these variables: $\Phi = \Phi\{T,P;\rho_i,\eta_j\}$. At equilibrium, the densities and order parameters take on specific values, which are functions of temperature and pressure, $\{\rho^E,\eta^E\} = \Xi(T,P)$, and can be found from the proper condition of thermal equilibrium. Away from equilibrium they become dependent on time and eventually relax back to these specific values. The difference between densities and order parameters is that the latter do not obey conservation conditions of the type of Eq. (1) and hence may serve as measures of deviation from equilibrium in the system. As the fundamental difference between the phases is their symmetries, the concept of an order parameter may also be used to define a *bulk phase* as a locally stable state of matter homogeneous in the order parameters.

The presence of defects in the form of precipitates of a second phase or different homo- or heterophase interfaces makes a system essentially inhomogeneous, that is, there appear gradients of the independent variables like densities and order parameters. There is a certain penalty on the inhomogeneous system in the form of the "gradient energy" contribution to the thermodynamic potentials, which appears because the densities of the thermodynamic potentials $\hat{\varphi}$ become functions of the gradients of the thermodynamic variables as well as variables themselves. Thereby, the thermodynamic potentials become functionals over the entire system:

$$\Phi\{T,P\} = \int \hat{\varphi}(T,P;\rho_i,\eta_j;\nabla\rho_i,\nabla\eta_j)d^3x. \tag{2}$$

We consider an open thermodynamic system, which is capable of exchanging energy, matter, or volume with the ambience that is, a grand canonical ensemble. The equilibrium conditions for an open system involve the grand canonical potential of the whole system Ω [11]. The derivation of such conditions in the framework of the continuum approach is given, e.g., in Ref. [12]:

$$\Omega \equiv \int \hat{\omega} d^3x \rightarrow \min, \quad \hat{\omega} = \hat{f} - \mu_i\rho_i. \tag{3}$$

Here $\hat{\omega}$ is the density of the grand canonical potential, the μ_i's are the chemical potentials of the components, and Einstein summation over the repeated indices is implied. In this paper the gradient-energy contribution is represented in the standard Ginzburg-Landau-Cahn-Hilliard form [1,2]. For the free energy density of a heterogeneous system, $\hat{f}$, this yields the following expression:

$$\hat{f} = f(T,\rho_i,\eta_j) + \frac{1}{2}\nabla\rho_i\kappa_{\rho,ij}\nabla\rho_j + \frac{1}{2}\nabla\eta_i\kappa_{\eta,ij}\nabla\eta_j, \tag{4}$$

where $\kappa_{\alpha,ij}$ ($\alpha = \eta$ or ρ) are symmetric matrices of the gradient free energy coefficients, which may depend on temperature and pressure. The cross terms have been retained, because they may be of the same order of magnitude as the diagonal ones. Then equilibrium in the heterogeneous system satisfies the simultaneous Euler-Lagrange equations:

$$\frac{\delta\Omega}{\delta\eta_j} \equiv \partial_{\eta_j} f - \kappa_{\eta,jk}\nabla^2\eta_k = 0, \tag{5a}$$

$$\frac{\delta\Omega}{\delta\rho_i} \equiv \partial_{\rho_i} f - \mu_i - \kappa_{\rho,ik}\nabla^2\rho_k = 0. \tag{5b}$$

Here and in the following $\partial_u\varphi$ is a partial derivative of φ with respect to u and $\delta\Phi/\delta u$ is a variational derivative of Φ with respect to $u(\cdot)$ while other variables are held constant.

At a constant temperature and pressure Eqs. (5) have solutions with different symmetries, e.g., planar [13], cylindrical, or spherical [14]. However, only one-dimensional translation-invariant solutions are subjected to the thermomechanical analogy discussed in this article. Using translation invariance of the one-dimensional solutions, the equilibrium Eqs. (5) may be integrated once to yield the first integral in the form [12]:

$$\breve{\omega} \equiv f(T,\rho_i,\eta_j) - \mu_i\rho_i - \frac{1}{2}\frac{d\rho_i}{dx}\kappa_{\rho,il}\frac{d\rho_l}{dx} - \frac{1}{2}\frac{d\eta_j}{dx}\kappa_{\eta,jk}\frac{d\eta_k}{dx} = \text{const.} \tag{6}$$

In Eqs. (3), (4), and (6) and all that follow, the bare quantities stand for local densities of thermodynamic functions, the careted quantities are defined as the sums of the local and gradient contributions and stand for nonlocal densities of thermodynamic functions, while the quantities with the breve ($\cup$) are defined as the differences of the local and gradient contributions.

Applying the first integral, Eq. (6), to a bulk phase, the constant of integration is identified as the negative of the hydrostatic pressure P:

$$P = \mu_i\rho_i^E - f(T,\rho_i^E,\eta_j^E). \tag{7}$$

Entropy, volume, and other thermodynamic functions may be found with the help of the corresponding Legendre transformation acting on the grand canonical potentials. For instance, the internal energy functions are found through the Legendre transformation in temperature:

$$\{E,\hat{e},\breve{e},\kappa_E\} = (1 - T\partial_T)\{\Omega,\hat{\omega},\breve{\omega},\kappa\}. \tag{8}$$

The approach outlined for Eqs. (1)–(8) describes a process of phase transitions if f represents a multiwell function of OP's. Depending on T and P, Eq. (6) has different periodic and nonperiodic one-dimensional solutions. The nonperiodic two-well solution describes a transition region between the two phases (α) and (β) coexisting at equilibrium, that is, an *interface*, while the nonperiodic one-well solution describes a *critical nucleus* [13].

As is known [15], all properties of an interface at equilibrium are completely determined by just one intensive quantity, the *surface tension* or specific surface energy, σ. The surface tension is defined as the excess of the appropriate thermodynamic potential of the system with an interface, per unit area of the interface A, compared to that of the homogeneous bulk phase occupying the same volume. The appropriate thermodynamic potential must be equal in both phases.

TABLE I. Dictionary of the thermomechanical analogy.

Continuum thermodynamics (1D systems)	Classical mechanics of many particles
Equilibrium in an open system	**Dynamics in a conservative system**
Clausius' principle	Hamilton's principle
Spatial coordinate x (1D system) $[x_1, x_2]$	Time t $[t_1, t_2]$
Thermodynamic variables $\{\rho_i, \eta_j\}$	Generalized coordinates
Gradient free energy coefficients $\kappa_{\alpha,ij}$	Generalized masses
Negative of the local density of the potential ω	Potential function Π
Density of the gradient energy	Kinetic energy K
Density of the grand canonical potential $\hat{\omega}$	Lagrangian
The quantity $\breve{\omega}$	Negative of the Hamiltonian
Equilibrium equations	Lagrange equations
Pressure P	Total mechanical energy $(K+\Pi)$
Total grand canonical potential Ω	Action
The surface energy	"Abbreviated action"
Particle conservation condition	No simple analogy
Relaxation dynamics	**Dissipative dynamics**
TDGLE	Lagrange equation with dissipation
Velocity over relaxation coefficient V/γ_i	Dissipative coefficient
Dissipative function $\mathcal{F}$	Rayleigh's function
Nonisothermal dynamics	**Dynamics in external fields**
Temperature	Time-dependent external field

This requirement caused Gibbs to select the grand canonical potential for the definition of surface tension. Thus the expression for the surface tension is

$$\sigma \equiv \frac{\Omega - \Omega_{\text{bulk}}}{A} = \int_{\alpha}^{\beta} (\hat{\omega} + P)\, dx. \tag{9}$$

Using Eqs. (3), (4), (6), and (7) with Eq. (9), we obtain that the surface energy of a flat interface may be expressed as follows [12]:

$$\sigma = \int_{\alpha}^{\beta} \left\{ \frac{d\rho_i}{dx} \kappa_{\rho,ij} \frac{d\rho_j}{dx} + \frac{d\eta_i}{dx} \kappa_{\eta,ij} \frac{d\eta_j}{dx} \right\} dx. \tag{10}$$

The boundaries of integration from x_α to x_β are equivalent to going from $-\infty$ to $+\infty$. Note that, although the bulk phases are included in the integration, the integral in Eq. (10) does not diverge because the integrand vanishes in both bulk phases.

B. Mechanical analogy

A profound physical analogy may be brought to bear between a one-dimensional (1D) thermodynamic system at equilibrium and a conservative classical-mechanical (Hamiltonian) system of several coupled point masses moving in a potential field. This analogy is based on the application of variational principles in thermodynamics and mechanics. Table I provides a summary of the analogous terms in thermodynamics and classical mechanics. According to this analogy the spatial coordinate x of a 1D thermodynamic system is analogous to the time t of a mechanical system; (ρ_i, η_j) are analogous to the generalized coordinates of the particles; gradient free energy coefficients are analogous to the generalized masses of the particles; and $(i+j-1)$ is the number of degrees of freedom of a mechanical system. In the framework of this analogy, the negative of the local density of the grand canonical potential $(-\omega)$ is analogous $(\doteq)$ to the mechanical potential function Π, while the sum of the gradient free energy terms is analogous $(\doteq)$ to the total kinetic energy of the particles of the mechanical system, K:

$$\Pi \doteq -\omega(\rho_i, \eta_j; T, \mu_i) = \mu_i \rho_i - f(T, \rho_i, \eta_j), \tag{11a}$$

$$K \doteq \frac{1}{2} \frac{d\rho_i}{dx} \kappa_{\rho,il} \frac{d\rho_l}{dx} + \frac{1}{2} \frac{d\eta_j}{dx} \kappa_{\eta,jk} \frac{d\eta_k}{dx}. \tag{11b}$$

The density of the grand canonical potential $\hat{\omega}$, Eqs. (3) and (4), is analogous to the Lagrangian of the mechanical system and the quantity $\breve{\omega}$, Eq. (6), to the negative of the Hamiltonian. Notice that $\breve{\omega}$ can be obtained from $\hat{\omega}$ with the aid of the Legendre transformation in $(\boldsymbol{\nabla}\rho_i, \boldsymbol{\nabla}\eta_j)$ [see Eqs. (3), (4), and (6)]. Then Eqs. (5) correspond to Newtonian equations of motion of a mechanical system in either Lagrange's or Hamilton's formulation. The pressure P is analogous to the total mechanical energy of the system $(K+\Pi)$ and the condition of thermodynamic equilibrium, Eq. (6), that is, the constancy of pressure throughout the system, is analogous to the conservation of the mechanical energy. The energy is conserved because the Hamiltonian does not depend explicitly on time and the pressure is constant because $\breve{\omega}$ does not depend explicitly on the coordinate x. The total grand canonical potential of the thermodynamic system Ω, Eq. (3), is analogous to the action of the mechanical system and the surface energy σ, Eq. (10), to the "abbreviated action" [16].

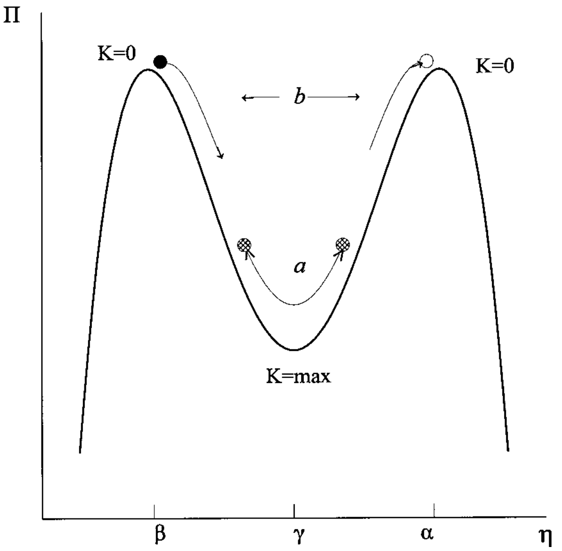

FIG. 1. Even potential function Π corresponds to thermodynamic equilibrium between phases α and β. Undamped oscillator is the mechanical analogue of an equilibrium heterogeneous 1D thermodynamic system. α, β, and γ are rest points of the point mass. (a) Periodic oscillator: the shaded circles indicate the turning points of the point mass. (b) Heteroclinic orbit: the filled (β) and open (α) circles indicate initial and final positions of the point mass (stable bulk phases).

Then the minimization of the surface energy is analogous to the principle of least action for the mechanical system.

The thermomechanical analogy can be used for better understanding the problem of phase transitions. For instance, application of the formalism of action-angle variables to a one-component thermodynamic system with a single scalar order parameter helps identify and interpret different equilibrium states in the system: the bulk phases α and β correspond to unstable (saddle-type) rest points separated by a stable (center-type) rest point γ of the mechanical system with one degree of freedom (see Fig. 1). Heterogeneous equilibrium states correspond to bound solutions of the mechanical system, e.g., periodic thermodynamic states to periodic mechanical solutions [Fig. 1(a)]. Due to unboundness of the free energy *f*, Eq. (4) and, hence, potential Π, Eq. (11a), only one type of periodic motion is possible, oscillation (no rotations). The interface between the bulk phases α and β corresponds to the *heteroclinic trajectory* that connects two different rest points with equal potential energies Π [Fig. 1(b)]. A critical nucleus corresponds to a *homoclinic orbit* that connects one rest point of lower potential energy Π to itself, which is possible only for a "tipped-off" potential Π (not equal depths of the wells), as shown in Fig. 2(a).

Notice that in the transformation from thermodynamics to mechanics the equilibrium states exchange their stabilities due to the negative sign in Eq. (11a). For instance, mechanical periodic solutions are stable, while their thermodynamic counterparts are not. The latter, however, do appear in the processes of phase transitions and the systems undergoing the transformation spend a great deal of time in the vicinity of the periodic states [5].

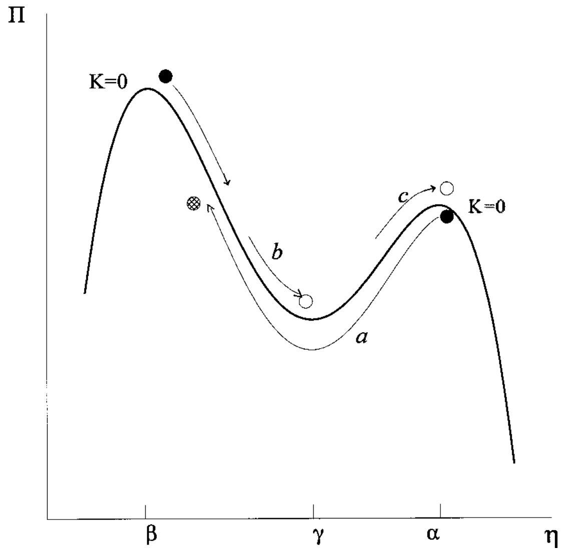

FIG. 2. Tipped-off potential function Π corresponds to thermodynamic preference of a stable phase β compared to a metastable phase α. Damped oscillator is the mechanical analog of a traveling wave in the thermodynamic system. The filled circles indicate the initial positions, the open circles indicate the final position, and the shaded circle indicates the turning point of the point mass. (a) Homoclinic orbit; (b) critically damped oscillator; (c) "marginally" damped oscillator.

III. DYNAMICS IN A ONE-COMPONENT SYSTEM

A. Isothermal dynamics

Away from equilibrium the thermodynamic system relaxes back to an equilibrium state, that is, one of the solutions of Eqs. (5). To characterize the response of a nonequilibrium system, in compliance with the second law of thermodynamics, Onsager assumed it to be linearly proportional to the thermodynamic driving force, which is the deviation of the system from equilibrium [17]. Mandel'shtam and Leontovitch implemented these ideas in a seminal paper [18], where they studied relaxations and scattering of sound in liquids without phase transitions. For the degree of relaxation they introduced the evolution equation $\dot{\eta} \propto -(\partial\Omega/\partial\eta)_{T,P}$, which Landau and Khalatnikov adopted later in their study of the absorption of sound in the vicinity of a second-order phase transition [19].

In heterogeneous media the gradient-energy contribution is essential and the thermodynamic potentials are functionals [see Eq. (2)]. Hence, the local thermodynamic forces are expressed as the variational derivatives of the grand potential [left-hand sides of Eqs. (5)] instead of the partial ones. The general equation of the order parameter evolution takes the form, which came to be known as the "time-dependent Ginzburg-Landau equation" (TDGLE):

$$\partial_t \eta_j = -\gamma_j \frac{\delta\Omega}{\delta\eta_j} \quad \text{(no summation)}. \tag{12}$$

The response coefficients γ_j set the relaxation time scales proportional to γ_j^{-1}. Relaxation of densities follows a different evolutionary path, which is described by the so-called

Cahn-Hilliard equation because the densities obey the particle conservation condition (1). Relaxation of density is not considered in this paper because we were not able to establish an analogy between the constraint (1) and classical mechanics.

An analogy can be established between translation-invariant motion in a relaxing thermodynamic system, which satisfies Eqs. (12), and motion of particles in a dissipative mechanical system with the frictional forces proportional to their velocities. Such a system is described by Rayleigh's dissipative function, whose partial derivatives yield the frictional forces that should be added to the right-hand sides of the Lagrange equations [20]. Translation-invariant solutions of Eq. (12) represent waves, $\{\eta_j=\eta_j(x-Vt)\}$, which travel with constant speed V and obey the simultaneous equations

$$\kappa_{\eta,jk}\frac{d^2\eta_k}{dx^2}+\frac{V}{\gamma_j}\frac{d\eta_j}{dx}-\partial_{\eta_j}\omega=0 \quad (\text{no summation in } j). \tag{13}$$

The sought thermomechanical analogy will be established if, on the top of the above described equilibrium analogy, the coefficients V/γ_i in Eq. (13) will be brought into correspondence with the dissipative coefficients of Rayleigh's function (see Table I).

The thermomechanical analogy helps develop an intuitive understanding of the dynamics of phase transitions. For instance, it clearly shows that in the dynamical case the equilibrium types of heterogeneous solutions, periodic, critical nucleus, and stationary interface, are destroyed because they correspond to the conservation of the mechanical energy (see Fig. 2). They are replaced, however, by traveling waves with different speeds V. The thermomechanical analogy also helps interpret the *principle of selection* of such waves, that is, to determine the unique velocity of a wave that will be realized in a physical or numerical experiment with given temperature and pressure. Decomposition of an unstable state γ, for instance, may propagate with many acceptable velocities V, according to Eq. (13) [21]. This corresponds to the damped oscillations of a particle about a stable rest point γ with different values of the friction coefficient (Fig. 2). Recall that the thermomechanical analogy changes the stabilities of the equilibrium states of the system (rest points). The asymptotically stable front solution, however, corresponds to the case of "marginal stability" [7,8], that is, the waves that move more slowly are unstable to perturbations while those that move faster are stable. From the standpoint of the thermomechanical analogy, the asymptotically stable wave of decomposition of an unstable state corresponds to a particle motion with *critical damping* [Fig. 2(b)].

An interface between a stable (β) and a metastable (α) state corresponds to a wave described by a heteroclinic trajectory between two rest points with different potential energies Π. It cannot move at a steady pace with an arbitrary speed. Instead, the speed V of the wave (interface) is *selected* as an eigenvalue of the boundary problem Eq. (13), that is, for dissipative coefficients smaller than the "marginal" trajectories are unbounded, while for greater ones trajectories never reach the rest point (α) [see Fig. 2(c)]. Hence, the selected wave (interface) also possesses a "marginal property," which is best revealed by the thermomechanical analogy.

The thermomechanical analogy also allows one to generalize the relaxational dynamics by including the cross terms between the thermodynamic "driving forces" and responses. The simultaneous generalized equations (GTDGLE's) take the form

$$\frac{\delta\Omega}{\delta\eta_j}+\frac{\partial\mathcal{F}}{\partial(\partial_t\eta_j)}=0, \tag{14}$$

where $\mathcal{F}$ is a positive definite dissipative function:

$$\mathcal{F}\equiv\frac{1}{2}(\partial_t\eta_j)\tau_{jk}(\partial_t\eta_k)>0,$$

$$\tau_{jk}=\tau_{kj}, \quad \tau_{jj}=\gamma_j^{-1}>0. \tag{15}$$

Using Eq. (14) and the Euler relation for homogeneous functions of the second order, it is easy to show that the rate of the "free energy" change in the system is

$$\frac{d\Omega}{dt}\equiv\int\frac{\delta\Omega}{\delta\eta_j}\partial_t\eta_j d^3x=-\int 2\mathcal{F}d^3x<0, \tag{16}$$

where the last inequality follows from Eq. (15). For a traveling wave $\{\eta_j=\eta_j(x-Vt)\}$, Eq. (16) can be represented as follows:

$$\frac{d}{dx}\breve{\omega}(T,\eta_i)=2V\mathcal{F}>0. \tag{17}$$

For a thermodynamic system, Eqs. (16) and (17) mean that $2\mathcal{F}$ is the local rate of dissipation, which is analogous to the dissipation of the mechanical energy due to friction in a mechanical system [20]. Thermodynamically, Eq. (17) can also be interpreted so that the wave speed V is proportional to the chemical potential gradient with $(2\mathcal{F})^{-1}$ as the mobility.

B. Nonisothermal dynamics

Many transitions in open systems occur under conditions of varying temperature, which is analogous to dynamics of a mechanical system in a changing external field. Temperature variations in the system may, however, occur naturally for purely internal reasons, because evolution of a thermodynamic system almost always entails release of heat, which is redistributed due to the thermal conduction. The recycled heat affects the rate of relaxation if the thermal conductivity is not infinitely large. In order to study nonisothermal dynamics, naturally, we need the heat equation, which would be thermodynamically consistent with the dynamics of phase transitions that take place in the system. Details of the derivation of a thermodynamically consistent generalized heat equation (GHE) compatible with the first and second laws of thermodynamics and the dynamics of phase transitions are presented in Ref. [22]. The GHE takes the form

$$C\partial_t T = \nabla(\lambda \nabla T) - \frac{\delta E}{\delta \eta_j}\partial_t \eta_j\,, \quad C = (\partial_T \hat{e})_{V,\eta}\,, \tag{18}$$

where C is the specific heat and λ is the thermal conductivity. The simultaneous coupling GTDGLE (14) and GHE (18) describe different regimes of interfacial dynamics. Equation (18) can be used not only for phase transitions but also for any thermodynamic process where internal parameters relax simultaneously with heat release, for instance, the problem of an excitable reaction-diffusion system [23].

For the purposes of thermomechanical analogy we consider again a 1D traveling wave where $\{\eta_i = \eta_i(x - Vt), T = T(x - Vt)\}$. Then Eq. (18) can be integrated once to yield the following simultaneous equations that describe nonisothermal dynamics in a heterogeneous thermodynamic medium with $\kappa_{E,ij} = \text{const}$ [24]:

$$\frac{d}{dx}\breve{\omega}(T,\eta_i) = 2V\mathcal{F} + \frac{dT}{dx}\partial_T \breve{\omega}, \tag{19a}$$

and

$$-\frac{dT}{dx} = \frac{V}{\lambda}(\breve{e} - \breve{e}_0), \tag{19b}$$

where $\breve{e}_0$ is the value of the quantity $\breve{e}$ far away from the wave. In the light of the thermomechanical analogy Eq. (19a) describes the dynamics of particles in a nonconservative mechanical system, where energy changes are due to Rayleigh's dissipation and the time-dependent field. Equation (19b) shows that the field T changes self-consistently with other variables of the system.

IV. DISCUSSION

In the present paper we describe the physical analogy between one-dimensional evolution in a continuum thermodynamical system with relaxation and a classical mechanical system of a few interacting particles moving with dissipation. This analogy can be extended to evolution in nonisothermal systems with temperature being analogous to time-dependent nonconservative field. However, a more specific mechanical interpretation of T and Eq. (19b) is still subject to inquiry. The principal difference between mechanical and thermodynamic systems is in the form of imposed constraints: mechanical constraints are usually given in algebraic (holonomic) or differential (nonholonomic) form, while thermodynamic ones are presented in an integral form, e.g., Eq. (1). The dimensionality of the thermodynamical system is limited to unity because of the obvious reason that the temporal coordinate in classical mechanics is one dimensional. It is of interest to see if this analogy holds for physical models, where time is a multidimensional quantity, or to look at a thermodynamic analog of a relativistic extension of the Hamilton principle.

A structural analogy between descriptions of different physical phenomena always improves our understanding of the subjects on both ends and allows for possible extensions into untested areas. It suffices to recall the electromechanical [25] and optomechanical [26] analogies. The thermomechanical analogy sheds light on the problem of pattern formation during phase transitions and provides an interpretation of the marginal stability principle of dynamical selection (at least in one dimension). A good use of the thermomechanical analogy may be made through application of the mechanical intuition developed in problems of small balls rolling on curved profiles to computer simulations of thermodynamic problems, e.g. [8,9,24]. In Ref. [24], Eqs. (19) were applied to phase transitions in an adiabatic system where the mechanical analog of temperature changes self-consistently with the particle coordinates. The author found that heteroclinic trajectories, which correspond to phase-transition waves, exist at two different speeds V for the same conditions in the system. However, only the wave with the greater speed was found to be stable with respect to variations of the velocity. The latter may be viewed as a selection principle in one dimension.

On the basis of the thermomechanical analogy one may also suggest generalizations of the thermodynamic description of a continuous system. In the present paper we suggested the generalized TDGLE, Eq. (14).

The source of the thermomèchanical analogy is identified as the applicability of the variational principles in different branches of physics, like Hamilton's principle in classical mechanics, Fermat's principle in optics, and Clausius' principle in thermodynamics. Variational principles play a role of selection principles and allow one to choose a unique solution (trajectory) out of a large set of solutions (trajectories) that satisfy all other constraints of the problem. Motivated by Noether's theorem [27], which establishes the relation between symmetry properties and conservation laws, we pose a question: What property of a system entails validity of variational principles? As known, Hamilton's and Fermat's principles may be derived from the variational formulation of quantum mechanics [28]: particles and photons, so to speak, "search" the neighboring paths to find the one with the maximum "action" and cancel out through interference on all others [29]. Hence, Hamilton's and Fermat's principles are consequences of the wave nature of light and matter. However, variational principles of thermodynamics are not reducible to the quantum mechanical ones [29]. The answer to the question posed may help find a solution to one of the most fundamental problems of physics, the problem of the arrow of time: how to obtain irreversibility in a thermodynamic system from a completely reversible quantum mechanical description of it.

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