Speed-gradient principle for nonstationary processes in thermodynamics

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The speed-gradient variational principle (SG-principle) is formulated and applied to thermodynamical systems. It is shown that Prigogine’s principle of minimum entropy production and Onsager’s symmetry relations can be interpreted in terms of the SG-principle and, therefore, are equivalent to each other. In both cases entropy of the system plays a role of the goal functional. The speed-gradient formulation of thermodynamic principles provide their extended versions, describing transient dynamics of nonstationary systems far from equilibrium. As an example a model of transient (relaxation) dynamics for maximum entropy principle is derived.

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I. INTRODUCTION

The equations of motion for physical systems are often derived from variational principles: principle of least action, maximum entropy principle, etc. 1, 2, 3. In thermodynamics two of such principles have become well known during last century: Prigogine’s principle of minimum entropy production and Onsager’s symmetry principle for kinetic coefficients. Authors of both results were awarded with Nobel prizes. Variational principles are based on specification of a functional (usually, integral functional) and determination of real motions as points in an appropriate functional space providing extrema of the specified functional.

In addition to integral principles, differential (local) ones were proposed: Gauss principle of least constraint, principle of minimum energy dissipation and others. It has been pointed out by M. Planck 4 that the local principles have some preference with respect to integral ones because they do not fix dependence of the current states and motions of the system on its later states and motions. In 5, 6, 7 a new local evolution principle, so called speed-gradient (SG) principle originated from the SG-design principle of nonlinear control theory 5, 8 was proposed and illustrated by a number of examples from mechanics. In 9 SG-principle was extended to the case of systems with constraints.

This paper is devoted to application of the SG-principle to thermodynamics. First, the formulation of the SG-principle is recalled. Then it is shown that Prigogine’s and Onsager’s principles can be interpreted in terms of the SG-principle and, therefore, are equivalent to each other. In both cases entropy of the system plays a role of the goal functional. The speed-gradient formulation of thermodynamic principles provide their extended versions, suitable for the systems far from equilibrium. Moreover, it may describe their nonstationary, transient dynamics. In the paper SG-principle is applied to derivation of transient (relaxation) dynamics for a system driven by maximum entropy principle.

II. SPEED-GRADIENT VARIATIONAL PRINCIPLE

Consider a class of physical systems described by systems of differential equations

\[ \dot{x} = f(x, u, t), \] (1)

where \( x \) is \( n \)-dimensional vector of the system state, \( u \) is \( m \)-dimensional vector of free (input) variables, \( \dot{x} = dx/dt, t \geq 0 \). The problem of modelling system dynamics can be posed as the search of a law of changing \( u(t) \) in order to meet some criterion of “natural”, or “reasonable” behavior of the system. Let such a behavior be specified as a tendency to achieve a goal, specified as decreasing the value of the goal functional \( Q(x) \), where \( Q(x) \) is given apriori. The first step of the speed-gradient procedure is to calculate the speed \( \dot{Q} = \frac{dQ}{dt} = \frac{\partial Q(x)}{\partial x} f(x, u, t) \). The second step is to evaluate the gradient of the speed \( \nabla_u \dot{Q} \) with respect to input vector \( u \) (speed-gradient vector). Finally the law of dynamics is formed as the feedback law in the finite form

\[ u = -\gamma \nabla_u \dot{Q}(x, u). \] (2)

or in the differential form

\[ \frac{du}{dt} = -\gamma \nabla_u \dot{Q}(x, u), \] (3)

where \( \gamma > 0 \) is a scalar or symmetric matrix gain (positivity of a matrix is understood as positive definiteness of associated quadratic form). The underlying idea of the choices (2) or (3) is that the motion along the antigradient of the speed \( \dot{Q} \) provides decrease of \( \dot{Q} \). It may eventually lead to negativity of \( \dot{Q} \) which, in turn, yields
decrease of $Q$. Now the speed-gradient principle can be formulated as follows.

**Speed-gradient principle:** Among all possible motions of the system only those are realized for which the input variables change proportionally to the speed gradient $\nabla_x Q(x,u)$ of an appropriate goal functional $Q(x)$. If there are constraints imposed on the system motion, then the speed-gradient vector should be projected onto the set of admissible (compatible with constraints) directions.

According to the SG-principle, to describe a system dynamics one needs to introduce the goal function $Q(x)$. The choice of $Q(x)$ should reflect the tendency of natural behavior to decrease the current value $Q(x(t))$. Systems obeying the SG-principle will be called SG-systems. Below only the models $\dagger$ in a special form are considered:

$$\dot{x} = u,$$  \hspace{1cm} (4)

i.e. a law of change of the state velocities is sought.

Note that the SG-direction is the direction of maximum growth for $\dot{Q}(x,u,t)$, i.e. direction of maximum production rate for $Q$. Respectively, the opposite direction corresponds to minimum production rate for $Q$. The finite form $\S$ may be used to describe irreversible processes, while differential form $\S$ corresponds to reversible ones. The SG-laws with nondiagonal gain matrices $\gamma$ can be incorporated if a non-Euclidean metric in the space of inputs is introduced by the matrix $\gamma^{-1}$. The matrix $\gamma$ can be used to describe spatial anisotropy. Admitting dependence of the matrix $\gamma$ on $x$ one can recover dynamics law for complex mechanical systems described by Lagrangian or Hamiltonian formalism. The SG-principle applies to spatially distributed systems where the state $x(t)$ is an element of an infinite dimensional space and allows one to model dynamics of spatial fields $\S$.

Consider a simple illustrating example: motion of a particle in the potential field. In this case the vector $x = \text{col}(x_1,x_2,x_3)$ consists of coordinates $x_1, x_2, x_3$ of a particle. Choose smooth $Q(x)$ as the potential energy of a particle and derive the speed-gradient law in the differential form. To this end, calculate the speed $\dot{Q} = [\nabla_x Q(x)]^T u$ and the speed-gradient $\nabla_u \dot{Q} = \nabla_x Q(x)$. Then, choosing differential SG-law $\S$, with the gain $\gamma = m^{-1}$, where $m > 0$ is a parameter, we arrive at familiar Newton’s law $\dot{u} = -m^{-1} \nabla_x Q(x)$ or $\dot{m} = -\nabla_x Q(x)$.

### III. GENERALIZED ONSAGER RELATIONS

Consider an isolated physical system whose state is characterized by a set of variables (thermodynamic parameters) $\xi_1, \xi_2, \ldots, \xi_n$. Let $x_i = \xi_i - \xi^*_i$ be deviations of the variables from their equilibrium values $\xi^*_1, \xi^*_2, \ldots, \xi^*_n$. Let the dynamics of the vector $x_1, x_2, \ldots, x_n$ be described by the differential equations

$$\dot{x}_i = u_i(x_1, x_2, \ldots, x_n), \hspace{1cm} i = 1, 2, \ldots, n.$$  \hspace{1cm} (5)

### Linearize equations $\S$ near equilibrium

$$\dot{x}_i = -\sum_{k=1}^{n} \lambda_{ik} x_k, \hspace{1cm} i = 1, 2, \ldots, n.$$  \hspace{1cm} (6)

The Onsager’s principle $\S$ claims that the values $\lambda_{ik}$ (kinetic coefficients) satisfy the equations

$$\lambda_{ik} = \lambda_{ki}, \hspace{1cm} i, k = 1, 2, \ldots, n.$$  \hspace{1cm} (7)

In general, the Onsager principle is not valid for all systems e.g. for systems far from equilibrium. Its existing proofs $\S$ require additional postulates. Below a simple new proof is given, showing that it is valid for irreversible speed-gradient systems without exceptions.

First of all, the classical formulation of the Onsager principle $\S$ should be extended to nonlinear systems. A natural extension is the following set of identities:

$$\frac{\partial u_i}{\partial x_k}(x_1, x_2, \ldots, x_n) = \frac{\partial u_k}{\partial x_i}(x_1, x_2, \ldots, x_n).$$  \hspace{1cm} (8)

Obviously, for the case when the system equations $\S$ have linear form $\S$ the identities $\S$ coincide with $\S$. However, since linearization is not used in the formulation $\S$ there is a hope that the extended version of the Onsager law holds for some nonlinear systems far from equilibrium. The following theorem specifies a class of systems for which this hope comes true.

**Theorem 1.** There exists a smooth function $Q(x)$ such that equations $\S$ represent the speed-gradient law in finite form for the goal function $Q(x)$ if and only if the identities $\S$ hold for all $x_1, x_2, \ldots, x_n$.

The proof of the theorem is very simple. Since $\S$ is the speed-gradient law for $Q(x)$, its right-hand sides can be represented in the form $u_i = -\gamma \frac{\partial Q}{\partial x_i}$, $i = 1, 2, \ldots, n$. Therefore $u_i = -\gamma \frac{\partial Q}{\partial x_i}$ (in view of $\dot{Q} = (\nabla_x Q)^T u$). Hence $\frac{\partial u_i}{\partial x_k} = -\gamma \frac{\partial^2 Q}{\partial x_i \partial x_k} = \frac{\partial u_k}{\partial x_i}$, and identities $\S$ are valid. Finally, the condition $\S$ is necessary and sufficient for potentiality of the vector-field of the right-hand sides of $\S$, i.e. for existence of a scalar function $Q$ such that $u_i = \gamma \nabla_x \dot{Q} = \gamma \nabla_u \dot{Q}$.

Thus, for SG-systems the extended form of the Onsager equations $\S$ hold without linearization, i.e., they are valid not only near the equilibrium state. In a special case the condition $\S$ was proposed in $\S$. The theorem means that generalized Onsager relations $\S$ are necessary and sufficient for the thermodynamics system to obey the SG-principle for some $Q$. On the other hand, it is known that different potential functions for the same potential vector-field can differ only by a constant: $\dot{Q} = Q + \text{const}$ and their stationary sets coincide. Therefore, if the system tends to maximize its entropy and the entropy serves as the goal function for the SG-evolution law, then at every time instant the direction of change of parameters coincides with the direction maximizing the rate of entropy change (gradient of the entropy rate). It
follows from Zigler’s version of maximum entropy principle [13] that at every time instant it tends to minimize its entropy production rate (Prigogine principle). That is, if Prigogine principle holds then the generalized Onsager principle [5] holds and vice versa. Note that for special case the relation between Prigogine principle and Onsager principle was established by D.Gyarmati [2].

For the SG-systems some other properties can be established. Let for example a system is governed by SG-law with a convex entropy goal function $S$. Then the decrease of the entropy production $\dot{S}$ readily follows from the identities $\dot{S} = dS/dt = (\nabla_x S) \dot{x} = \gamma(\nabla_x ||\nabla_x S||^2)\nabla_x S = 2\gamma(\nabla_x S)^\top||\nabla_x S||(\nabla_x S)$.

If the entropy $S(x)$ is convex then its Hessian matrix $\nabla_x^2 S$ is negative semidefinite: $\nabla_x^2 S \preceq 0$. Hence $\dot{S}(x) \leq 0$ and $S$ cannot increase [3].

**IV. SPEED-GRADIENT ENTROPY MAXIMIZATION**

It is worth noticing that the speed-gradient principle provides an answer to the question: how the system will evolve? It differs from the principles of maximum entropy, maximum Fisher information, etc. providing and answer to the questions: where? and how far? Particularly, it means that SG-principle generates equations for the transient (nonstationary) mode rather than the equations for the steady-state mode of the system. It allows one to study nonequilibrium and nonstationary situations, stability of the transient modes, maximum deviations from the limit mode, etc. Let us illustrate this feature by example of entropy maximization problem.

According to the 2nd thermodynamics law and to the Maximum Entropy Principle of Gibbs-Jaynes the entropy of any physical system tends to increase until it achieves its maximum value under constraints imposed by other physical laws. Such a statement provides knowledge about the final distribution of the system states, i.e. about asymptotic behavior of the system when $t \to \infty$. However it does not provide information about the way how the system moves to achieve its limit (steady) state.

In order to provide motion equations for the transient mode employ the SG-principle. Assume for simplicity that the system consists of $N$ identical particles distributed over $m$ cells. Let $N_i$ be the number of particles in the $i$th cell and the mass conservation law holds:

$$\sum_{i=1}^{m} N_i = N.$$  (9)

Assume that the particles can move from one cell to another and we are interested in the system behavior both in the steady-state and in the transient modes. The answer for the steady-state case is given by the Maximum Entropy Principle: if nothing else is known about the system, then its limit behavior will maximize its entropy [14]. Let the entropy of the system be defined as logarithm of the number of possible states:

$$S = \ln \frac{N!}{N_1! \cdots N_m!}. \quad (10)$$

If there are no other constraints except normalization condition $\sum_{i=1}^{m} N_i = N$ it achieves maximum when $N_i^* = N/m$. For large $N$ an approximate expression is of use. Namely, if the number of particles $N$ is large enough, one may use the Stirling approximation $N_i^! \approx (N_i/e)^N$. Then

$$S \approx N \ln \frac{N}{e} - \sum_{i=1}^{m} N_i \ln \frac{N_i}{e} = - \sum_{i=1}^{m} N_i \ln \frac{N_i}{N}$$

which coincides with the standard definition for the entropy $S = -\sum_{i=1}^{m} p_i \ln p_i$, modulo a constant multiplier $N$, if the probabilities $p_i$ are understood as frequencies $N_i/N$.

To get an answer for transient mode apply the SG-principle choosing the entropy law $S(X) = -\sum_{i=1}^{m} N_i \ln N_i$ as the goal function to be maximized, where $X = \text{col}(N_1, \ldots, N_m)$ is the state vector of the system. Assume for simplicity that the motion is continuous in time and the numbers $N_i$ are changing continuously, i.e. $N_i$ are not necessarily integer (for large $N_i$ it is not a strong restriction). Then the sought law of motion can be represented in the form

$$\dot{N}_i = u_i, \quad i = 1, \ldots, m,$$  (11)

where $u_i = u_i(t), \quad i = 1, \ldots, m$ are controls – auxiliary functions to be determined. According to the SG-principle one needs to evaluate first the speed of change of the entropy [10] with respect to the system [11], then evaluate the gradient of the speed with respect to the vector of controls $u_i$ considered as frozen parameters and finally define actual controls proportionally to the projection of the speed-gradient to the surface of constraints [10]. In our case the goal function is the entropy $S$ and its speed coincides with the entropy production $\dot{S}$. In order to evaluate $\dot{S}$ let us again approximate $S$ from the Stirling formula $N_i^! \approx (N_i/e)^N$:

$$\dot{S} = N \ln N - N - \sum_{i=1}^{m} (N_i \ln N_i - N_i) = N \ln N - \sum_{i=1}^{m} N_i \ln N_i.$$  (12)

Evaluation of $\dot{S}$ yields

$$\dot{\dot{S}} = - \sum_{i=1}^{m} \left((u_i \ln N_i + N_i \frac{u_i}{N_i}) - \sum_{i=1}^{m} u_i (\ln N_i + 1). \right.$$  

It follows from (10) that $\sum_{i=1}^{m} u_i = 0$. Hence $\dot{S} = - \sum_{i=1}^{m} u_i \ln N_i$. Evaluation of the speed-gradient yields

$$\frac{\delta \dot{S}}{\delta u_i} = - \ln N_i$$

and the SG-law $u_i = \gamma(- \ln N_i + \lambda), \quad i = 1, \ldots, m$, where Lagrange multiplier $\lambda$ is chosen in order to fulfill the constraint $\sum_{i=1}^{m} u_i = 0$, i.e. $\lambda =$
According to the SG-principle the equation (13) determines transient dynamics of the system. To confirm consistency of the choice (13) let us find the steady-state mode, i.e. evaluate asymptotic behavior of the variables $N_i$. To this end note that in the steady-state $\dot{N}_i = 0$ and $\sum_{i=1}^{m} \ln N_i = \ln N$. Hence all $N_i$ are equal: $N_i = N/m$ which corresponds to the maximum entropy state and agrees with thermodynamics.

The next step is to examine stability of the steady-state mode. It can be done by means of the entropy Lyapunov function $V(X) = S_{\text{max}} - S(X) \geq 0$, where $S_{\text{max}} = N \ln m$. Evaluation of $V$ yields

$$
\dot{V} = -\dot{S} = \sum_{i=1}^{m} u_i \ln N_i = \gamma \sum_{i=1}^{m} \left( \frac{m}{m} \left[ \sum_{i=1}^{m} \ln N_i \right]^2 \right) - \gamma \sum_{i=1}^{m} \left( \ln N_i \right)^2.
$$

It follows from the Cauchy-Bunyakovsky-Schwarz inequality that $V(X) \leq 0$ and the equality $V(X) = 0$ holds if and only if all the values $N_i$ are equal, i.e. only at the maximum entropy state. Thus the law (13) provides global asymptotic stability of the maximum entropy state. The physical meaning of the law (13) is moving along the direction of the maximum entropy production rate (direction of the fastest entropy growth).

The case of more than one constraint can be treated in the same fashion. Let in addition to the mass conservation law (19) the energy conservation law hold. Let $E_i$ be the energy of the particle in the $i$th cell and the total energy $E = \sum_{i=1}^{m} N_i E_i$ be conserved. The energy conservation law

$$
E = \sum_{i=1}^{m} N_i E_i
$$

appears as an additional constraint. Acting in a similar way, we arrive at the law (13) which needs modification to ensure conservation of the energy (14). According to the SG-principle one should form the projection onto the surface (in our case – subspace of dimension $m-2$) defined by the relations

$$
\sum_{i=1}^{m} u_i E_i = 0, \quad \sum_{i=1}^{m} u_i = 0.
$$

It means that the evolution law should have the form

$$
\dot{u}_i = \gamma (-\ln N_i) + \lambda_1 E_i + \lambda_2, \quad i = 1, \ldots, m,
$$

where $\lambda_1, \lambda_2$ are determined by substitution of (16) into (15). The obtained equations are linear in $\lambda_1, \lambda_2$ and their solution is given by formulas

$$
\begin{cases}
\lambda_1 = \gamma \frac{m \sum_{i=1}^{m} E_i \ln N_i - \gamma (\sum_{i=1}^{m} E_i)(\sum_{i=1}^{m} \ln N_i)}{m \sum_{i=1}^{m} E_i^2 - (\sum_{i=1}^{m} E_i)^2}, \\
\lambda_2 = \gamma \frac{m \sum_{i=1}^{m} \ln N_i - \lambda_1 \sum_{i=1}^{m} E_i}{m \sum_{i=1}^{m} E_i^2 - (\sum_{i=1}^{m} E_i)^2}.
\end{cases}
$$

The solution of (17) is well defined if $m \sum_{i=1}^{m} E_i^2 - (\sum_{i=1}^{m} E_i)^2 \neq 0$ which holds unless all the $E_i$ are equal (degenerate case).

Let us evaluate the equilibrium point of the system (11), (16) and analyze its stability. At the equilibrium point of the system the following equalities hold:

$$
\gamma (-\ln N_i) + \lambda_1 E_i + \lambda_2 = 0, \quad i = 1, \ldots, m.
$$

Hence

$$
N_i = C \exp(-\mu E_i), \quad i = 1, \ldots, m,
$$

where $\mu = \lambda_1 / \gamma$ and $C = \exp(-\lambda_2 / \gamma)$.

The value of $C$ can also be chosen from the normalization condition $C = N(\sum_{i=1}^{m} \exp(-\mu E_i))$. We see that equilibrium of the system with conserved energy corresponds to the Gibbs distribution which agrees with classical thermodynamics. Again it is worth to note that the direction of change of the numbers $N_i$ coincides with the direction of the fastest growth of the local entropy production subject to constraints. As before, it can be shown that $V(X) = S_{\text{max}} - S(X)$ is Lyapunov function for the system and that the Gibbs distribution is the only stable equilibrium of the system in nongenerate cases. Similar results are valid for continuous (distributed) systems even for more general problem of minimization of relative entropy (Kullback divergence) [9].

Conclusions

Speed-gradient variational principle provides a useful yet simple addition to classical results in thermodynamics. Whereas the classical results allow researcher to answer the question "Where it goes to?", the speed-gradient approach provides an answer to the question: "How it goes and how it reaches its steady-state mode?" SG-principle may be applied to evaluation of nonequilibrium stationary states and study of system internal structure evolution [15], description of transient dynamics of complex networks [16, 17], etc. A different approach to variational description of nonstationary nonequilibrium processes is proposed in [18].

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