Thermodynamic framework for discrete optimal control in multiphase flow systems

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Bellman's method of dynamic programming is used to synthesize diverse optimization approaches to active (work producing) and inactive (entropy generating) multiphase flow systems. Thermal machines, optimally controlled unit operations, nonlinear heat conduction, spontaneous relaxation processes, and self-propagating wave fronts are all shown to satisfy a discrete Hamilton-Jacobi-Bellman equation and a corresponding discrete optimization algorithm of Pontryagin's type, with the maximum principle for a Hamiltonian. The extremal structures are always canonical. A common unifying criterion is set for all considered systems, which is the criterion of a minimum generated entropy. It is shown that constraints can modify the entropy functionals in a different way for each group of the processes considered; thus the resulting structures of these functionals may differ significantly. Practical conclusions are formulated regarding the energy savings and energy policy in optimally controlled systems. [S1063-651X(99)14508-2]

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I. INTRODUCTION: DYNAMIC PROGRAMMING FOR THERMODYNAMIC OPTIMIZATION

In this paper we present a synthesis of dynamic optimization approaches to active (work producing) and inactive (mechanical energy degrading) multiphase flow systems. The mathematical framework is essentially Bellman's method of dynamic programming and associated maximum principles. Endoreversible multistage processes which yield maximum mechanical work, optimally controlled unit operations that minimize energy costs, spontaneous relaxation processes towards equilibrium, thermal rays, and self-propagating reaction-diffusion fronts are all shown to satisfy a discrete algorithm of Pontryagin's type, with the maximum principle for a Hamiltonian with respect to controls. The minimum entropy generation is a common unifying criterion; the extremal structure is always canonical. Both multistage and continuous processes are considered; all discrete characteristics reach their continuous counterparts in the limit of an infinite number of stages. The dynamic programming approach (DP) leads to a discrete Hamilton-Jacobi-Bellman equation, a discrete canonical set, and extends to discrete finite-stage processes Pontryagin's classical method in which a Hamiltonian H is maximized with respect to controls. Optimal performance functions (which describe extremal work, minimal entropy generation, minimum resistance, etc.) are found in terms of end states, process duration, and number of stages. Alternatively, the Legendre transforms of the original functions with respect to the time can be generated; in this case the optimal functions are found in terms of end states, Hamiltonian, and number of stages. We also predict that our theory could be of use for quantum phenomena and for the multistage cooling processes necessary to reach conditions in which quantum effects become observable in cold systems.

Despite a common mathematical framework, optimization goals are quite different for the variety of the processes considered. For a class of energy-converting endoreversible processes, the principal goal is to determine bounds for work produced by an engine system or consumed by a heat-pump system in high-rate regimes. For a class of optimally controlled unit operations, the principal goal is to find optimal controls and optimal trajectories which minimize energy costs, whereas the optimal data of these costs may be of secondary importance. For a class of spontaneously relaxing nonequilibrium processes, whose dynamics are known, the principal goal is to form the entropy production functional which assures that dynamics. For inhomogeneous heat-conducting solids, the principal goal is to assess nonlinear effects caused by spatially distributed thermal resistances. For the self-propagating reaction-diffusion fronts with kinetics governed by the mass action law and diffusion-reaction couplings, the principal goal is to transform an exact field model into an optimal lumped model which satisfies the second law in terms of relationships for wave fronts and rays, as an admissible approximation.

It is worth noting that the analytical expressions which describe the formal Lagrangians in terms of the state and control variables are different for each class investigated, and so are resulting equations of optimal dynamics. This proves that, while the entropy production can be accepted as a governing quantity, in each of the considered cases constraints modify resulting functionals in a different way, or, formally speaking, the entropy generation minimization always works with different subsets in the state space. Practical aspects of the theory are illustrated by optimization of multistage thermal machines and heat and mass heat exchangers, especially for processes of fluidized bed evaporation from porous solids. Applications also involve a finite-size extension of the classical problem of minimal work to discrete processes.

To derive necessary optimality conditions for both continuous and discrete processes, Bellman's method of dynamic programming (DP) is applied [1,2]. An original discrete approach to sequential systems allows us to pass from DP results to the discrete maximum principle, which is another powerful computational tool. To accomplish the multistage optimization, it is essential to define a class of discrete optimal control processes linear with respect to the residence

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time interval. With the discrete version of Bellman's dynamic programming, necessary conditions of optimality arise in a form which contains an equation of Hamilton-Jacobi type with a delayed time argument. To overcome difficulties associated with solving equations of this sort, the necessary conditions are transformed to a form governed by a discrete Hamiltonian. It is then shown that, in multistage autonomous systems, a Pontryagin-like Hamiltonian emerges, which is constant along an optimal discrete trajectory. From a physical standpoint, this constant Hamiltonian condition is a generalization of the energy conservation condition to optimal discrete systems with free intervals of time. On this basis, a discrete canonical formalism, strongly analogous to those in analytical mechanics and the theory of optimal continuous systems, is introduced and applied for the multistage optimization.

Bellman's principle of optimality is crucial for both the existence of the optimal performance functions and the derivation of the pertinent dynamic programming equation, which describe these functionals. When the optimal performance function is generated in terms of the initial states and initial time, the principle of optimality may be stated as follows: In a continuous or discrete process, which is described by an additive performance criterion, the optimal strategy and the optimal profit function are functions of the initial state, initial time, and (in a discrete process) the total number of stages. Therefore, each final segment of an optimal path (continuous or discrete) is optimal for its own initial state and initial time and (in a discrete process) the corresponding number of stages. The proof of this formulation is by contradiction; it uses the additivity property of the performance criterion.

The formulation of the principle of optimality, stated above, refers to the so-called backward algorithm of the DP method. In this algorithm, the recursive optimization procedure that solves Bellman's functional equation begins at the final process state and terminates at its initial state. The process to which this is applied may be arbitrary: it may be discrete by nature or may be obtained by discretizing an original continuous process. The state transformations possess, in this algorithm, their most natural form, as they describe output states in terms of input states and controls at a stage. The optimization at a stage and the optimal functions do recursively involve the information generated in earlier subprocesses. It is well known [3] that, in the continuous case, this method leads to a basic equation of optimal continuous processes, which is the so-called Hamilton-Jacobi-Bellman equation. However, a similar equation can be derived only for special discrete processes, those which are linear in the free time intervals θ^n. The optimality principle makes it possible to replace a simultaneous evaluation of all optimal controls by a sequence of local evaluations of optimal controls at stages, for evolving subprocesses.

On the other hand, the optimal profit function can be generated in terms of the final states and final time. The optimality principle has then a dual form: In a continuous or discrete process, which is described by an additive performance criterion, the optimal strategy and the optimal profit function are functions of the final state, final time, and (in a discrete process) the total number of stages. Thus each initial segment of the optimal path is optimal for its own final state and final time and (in a discrete process) the corresponding number of stages.

The dual formulation refers to the so-called forward algorithm of the DP method, which we apply here to multistage processes. In this algorithm, recursive optimizations that solve the functional equation begin at the initial state and terminate at its final state. The state transformations have the form which describes state inputs in terms of state outputs and controls at a stage. While this is not the most typical representation of the state transformations, it is directly obtainable for multistage processes with an ideal mixing at the stage. On the other hand, inverse transformations (used in the backward algorithm) may be difficult to apply in an explicit form. With the forward DP algorithm, local optimizations proceed in the direction of real time.

II. HAMILTON-JACOBI-BELLMAN EQUATIONS FOR CONTINUOUS SYSTEMS

In many physical phenomena and processes in practical systems, a general problem of optimal control can be associated with the Bolza form of the performance index,

$$S=\int_{t^i}^{t^f} f_0(\mathbf{x},t,\mathbf{u})dt+G(\mathbf{x}^f(t^f),t^f)-G(\mathbf{x}^i(t^i),t^i), \qquad (1)$$

where f_0 is the profit intensity and $G(\mathbf{x},t)$ is a gauging function that depends on the state $\mathbf{x}$ and the time t. For Eq. (1), a maximum of the criterion S is sought with respect to a suitable choice of the vector functions $\mathbf{x}(t)$ and $\mathbf{u}(t)$. The function G influences an optimal solution only if some of the end coordinates of the state vector or time are undetermined. Working with all initial coordinates $\mathbf{x}^i$ and initial time t^i as independent variables, we can generate a function describing the maximum value of S in terms of $\mathbf{x}^i$ and t^i. This is called the original optimization problem. However, one can also consider the maximum of S as a function generated in terms of the final coordinates and final time $\mathbf{x}^f$ and t^f. This is called the dual optimization problem. It is insightful to confront properties of the original problem with those of the dual problem. For this purpose, we introduce the optimal performance function $V(\mathbf{x}^i,t^i,\mathbf{x}^f,t^f)$,

$$V(\mathbf{x}^i,t^i,\mathbf{x}^f,t^f)\equiv \max S = \max\left\{\int_{t^i}^{t^f} f_0(\mathbf{x},t,\mathbf{u})dt+G(\mathbf{x}^f,t^f)-G(\mathbf{x}^i,t^i)\right\}. \qquad (2)$$

The function V describes the maximum of S in terms of the end states and end times, and it is common for both the original and the dual problem.

The optimization in Eq. (1) is subject to constraints resulting from a set of differential equations,

$$\frac{dx_i}{dt}=f_i(\mathbf{x},t,\mathbf{u}), \qquad (3)$$

where $\mathbf{x}=(x_1,x_2,\ldots,x_i,\ldots,x_s)$ is the s-dimensional state vector and $\mathbf{f}=(f_1,f_2,\ldots,f_i,\ldots,f_s)$ is the vector of rates. The r-dimensional vector $\mathbf{u}=(u_1,u_2,\ldots,u_r)$ is the control vector.

The admissible control usually satisfies certain local constraints, the most typical being

$$\mathbf{u}(t) \in \mathbf{U}, \tag{4}$$

where $\mathbf{U}$ is an admissible set in the control space. There may also be some additional constraints which link coordinates of the state vector, $\mathbf{x}$, and the control vector, $\mathbf{u}$. They are usually of the type $\mathbf{g}(\mathbf{x},\mathbf{u},t)=0$ or $\mathbf{g}(\mathbf{x},\mathbf{u},t)\leqslant 0$. However, they may be included into the model by using Lagrange multipliers, a special sort of control variable which resides linearly in the model. These multipliers will increase the dimensionality of $\mathbf{u}$ without changing the general structure of the model, given above. Thus the model (1)–(4) is sufficient for general considerations. To include the time coordinate into the state vector, we can use the enlarged $(s+1)$-dimensional vector of state $\tilde{\mathbf{x}}=(x_1,x_2,\ldots,x_i,\ldots,x_s,x_{s+1})$ in which case $x_{s+1}\equiv t$ and $(s+1)$-dimensional vector of rates $\tilde{\mathbf{f}}=(f_1,f_2,\ldots,f_i,\ldots,f_s,f_{s+1})$ with $f^n_{s+1}=1$.

The use of Bellman's optimality principle for continuous systems is known from many sources [1,3–6]. Maximizing S along a trajectory that starts at $(\mathbf{x}^i,t^i)$, the principle yields the so-called Hamilton-Jacobi-Bellman equation (HJB equation)

$$\max_{\mathbf{u}^i}\left\{ f^i_0+\sum_{i=1}^{n}\frac{\partial P}{\partial x^i}f^i+\frac{\partial P}{\partial t^i}\right\}=0, \tag{5}$$

where

$$P(\mathbf{x}^i,t^i,\mathbf{x}^f,t^f)\equiv G(\mathbf{x}^i,t^i)-G(\mathbf{x}^f,t^f)+V(\mathbf{x}^i,t^i,\mathbf{x}^f,t^f). \tag{6}$$

(Of course, $P\equiv V$ when $G=0$.) Expressing a HJB equation in terms of P rather than V is convenient, because P summarizes all gauging effects.

Now, we consider an optimal trajectory which terminates at $(\mathbf{x}^f,t^f)$. The optimality principle yields the HJB equation in the form

$$\max_{\mathbf{u}^f}\left\{ f^f_0-\sum_{i=1}^{n}\frac{\partial P}{\partial x^f}f^f-\frac{\partial P}{\partial t^f}\right\}=0. \tag{7}$$

We can interpret the meaning of extremum operations in HJB equations as a maximization of the profit intensity gauged by the total derivative of the optimal performance function P. A mnemonic rule is helpful which states that the total differentiation of P is allowed at the end of the process where the complete state can be fixed (cannot be optimized), and that this differentiation yields the related HJB equation.

It is also worth noting that the optimal function V, Eq. (2), that is related directly to the original criterion S, can be used to yield the HJB equation. Indeed, we find from Eqs. (5)–(7)

$$\max_{\mathbf{u}^f}\left\{ \tilde{f}^f_0-\sum_{i=1}^{n}\frac{\partial V}{\partial x^f}f^f-\frac{\partial V}{\partial t^f}\right\}=\max_{\mathbf{u}^i}\left\{ \tilde{f}^i_0+\sum_{i=1}^{n}\frac{\partial V}{\partial x^i}f^i+\frac{\partial V}{\partial t^i}\right\}=0, \tag{8}$$

where in either case a gauged profit intensity

$$\tilde{f}_0(\mathbf{x},t,\mathbf{u})\equiv f_0(\mathbf{x},t,\mathbf{u})+\partial G/\partial t+\sum_{i=1}^{s}\frac{\partial G}{\partial \mathbf{x}_i}f_i(\mathbf{x},t,\mathbf{u}) \tag{9}$$

appears in a HJB equation describing V.

The HJB equation is a quasilinear partial differential equation with the extremizing sign that governs the characteristic functions P or V via the control $\mathbf{u}$, which achieves the optimization. The definition of the performance potential V in Eq. (2) is the most suitable to processes producing a profit, in which case V is positive. For processes described in terms of cost, the most suitable definition assuring a positive potential involves an optimal function R, which is the negative of V. Indeed, for an arbitrary functional S and the same end states and times,

$$R\equiv\min(-S_{[\tilde{\mathbf{x}}^i,\tilde{\mathbf{x}}^f]})=-\max S_{[\tilde{\mathbf{x}}^i,\tilde{\mathbf{x}}^f]}=-V, \tag{10}$$

where tildes refer to the enlarged vector of state that includes the time t. Thus, the single external function $V(t^i,\mathbf{x}^i,t^f,\mathbf{x}^f)$ is sufficient to describe the extremum of the functional S. In analytical mechanics such equations are usually derived by the method of variational calculus [7]. The DP approach allows for more general derivations, which take into account local constraints imposed on control variables, Eq. (4). Our treatment here develops a search for properties and implications of HJB equations in physics, chemistry, and thermodynamics of multiphase systems. For discrete problems, the dynamic programming will effectively be applied in the next section.

The partial derivative of the characteristic function V with respect to time can be taken out of the bracket of a HJB equation, and the indices f or i are conveniently omitted in equations of this sort for various end states. Changing the signs of extremized expressions, whenever the change of the extremum operation takes place, yields in terms of final states and times

$$\frac{\partial V}{\partial t}+\min_{\mathbf{u}}\left\{\frac{\partial V}{\partial \mathbf{x}}\cdot\mathbf{f}(\mathbf{x},t,\mathbf{u})-\tilde{f}_0(\mathbf{x},t,\mathbf{u})\right\} \equiv\frac{\partial R}{\partial t}+\max_{\mathbf{u}}\left\{\frac{\partial R}{\partial \mathbf{x}}\cdot\mathbf{f}(\mathbf{x},t,\mathbf{u})+\tilde{f}_0(\mathbf{x},t,\mathbf{u})\right\}=0. \tag{11}$$

In terms of initial states and times we find similar relationships. Note that functions R represent extremum actions of classical mechanics, where $\tilde{l}_0(\mathbf{x},t,\mathbf{u})\equiv-\tilde{f}_0(\mathbf{x},t,\mathbf{u})$ is a Lagrangian [8].

In all HJB equations, the extremized expressions are Hamiltonians. In fact, they are ''nonextremal'' Hamiltonians of Pontryagin's type. The optimal control $\mathbf{u}$, which solves the optimal work problem, is chosen in order to extremize the Hamiltonian at each point of the extremal path, which means extremizing a wave-front velocity in the HJB equation. The power of approaches based on the HJB equation is caused by the fact that the *optimal* performance functions satisfy this equation with the same state variables as those found in the related unconstrained problem. Only dimensionalities and numerical values of optimizing control sets and the numerical values of the functions P or V may differ in constrained and unconstrained cases. Methods which serve to obtain so-

lutions of a HJB equation can be both analytical and numerical. For some special models, e.g., for thermal machines with heat transfer, solutions can be obtained analytically. A standard numerical procedure, which works with Bellman's recurrence equation, is the most usual tool to solve a HJB equation in the case of low dimensionality of the state vector [1,9].

III. TRANSITION TO HAMILTON-JACOBI EQUATIONS IN CONTINUOUS SYSTEMS

We now consider a transition to a Hamilton-Jacobi equation for Eq. (11). For a definite physical problem, a single common formula can summarize the effect of varying the final states and final time and that of initial states and initial time. To derive the formula, we first need to define an adjoint vector, $\mathbf{p}$, as the negative partial derivative $-\partial V/\partial \mathbf{x}$ when the varied $\mathbf{x}$ is the final state $\mathbf{x}^f$. It may be realized that these adjoints, resembling mechanical momenta, do not coincide with other possible adjoints, based on gradients of the function P, which can also be used. An important fact is the equality $\partial V/\partial \mathbf{x}^i = -\partial V/\partial \mathbf{x}^f$ arising whenever two end states $\mathbf{x}^i$ and $\mathbf{x}^f$ tend to coincide. This proves that both derivatives $\partial V/\partial \mathbf{x}^i$ and $-\partial V/\partial \mathbf{x}^f$ (or $\partial P \partial \mathbf{x}^i$ and $-\partial P/\partial \mathbf{x}^f$) represent, in fact, the same physical quantity. Thus, it is enough if we test Eq. (11), which deals with final states and times.

For the process Lagrangians, i.e., the integrands $\tilde{l}_0(\mathbf{x},t,\mathbf{u}) \equiv -\tilde{f}_0(\mathbf{x},t,\mathbf{u})$, the extremum conditions in Eqs. (5) and (7) determine the link between the derivatives $\partial \tilde{f}_0/\partial \mathbf{u}$ (or $-\partial \tilde{l}_0/\partial \mathbf{u}$) and the state adjoints $\mathbf{p} = -\partial V/\partial \mathbf{x}$. The formulas that follow refer to the final-state variations in Eq. (11). Its extremizing with respect to the control $\mathbf{u}$ (in fact $\mathbf{u}^f$) leads to two equations. The first express the optimal control $\mathbf{u}$ through $\mathbf{x}$, t, and $-\partial V/\partial \mathbf{x}$; for an unconstrained vector $\mathbf{u}$,

$$\frac{\partial V}{\partial \mathbf{x}} = \frac{\partial \tilde{f}_0(\mathbf{x},t,\mathbf{u})}{\partial \mathbf{u}} \tag{12}$$

and the second is the original equation (11) without the extremizing sign; in terms of V,

$$\frac{\partial V}{\partial t} + \frac{\partial V}{\partial \mathbf{x}} \cdot \mathbf{f}(\mathbf{x},t,\mathbf{u}) - \tilde{f}_0(\mathbf{x},t,\mathbf{u}) = 0. \tag{13}$$

With the momentum-type variable $\mathbf{p} \equiv -\partial V/\partial \mathbf{x} = \partial R/\partial \mathbf{x}$ and Eq. (12) written in the form

$$\mathbf{p} = -\frac{\partial \tilde{f}_0(\mathbf{x},t,\mathbf{u})}{\partial \mathbf{u}} = \frac{\partial \tilde{l}_0(\mathbf{x},t,\mathbf{u})}{\partial \mathbf{u}}, \tag{14}$$

we can solve Eq. (14) in terms of $\mathbf{u}$ to obtain the function $\mathbf{u}(\mathbf{p},t,\mathbf{x})$. When we substitute this function into Eq. (13), an energylike Hamiltonian of the extremal process emerges:

$$\mathcal{H}(\mathbf{x},t,\mathbf{p}) \equiv \mathbf{p} \cdot \mathbf{f}(\mathbf{x},t,\mathbf{p}) + \tilde{f}_0(\mathbf{x},t,\mathbf{p}) = \mathbf{p} \cdot \mathbf{f}(\mathbf{x},t,\mathbf{p}) - \tilde{l}_0(\mathbf{x},t,\mathbf{p}). \tag{15}$$

This structure is also valid for the extremal function $\mathcal{H}$ if the control $\mathbf{u}$ is constrained, i.e., when the link between $\mathbf{p}$ and $\mathbf{u}$ is no longer given by Eq. (14). Along with the HJB equation (11), the definition assures that H has a positive maximum in an extremal process. Yet, for the same $\mathbf{x}$, the numerical values of H may be different when the process evolves from the state $\mathbf{x}^i$ to the state $\mathbf{x}^f$ and then goes back, from $\mathbf{x}^f$ to $\mathbf{x}^i$, in the same amount of time. With the optimal $\mathcal{H}$ and using $\mathbf{p} \equiv -\partial V/\partial \mathbf{x}$ in Eqs. (13) and (15), we obtain the Hamilton-Jacobi equation for the characteristic function V:

$$-\frac{\partial V}{\partial t} + \mathcal{H}\left(\mathbf{x},t,-\frac{\partial V}{\partial \mathbf{x}}\right) = 0. \tag{16}$$

This form refers to variations of final states and times. We can express Eq. (16) also in terms of the derivatives $\partial R/\partial \mathbf{x}$, replacing $-\partial V/\partial \mathbf{x}$. Equation (16) differs from its HJB equation insofar as it refers only to extremal paths and $\mathcal{H}$ is the *extremal* Hamiltonian. This equation should be solved subject to the boundary condition

$$\lim_{x \to x_i} V(\mathbf{x}^i,t^i,\mathbf{x},t) = 0. \tag{17}$$

Associated with the canonical set, the free boundary condition for $\mathcal{H}$ and $\mathbf{p}$ follows from the definition of $V = \max S$ in the form $-\mathcal{H} = p_t = -\partial V/\partial t = 0$ and $\mathbf{p} = -\partial V/\partial \mathbf{x} = 0$. However, in terms of the potential P, Eq. (6), the free boundary conditions are different; the condition $\partial V/\partial t = 0$ implies $\partial P/\partial t = \partial G/\partial t$ at the initial point and $\partial P/\partial t = -\partial G/\partial t$ at the final point. Thus, we find $\partial P/\partial t = -\partial G/\partial t$ and $\partial P/\partial \mathbf{x} = -\partial G/\partial \mathbf{x}$ for variations that refer to the final points.

When the vector of initial values $\mathbf{x}(t^i) = \mathbf{x}^i$ is given, the function $V(\mathbf{x}^i,t^i,\mathbf{x},t)$ is determined as the solution to Eq. (16) in terms of the final states. The optimal trajectory, or the vector $\mathbf{x}(t)$, is then found from the initial relationship $\mathbf{p}^i = \partial V/\partial \mathbf{x}^i$, which yields $\mathbf{x} = \mathbf{x}(t,t^i,\mathbf{x}^i,\mathbf{p}^i)$. Otherwise, the adjoint vector follows for current states in the form $\mathbf{p} = -\partial V/\partial \mathbf{x}$; this yields $\mathbf{p} = \mathbf{p}(t^i,\mathbf{x}^i,t,\mathbf{x})$. Substituting into the latter expression the trajectory $\mathbf{x} = \mathbf{x}(t,t^i,\mathbf{x}^i,\mathbf{p}^i)$, we find the evolution of $\mathbf{p}$ in time; $\mathbf{p} = \mathbf{p}(t,t^i,\mathbf{x}^i,\mathbf{p}^i)$. Thus, we obtain both the optimal trajectory and the adjoint vector as functions of the current time t and the initial values $(t^i,\mathbf{x}^i,\mathbf{p}^i)$.

IV. DISCRETE THEORY OF PONTRYAGIN'S TYPE WITH OPTIMAL INTERVALS OF TIME

Now we shall outline an analogous theory for multistage processes: a discrete optimization theory based on the so-called discrete maximum principle with a constant Hamiltonian [5,10–12]. The previous continuous theory will appear as the limit of the discrete theory for an infinite number of stages. Still, our approach will made it possible to treat multistage processes with a small number of finite stages. These latter processes are discrete by nature; they occur in many engineering systems, e.g., cascades of extractors, evaporators, fluidized dryers, multistage thermal machines, etc. A continuous-discrete analogy is derivable for discrete models which are linear with respect to a particular unconstrained control variable. This control may be an unconstrained interval of one of the state variables, especially the interval of time, θ^n, or an interval of a length. The model's linearity with respect to θ^n is crucial for the formal similarity of the necessary optimality conditions in discrete and continuous processes because, broadly speaking, this linearity eliminates the second order and higher terms in Taylor ex-

pansions of characteristic functions for discrete processes. The standard discrete theory of optimal control [13,14] does not predict a special similarity between discrete and continuous cases. This is why such characteristic features of the continuous theory as constancy of an autonomous Hamiltonian or a Hamilton-Jacobi equation remainded unknown in discrete systems for a long time. However, when a discrete model has a structure linear in θ^n, a remarkable discrete-continuous analogy emerges. In particular, discrete optimal functions satisfy Hamilton's and Hamilton-Jacobi formalisms and a discrete maximum principle emerges in a form analogous to that known for continuous systems. An analytical theory of discrete optimization is given below.

To develop an analogy with Eq. (1), we consider the discrete Bolza functional,

$$S^N \equiv \sum_{n=1}^{N} f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n + G(\mathbf{x}^N,t^N) - G(\mathbf{x}^0,t^0). \quad (18)$$

The optimization in Eq. (18) is subject to constraints resulting from difference equations,

$$x_i^n - x_i^{n-1} = f_i(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n, \quad t^n - t^{n-1} = \theta^n, \quad (19)$$

where $\mathbf{x}=(x_1,x_2,\ldots,x_i,\ldots,x_s)$ is the s-dimensional state vector and $\mathbf{f}=(f_1,f_2,\ldots,f_i\ldots,f_s)$ is the vector of rates. The r-dimensional control vector $\mathbf{u}=(u_1,u_2,\ldots,u_r)$ is constrained, i.e.,

$$\mathbf{u}^n \in \mathbf{U}, \quad (20)$$

where $\mathbf{U}$ is the admissible set in the control space. Generalizations are possible to include local constraints on the state and controls in the way described for the continuous case.

The optimization problem can be stated as that of maximizing S for $n=N$ when the initial point $(\mathbf{x}^0,t^0)$ is fixed. However, a difficulty arises if we want to obtain a difference analog of Eq. (9); in fact, it is not clear whether such an analog exists, because the differential calculus cannot be applied to finite differences in the discrete case. It is precisely for this reason that we prefer to use the potential function P rather than V when discrete processes are analyzed. It is also essential to recognize the importance of the necessary optimality condition for free intervals of time, θ^n, which yields a vanishing ''enlarged Hamiltonian,'' and the significance of generalization of Bellman's recurrence equation into the so-called stage criterion. The latter includes variations of end states and times, thus yielding simultaneously the discrete characteristics and the conditions for an optimal control. We concentrate here on the dual problem in which a maximum of S is sought at a fixed final point (x^N,t^N), subject to the constraints set by Eqs. (19) and (20).

We define the optimal performance function of the discrete problem,

$$V^N(\mathbf{x}^0,t^0,\mathbf{x}^N,t^N) \equiv \max\left\{ \sum_{n=1}^{N} f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n + G(\mathbf{x}^N,t^N) - G(\mathbf{x}^0,t^0) \right\}. \quad (21)$$

An alternative definition of V states this function in the form

$$\begin{aligned} V^n(\mathbf{x}^0,t^0,\mathbf{x}^n,t^n) &\equiv \max\left\{ \sum_{k=1}^{n} [f_0^k(\mathbf{x}^k,t^k,\mathbf{u}^k)\,\theta^k \right. \\ &\quad \left. + G(\mathbf{x}^k,t^k) - G(\mathbf{x}^{k-1},t^{k-1})] \right\} \\ &= \max\left\{ \sum_{k=1}^{n} \left[f_0^k(\tilde{\mathbf{x}}^k,\mathbf{u}^k) \right.\right. \\ &\quad \left.\left. + \frac{G(\tilde{\mathbf{x}}^k) - G(\tilde{\mathbf{x}}^k - \tilde{\mathbf{f}}^k(\tilde{\mathbf{x}}^k,\mathbf{u}^k)\,\theta^k)}{\theta^k} \right] \theta^k \right\} \\ &\equiv \max\left\{ \sum_{m=1}^{n} \tilde{f}_0^k \theta^k \right\}, \end{aligned} \quad (22)$$

where $\tilde{f}_0^k$ is the gauged profit intensity, a discrete analog of that in Eq. (9).

To solve the optimization problem, a generalization of Bellman's recurrence equation to the form of the so-called stage criterion [5] is essential,

$$\max_{\mathbf{u}^n,\theta^n,\mathbf{x}^n,t^n} \{ f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n - [P^n(\mathbf{x}^n,t^n) - P^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n, t^n - \theta^n)] \} = 0, \quad (23)$$

where, by definition,

$$P^n(\mathbf{x}^0,t^0,\mathbf{x}^n,t^n) \equiv G(\mathbf{x}^0,t^0) - G(\mathbf{x}^n,t^n) + V^n(\mathbf{x}^0,t^0,\mathbf{x}^n,t^n). \quad (24)$$

With Eq. (23), a complete set of necessary optimality conditions is determined, including those with respect to state $\mathbf{x}^n$ and time t^n (see Ref. [6] for an analogous continuous approach). Equation (23) yields all relevant information: it leads to HJB equations, definition of H, state adjoints, and canonical set. Bellman's equation follows from the criterion (23) for the fixed final state and time,

$$\begin{aligned} P^n(\mathbf{x}^n,t^n) = \max_{\mathbf{u}^n,\theta^n} \{ & f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n \\ & - P^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n, t^n - \theta^n) \}. \end{aligned} \quad (25)$$

Equation (25) is in the ''forward'' form; its backward counterpart represents the most popular form of recurrence equations for multistage optimization. Starting with $V^0=0$, the sequence $V^1,\ldots,V^N$ is found by a well-known iterative procedure [2,9], in which extremizing is with respect to controls at the constant coordinates $(\mathbf{x}^n,t^n)$. Analytical solutions are rare. For example, an analytical solution to Eq. (25) exists for a cascade of thermal engines; see Sec. VI.

Let us first fix state x^n and time t^n in Eq. (23), or, equivalently, deal with Eq. (25). For an unconstrained θ^n and constrained $\mathbf{u}^n \in \mathbf{U}$, these equations yield the following set of necessary conditions of optimality:

$$f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n - [P^n(\mathbf{x}^n,t^n) - P^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)\,\theta^n, t^n - \theta^n)] = 0, \quad (26)$$

$$f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial \mathbf{x}^{n-1}}\cdot\mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial t^{n-1}}=0, \quad (27)$$

and

$$\left\{\frac{\partial f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)}{\partial \mathbf{u}^n}-\frac{\partial P^{n-1}}{\partial \mathbf{x}^{n-1}}\cdot\frac{\mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)}{\partial \mathbf{u}^n}\right\}\cdot\delta\mathbf{u}^n\leqslant 0. \quad (28)$$

The weak maximum condition with respect $\mathbf{u}^n$, which follows as the necessary condition for the negative variation of S, is sufficient in applications in most practical cases.

Equation (27) is the stationarity condition for the optimal intervals θ^n. Whenever θ^n is finite and positive, then it follows from Eqs. (26)–(28) that Eq. (28) can be derived from the following maximum condition:

$$\max_{\mathbf{u}^n}\left\{f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial \mathbf{x}^{n-1}}\cdot\mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial t^{n-1}}\right\}=0. \quad (29)$$

This is a discrete HJB equation which represents a weak maximum principle with respect to $\mathbf{u}^n$ for the ''enlarged Hamiltonian''

$$\tilde{H}^{n-1}=f_0^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial \mathbf{x}^{n-1}}\cdot\mathbf{f}^n(\mathbf{x}^n,t^n,\mathbf{u}^n)-\frac{\partial P^{n-1}}{\partial t^{n-1}}, \quad (30)$$

where P^n is defined by Eq. (24). Equation (29) states that the necessary condition for the maximum of S^N with respect to the control sequence $\{\mathbf{u}^n\}$ is that for the enlarged Hamiltonian (30). As $f_{s+1}(=1)$ is $\mathbf{u}$-independent, the optimality condition (29) can also be expressed in terms of an energylike Hamiltonian that has excluded the partial derivative of P^{n-1} with respect to t^{n-1},

$$H^{n-1}\left(\mathbf{x}^n,t^n,-\frac{\partial P^{n-1}}{\partial \mathbf{x}^{n-1}},\mathbf{u}^n\right)\equiv f_0^n-\sum_{i=1}^{s}\frac{\partial P^{n-1}}{\partial x_i^{n-1}}f_i^n. \quad (31)$$

Equation (31) rejects the $\mathbf{u}$-independent term $\partial P^{n-1}/\partial t^{n-1}$ from the Hamiltonian (30).

When the optimal control $\mathbf{u}^n$ is evaluated from Eq. (28) and substituted into Eq. (27), the latter becomes a discrete Hamilton-Jacobi equation,

$$-\frac{\partial P^{n-1}}{\partial t^{n-1}}+\mathcal{H}^{n-1}\left(x_1^n,\ldots,x_s^n,t^n,-\frac{\partial P^{n-1}}{\partial x_1^{n-1}}\cdots-\frac{\partial P^{n-1}}{\partial x_s^{n-1}}\right)=0, \quad (32)$$

which is nonlinear in terms of the derivatives $\partial P^{n-1}/\partial x^{n-1}$. It is written for the *extremum* H^{n-1} of the Hamiltonian function of energy type, Eq. (31), rather than in terms of the enlarged Hamiltonian $\tilde{H}^{n-1}$. In the limiting case of an infinitesimal sequence of θ^n, this equation yields the Hamilton-Jacobi equation of corresponding continuous process, consistent with Eq. (16). Note that for the gauging function $G=0$, the limiting form of Eq. (32) coincides with Eq. (16).

The state adjoints are now defined as

$$z_1^{n-1}\equiv-\frac{\partial P^{n-1}(\mathbf{x}^{n-1})}{\partial x_i^{n-1}}=\frac{\partial K^{n-1}(\mathbf{x}^{n-1})}{\partial x_i^{n-1}} \quad (33)$$

$(i=1,\ldots,s,s+1)$. Here $K^n\equiv -P^n$ is the costlike optimal function. In terms of the state and adjoint variables, the Hamiltonian (30) is

$$\tilde{H}^{n-1}(\mathbf{x}^n,t^n,\mathbf{z}^{n-1},z_t^{n-1},\mathbf{u}^n)\equiv\sum_{\nu=0}^{s+1}z_\nu^{n-1}f_\nu^n=z_0^{n-1}f_0^n+\sum_{i=1}^{s}z_i^{n-1}f_i^n+z_t^{n-1}, \quad (34)$$

where $z_0^{n-1}=1$, $z_i^{n-1}=-\partial P^{n-1}/\partial x_i^{n-1}=\partial K^{n-1}/\partial x_i^{n-1}$, $z_{s+1}^{n-1}\equiv z_t^{n-1}=-\partial P^{n-1}/\partial t^{n-1}=\partial K^{n-1}/\partial t^{n-1}$, and $f_{s+1}=1$ for $i=1,2,\ldots,s$ and $n=1,2,\ldots,N$. This Hamiltonian has to attain a maximum with respect to the controls $\mathbf{u}^n$ which maximize a performance index of the profit type, such as the production criterion S^N, whose optimal function P^n satisfies Eq. (24). In an equivalent formulation, we minimize a performance index of the cost type, such as the consumption criterion $(-S^N)$, whose optimal function $K^n=-P^n$. The Hamiltonian (34) is a basis for the method using canonical equations, which emerges from the stage criterion (23) as shown below.

Let us now fix controls $\mathbf{u}^n$ and θ^n in Eq. (23) and differentiate the expression in curly brackets of this equation to determine its stationarity conditions with respect to the final state and time. We obtain an optimal difference set which is canonical with respect to two sorts of equations, one defining the changes of state and the other the corresponding changes of the adjoint variables. Using the most popular energylike Hamiltonian, Eq. (31), expressed in terms of the adjoint variables.

$$H^{n-1}(\mathbf{x}^n,\mathbf{z}^{n-1},\mathbf{u}^n,t^n)\equiv f_0^n(\mathbf{x}^n,\mathbf{u}^n,t^n)+\sum_{i=1}^{s}z_i^{n-1}f_i^n(\mathbf{x}^n,\mathbf{u}^n,t^n), \quad (35)$$

the algorithm of the discrete maximum principle is represented by the equations

$$\frac{x_i^n-x_i^{n-1}}{\theta^n}=\frac{\partial H^{n-1}}{\partial z_i^{n-1}}, \quad (36)$$

$$\frac{z_i^n-z_i^{n-1}}{\theta^n}=-\frac{\partial H^{n-1}}{\partial x_i^n}, \quad (37)$$

$$\frac{z_t^n-z_t^{n-1}}{\theta^n}=-\frac{\partial H^{n-1}}{\partial t^n}, \quad (38)$$

and

$$z_t^{n-1}+\max_{\mathbf{u}^n}H^{n-1}(\mathbf{x}^n,\mathbf{z}^{n-1},\mathbf{u}^n,t^n)=0 \quad (39)$$

$(n=1,\ldots,N;\ i=1,\ldots,s$ and $l=1,\ldots,r)$. As shown by Eq. (28), the weak or local maximum conditions in Eqs. (29) and (39) can be proven easily, otherwise the strong or global maximum condition requires a subtle proof of validity of Eq.

(29) in the whole admissible region of **u**, Eq. (20); for this issue, see Ref. [15, 16]. Nonetheless, it is the weak maximum principle which is sufficient in most applications.

Equation (36) constitutes the Hamiltonian form of the state equations, and Eq. (37) is its adjoint equation. Equation (38) describes the Hamiltonian interval at the stage n, whereas Eq. (39) states that in an extremal process the enlarged Hamiltonian $\tilde{\mathcal{H}}^{n-1}=\mathcal{H}^{n-1}+z_t^{n-1}$ is always constant and equals zero. Equation (39) includes the necessary condition for the stationary optimality of the decision vector $\mathbf{u}^n$ if its optimal value falls in the interior of the allowable range **U**. Quite importantly, Eq. (38), which describes the change of the Hamiltonian through a finite stage, does not follow (as in the continuous version) from the canonical equations for x_i and z_i, but it represents an independent extremum condition associated with the optimal choice of t^n. In autonomous systems, $\mathcal{H}^n=\mathcal{H}^{n-1}$, i.e., the energylike Hamiltonian is constant along an optimal discrete path. In nonautonomous systems, only the enlarged Hamiltonian (30) is constant of the optimal discrete motion; the value of this constant always equals zero, $\tilde{\mathcal{H}}^{n-1}=0$.

The boundary conditions are determined as vanishing stationarity conditions for the extremum of S^N with respect to end state coordinates and times. By applying Eq. (24), which links the functions V and P, in an equation defining the variation of S^N caused by end states,

$$dS^N=\sum_{i=1}^{s+1}\frac{\partial V^N}{\partial \tilde{x}_i^N}d\tilde{x}_i^N+\sum_{i=1}^{s+1}\frac{\partial V^N}{\partial \tilde{x}_i^0}d\tilde{x}_i^0, \tag{40}$$

we obtain

$$dS^N=\sum_{i=1}^{s+1}\left(\frac{\partial P^N}{\partial \tilde{x}_i^N}+\frac{\partial G}{\partial \tilde{x}_i^N}\right)d\tilde{x}_i^N+\sum_{i=1}^{s+1}\left(\frac{\partial P^N}{\partial \tilde{x}_i^0}+\frac{\partial G}{\partial \tilde{x}_i^0}\right)d\tilde{x}_i^0. \tag{41}$$

(In these equations, $\tilde{x}_i^{s+1}\equiv t$.) Hence after invoking the definition of adjoint variables, Eq. (33),

$$dS^N=\sum_{i=1}^{s+1}\left(\frac{\partial G}{\partial \tilde{x}_i^N}-\tilde{z}_i^N\right)d\tilde{x}_i^N+\sum_{i=1}^{s+1}\left(\frac{\partial G}{\partial \tilde{x}_i^0}-\tilde{z}_i^0\right)d\tilde{x}_i^0. \tag{42}$$

Setting to zero respective partial derivatives of the performance function S^N for one end, either for $n=0$ or for $n=N$, yields for free-end state variables

$$z_i^N=\frac{\partial G^N}{\partial x_i^N},\quad i\neq\beta,\quad z_i^0=\frac{\partial G^0}{\partial x_i^0},\quad i\neq\alpha, \tag{43}$$

and for free-end time t

$$\mathcal{H}^N=-\frac{\partial G^N}{\partial t^N},\quad \mathcal{H}^0=-\frac{\partial G^0}{\partial t^0}. \tag{44}$$

Equation (43) prescribes boundary conditions for the adjoint vector z^n, and Eq. (44) prescribes boundary conditions for the Hamiltonian H^n. As expressed in Eq. (43), if the βth component of the final state vector, x_i^N, or the αth component of the initial state vector, x_i^0, is fixed, the respective component of the adjoint vector, z_β^N or z_α^0, is undetermined. Likewise, if the boundary time, t^N or t^0, is fixed, the respective Hamiltonian, $\mathcal{H}^N$ or $\mathcal{H}^0$, is undetermined. When N tends to infinity, the discrete algorithm becomes that of Pontryagin.

V. OUTLINE OF THE COMPUTATIONAL APPROACH

Now we shall describe the basic principles of solving methods. The primary idea is to solve certain underlying equations [such as Bellman's equation (25), the stage criterion equation (23), or the maximum principle equations (35)–(39)], rather than the related HJB equation (29) or Hamilton Jacobi equation (32). This is because the solving methods for the preferred equations are those most efficient, although they still have some shortcomings: DP is restricted to problems with low dimensionality of state, whereas maximum principles do not generate optimal profit functions directly. The control theory approach used here differs from the traditional approach encountered in mechanics, in which Hamilton-Jacobi equations are solved [17].

We begin with the basic numerical method in which the DP is applied. In the control theory, both continuous and discrete processes with a single independent variable can be treated in the framework of a common discrete formalism. As we aim to work with a discrete set of equations, in the continuous case prior discretizing of the process differential equations is required. Then, it is appropriate to focus on multistage optimization. Here we describe the generation of the optimal function $V^n=\max S$ as a quantity directly related to the optimization criterion. Assume that at the stage n, a profit $\tilde{D}^n=\tilde{D}(\mathbf{x}^n,t^n,\mathbf{u}^n,\theta^n,n)$ is given; in our case $\tilde{D}^n=\tilde{f}_0^n\theta^n$, where tildes over the symbol D^n refer to the gauged profit in Eq. (22), and hence to the optimal function V^n rather than P^n. (To deal with the optimal function P^n, the bare profit $D^n=f_0^n\theta^n$ should be used.) The total profit of the n-stage subprocess is $\Sigma\tilde{D}^k=\Sigma\tilde{f}_0^k\theta^k$, for $k=1,2,\ldots,n$. With the state equations and local constraints at our disposal, any data of $\tilde{D}^n$—analytic, graphic, or tabular—are sufficient. It is, however, important that the data of $\tilde{D}^n$ represent this function completely in terms of the state $\mathbf{x}^n$, time t^n, and controls $(\mathbf{u}^n,\theta^n)$. Data of optimal functions $V^1,\ldots,V^n,\ldots,V^N$ are generated over subprocesses composed of the stages $1,\ldots,n,\ldots$ and N.

For the given set of difference constraints (19), each profit function of the problem, P^n or V^n, is found from Bellman's equation of dynamic programming, Eq. (25). This equation links the optimal functions V^n and V^{n-1} or P^n and P^{n-1} with the related profit at the stage n. The simultaneous generation of data for V^n and P^n is due to the fact that both these functions differ by the path-independent increment of the state function G. In terms of V^n, as the quantity directly connected with the optimization criterion S, the recurrence equation (25) may be written as

$$V^n(\tilde{\mathbf{x}}^n)=\max_{\mathbf{u}^n,\theta^n}\{\tilde{D}^n(\tilde{\mathbf{x}}^n,\mathbf{u}^n,\theta^n)+V^{n-1}(\tilde{\mathbf{x}}^n-\tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}^n,\mathbf{u}^n)\,\theta^n)\}, \tag{45}$$

where the symbol $\tilde{\mathbf{x}}^n$ denotes the enlarged vector $(\mathbf{x}^n,t^n)$ and the tilde over the symbol D^n refers to the gauged profit in-

cluding the effect of the state function G. As shown by Eq. (22), the gauged profit $\tilde{D}^n=\tilde{f}_0^n\theta^n$ is a discrete counterpart of the continuous profit (9).

By an iterating procedure starting with $V^0=0$, a function sequence $V^n(\tilde{\mathbf{x}})\equiv V^n(\mathbf{x},t)$ is obtained for $n=1,2,\ldots,N$, as a solution to Eq. (45). Organization of computations requires a grid of $\tilde{\mathbf{x}}$ in nodes of which data of optimal functions and optimal controls are computed and stored. A total number of stages, N, is assumed. The numerical DP algorithm generates the potential function $V^n(\tilde{\mathbf{x}})$ describing the total profit for the n-stage subprocess from the function $V^{n-1}(\tilde{\mathbf{x}})$ of the $n-1$ stage subprocess and the state transformations, Eq. (19). $V^n(\tilde{\mathbf{x}})$ is obtained by maximizing the sum of the optimal profit of all previous $n-1$ stages (the optimal function V^{n-1}) and the nonoptimal profit $\tilde{D}^n$ at the stage n. To determine the function $V^n(\tilde{\mathbf{x}})$ exactly for a definite n, we would have to numerically determine its values for every value of $\tilde{\mathbf{x}}$, an impossible task. Therefore, we must determine these values on a discrete subset of $\tilde{\mathbf{x}}$, and use the data in the way that enables evaluation of $V^n(\tilde{\mathbf{x}})$ everywhere. This is accomplished by an interpolation. The discrete subset of controls $\mathbf{u}^n$ is treated in a similar way. For example, when the constrains imposed on $\mathbf{u}^n$ satisfy the inequality $\mathbf{u}^*\leqslant\mathbf{u}^n\leqslant\mathbf{u}^*$, the tested variables $\mathbf{u}^n$ may assume only certain discrete values. This refers to the linear grid of controls.

The first optimal function, $V^1(\tilde{\mathbf{x}})$, and the corresponding optimal controls for $n=1$ follow from the application of the initial condition $V^1(\tilde{\mathbf{x}})=0$ in Eq. (45); this yields

$$V^1(\tilde{\mathbf{x}})=\max_{\mathbf{u}^n,\theta^n}\{\tilde{D}^1(\tilde{\mathbf{x}},\mathbf{u}^1,\theta^1)\} \tag{46}$$

and

$$\{\mathbf{u}^1(\tilde{\mathbf{x}}),\theta^1(\tilde{\mathbf{x}})\}=\arg\max_{\mathbf{u}^1,\theta^1}\{\tilde{D}^1(\tilde{\mathbf{x}},\mathbf{u}^1,\theta^1)\}. \tag{47}$$

To find these functions, the computer chooses the first point, say $\tilde{\mathbf{x}}=\mathbf{A}\delta=(A_1\delta,A_2\delta)$, assumes the first $\mathbf{u}=(E_1\gamma,E_2\gamma)$, and compares $\tilde{D}^1(\mathbf{A}\delta,E_1\gamma,E_2\gamma)$ with $\tilde{D}^1(\mathbf{A}\delta,(E_1+1)\gamma,E_2\gamma)$, for a fixed θ^1, in agreement with Eq. (46). The larger of these values is stored, and, in turn, compared with $\tilde{D}^1(\mathbf{A}\delta,(E_1+2)\gamma,E_2\gamma)$. This process is continued until the whole discrete set of controls $\mathbf{u}^1$ is exhausted. The largest of the stored values of $\tilde{D}^1$ is the maximum of $\tilde{D}^1$ with respect to $\mathbf{u}^1$ for the fixed discrete point $\tilde{\mathbf{x}}$ and for the fixed θ^1. At the same time, the coordinates of $\mathbf{u}^1$ which maximize $\tilde{D}^1$ are stored. The computations are then repeated for another fixed value of θ^1, and the best profits $\tilde{D}^1$ are compared until an optimal θ^1 is found for which $\tilde{D}^1$ is the largest. This leads to the absolute maximum of $\tilde{D}^1$ with respect to $\mathbf{u}^1$ and θ^1, for the fixed discrete point $\tilde{\mathbf{x}}$. The resulting coordinates of $\mathbf{u}^1$ and θ^1, which maximize $\tilde{D}^1$, are stored.

Analogous operations are next performed for $\tilde{\mathbf{x}}=((A_1+1)\delta,A_2\delta)$, $((A_1+2)\delta,A_2\delta)$, and so on. This leads again to the maximum of $\tilde{D}^1$ and the optimal values of $\mathbf{u}^1$ and θ^1. The data of the same quantity differ as they refer to various points $\tilde{\mathbf{x}}$ (different nodes of the grid). The computer outputs are the DP tables which contain only the optimal data: $V^1(\tilde{\mathbf{x}})$, $\theta^1(\tilde{\mathbf{x}})$, and $\mathbf{u}^1(\tilde{\mathbf{x}})$.

For $n=2$ (two-stage process), as well as for the larger n, the procedure is analogous but uses the recurrence equation (45) in its complete form. The function V^{n-1} is known in the form of tables describing the previous computations (for the cascade with $n-1$ stages). When its data are used, a difficulty can appear, which is called the ''danger of the grid expansion.'' This means that for some forms of the rate functions $\tilde{\mathbf{f}}$ the computation of $V^n(\tilde{\mathbf{x}})$ will require the knowledge of values $V^{n-1}(\tilde{\mathbf{x}})$ for $\tilde{\mathbf{x}}$ located outside the range $\tilde{\mathbf{x}}_I\leqslant\tilde{\mathbf{x}}\leqslant\tilde{\mathbf{x}}_{II}$, which was required for $V^n(\tilde{\mathbf{x}})$. Therefore, to evaluate $V^n(\tilde{\mathbf{x}})$ within the required range, it may be necessary to determine the function $V^{n-1}(\tilde{\mathbf{x}})$ within a boundary larger than that described by the inequality $\tilde{\mathbf{x}}_I\leqslant\tilde{\mathbf{x}}\leqslant\tilde{\mathbf{x}}_{II}$.

The procedure leads to the optimal values of V^n, θ^n, and $\mathbf{u}^n$ for each node of the grid of $\tilde{\mathbf{x}}$, for each n. These values are stored as the discrete representations of the optimal functions $V^n(\tilde{\mathbf{x}})$, $\theta^n(\tilde{\mathbf{x}})$, and $\mathbf{u}^n(\tilde{\mathbf{x}})$. Coordinates of the transformed states, $T^n(\tilde{\mathbf{x}})\equiv\tilde{\mathbf{x}}-\tilde{\mathbf{f}}^n(\tilde{\mathbf{x}},\mathbf{u}^n)\theta^n$, can also be stored. The computations terminate for $n=N$. Then, by a backward procedure which starts from the given final point $\tilde{\mathbf{x}}^N$, one obtains an optimal solution for the sequence of the optimal controls $\mathbf{u}^N$, $\mathbf{u}^{N-1},\ldots,\mathbf{u}^1$ and $\theta^N,\theta^{N-1},\ldots,\theta^1$, and the optimal discrete trajectory, $\tilde{\mathbf{x}}^N,\tilde{\mathbf{x}}^{N-1},\ldots,\tilde{\mathbf{x}}^1,\tilde{\mathbf{x}}^0$. The sequence of the optimal profits describing the whole process and all its subprocesses, $V^N,V^{N-1},\ldots,V^1$, also follows.

A virtue of the DP method is that it always leads to the absolute maximum, and, as opposed to other methods, an increase in number of constraints simplifies the numerical solution obtained with a computer (fewer points to be tested). The functions describing the profit and state transformation need not be continuous or analytical; they may be given in a graphic or tabular form. Also, the two-point boundary values do not cause problems, as the recurrence equation is not influenced by boundary conditions. Large dimensionality of the control vector does not cause essential troubles. There exists, however, a very serious difficulty connected with the use of the dynamic programming. This is the so-called ''curse of dimensionality,'' referred to the large dimensionality of the state vector, $\tilde{\mathbf{x}}$. Clearly, the number of computational points, and hence the memory requirements for the computer, increase tremendously with the state dimensionality s. Problems with $s=1$ and $s=2$ are quite easy to solve numerically, problems with $s=3$ may be troublesome, problems with $s=4$ are already serious, and problems with $s\geqslant5$ are practically intractable if good accuracy is required. Thus the numerical dynamic programming can effectively be applied only to problems characterized by the small dimensionality of the state vector $\tilde{\mathbf{x}}$; problems of large dimensionality, such as those encountered in the static optimization, are excluded. In the latter case, other methods, especially maximum principle algorithms, must be applied. Sometimes, however, a dimensionality reduction is possible in DP problems. For the problems considered here, a dimensionality reduction is possible, among others, in autonomous systems, in view of the constancy of the discrete $\mathcal{H}$ along an optimal path.

For V^n regarded as a production profit, a net economic profit, or the difference between V^n and the ''time penalty cost'' $h(t^n-t^0)$, can be defined. We will designate by an asterisk subscript the modified profits or costs of this sort, and will focus on their properties in the case of the constant Hamiltonian $\mathcal{H}^{n-1}=\mathcal{H}$. (This case is both the most important and the simplest.) Thus, we will deal with optimal functions describing net profits $V_*^n \equiv V^n - h(t^n - t^0)$ or with analogous functions describing net costs $R_*^n \equiv R^n + h(t^n - t^0)$, both criteria being equivalent. The quantity h is the constant numerical value of $\mathcal{H}^n$. It describes the decrease of the process profit when the process time is increased by one unit.

For the net profit $\tilde{D}_*^n \equiv \tilde{D}^n - h\theta^n$ the optimal behavior at the stage n is governed by the sequence of the asterisk functions: $V_*^1,\ldots,V_*^n,\ldots,V_*^{N-1}$ and V_*^N. An optimal function obeys the equation

$$V_*^n(\mathbf{x}^n,h) = \max_{\mathbf{u}^n,\,\theta^n}\{\tilde{D}_*^n(\mathbf{x}^n,\mathbf{u}^n,\theta^n,h) + V_*^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n,\mathbf{u}^n)\theta^n,h)\}. \tag{48}$$

It differs from Eq. (45) by the presence of the vector $\mathbf{x}$ rather than $\tilde{\mathbf{x}} \equiv (\mathbf{x},t)$. Because of the constancy of $\mathcal{H}^{n-1}=h$ along a discrete optimal path, the state dimensionality of the problem described by Eq. (48) is decreased by 1 in comparison with that described by Eq. (45).

The profits V^n and V_*^n preserve a number of the basic qualitative properties of the (economic) production profits and the total profits. (In the cost representation this is true for the optimal cost functions $R^n \equiv -V^n$ and $R_*^n \equiv -V_*^n$.) For multistage control processes, the optimal profits generated by the dynamic programming always have the structure of the sequence of functions $V^n(\mathbf{x},t)$ or their duals $V_*^n(\mathbf{x},h)$. The profit functions $V^n(\mathbf{x},t)$ and $V_*^n(\mathbf{x},h)$, or cost functions $R^n(\mathbf{x},t)$ and $R_*^n(\mathbf{x},h)$, which describe production and total profits (costs) of processes with one independent variable (time or length), are related by a Legendre transformation with respect to this independent variable [18,19]. The limiting case of a continuous process is characterized by the functions $V(\mathbf{x},t)$ and $V_*(\mathbf{x},h)$, which are mathematical equivalents of Hamilton's principal action and the ''abbreviated action'' of classical mechanics or related phase functions in optics [8]. The relation between the optimal cost functions generated by the DP and Pontryagin's maximum principle is now well understood [20]. The optimal trajectories of a control problem are equivalent to mechanical trajectories in mechanics or light rays in optics. The use of dynamic programming for constructing the finite-time potentials of discrete and continuous control separation processes has been summarized [5].

Now we outline the second basic numerical method. It applies the discrete maximum principle with the energy-type Hamiltonian (31). The necessary extremum conditions are Eqs. (35)–(39) with $\theta^n = t^n - t^{n-1}$, whose form suitable for numerical considerations is

$$F_1(\mathcal{H}^{n-1},\mathbf{x}^n,\mathbf{z}^{n-1},t^n,\mathbf{u}^n)=0$$

[definition of $\mathcal{H}^{n-1}$, Eq. (35)],

$$\mathbf{F}_2(\mathbf{x}^n,\mathbf{x}^{n-1},t^n,t^{n-1},\mathbf{u}^n)=0$$

[state equations, Eq. (36)],

$$\mathbf{F}_3(\mathbf{x}^n,\mathbf{z}^n,\mathbf{z}^{n-1},t^n,t^{n-1},\mathbf{u}^n)=0$$

[adjoint equations, Eq. (37)],

$$F_4(\mathcal{H}^n,\mathcal{H}^{n-1},\mathbf{x}^n,\mathbf{z}^{n-1},t^n,t^{n-1},\mathbf{u}^n)=0$$

[rate change of $\mathcal{H}^{n-1}$, Eq. (38)],

$$\mathbf{F}_5(\mathbf{x}^n,t^n,\mathbf{z}^{n-1},\mathbf{u}^n)=0$$ [extremality of $\mathcal{H}^{n-1}$, Eq. (39)].

These are algebraic equations which should be solved with a computer. Note that in the case of an autonomous process, Eq. (38) simplifies to the form $\mathcal{H}^n=\mathcal{H}^{n-1}$.

Typical optimal control problems lead to two-point boundary conditions, and procedures matching these boundary conditions should be designed. Contrary to DP algorithms, two-point boundary conditions increase the difficulty of the numerical solution when the maximum principle is used. Due to a strong analogy with Pontryagin's algorithm, both trial and error procedures which deal with two-point boundary values and control improvement procedures are identical with those applied in the standard continuous algorithm [3,4,21]. Methods of trajectory improvement in the state space and gradient methods in the control space are effective.

Quite generally, an approach transforms Eqs. (35)–(39) into a final set,

$$\tilde{\mathbf{F}}_1(\mathbf{x}^n,\mathbf{x}^{n-1},\mathbf{z}^n,t^n)=0 \tag{49}$$

and

$$\tilde{\mathbf{F}}_2(\mathbf{x}^n,\mathbf{z}^n,\mathbf{z}^{n-1},t^n)=0. \tag{50}$$

From this set the state and adjoints before the nth stage, $\mathbf{x}^{n-1}$ and $\mathbf{z}^{n-1}$, and all other quantities entering the stage n are determined, thus the computer may pass to the stage $n-1$. This backward procedure is necessary from the practical viewpoint in the case of a complex (nonlinear) dependence of the rate functions on the state $\mathbf{x}^n$.

VI. EXTENDED APPLICATION TO MULTISTAGE THERMAL MACHINES

We begin a brief review of applications of HJB equations with multistage systems in which work can be produced by cascade thermal machines operating sequentially between a fluid and a bath, i.e., an infinite reservoir. The multistage process is, in fact, a steady sequence of Novikov-Curzon-Ahlborn engines (NCA processes [22,23]). The sequential NCA process is a finite-stage counterpart of the recently considered continuous process [24]. The system contains the driving fluid with gradually decreasing temperatures $T^1,\ldots,T^N$; the environment at the constant temperature T^e; the boundary layers which act as thermal conductances; and the set of the Carnot engines, $C^1,\ldots,C^N$, which generate the mechanical work at each stage n. An analytical formulation

of the multistage problem deals with maximizing of the work criterion

$$S^N=\sum_1^N f_0(T^n,u^n)\,\theta^n\equiv\sum_1^N c\left(\frac{T^e}{T^n+\chi u^n}-1\right)u^n\theta^n, \quad (51)$$

where the coefficient $\chi=\rho c/(\alpha' a_v)$, ρ is the fluid's density, c its specific heat, α' the overall heat transfer coefficient associated with the overall conductance g, and a_v is the total exchange area per unit volume of the fluid [24]. Our task is to achieve an extension of this problem that could take into account variability in time of thermal and transfer coefficients (such as the specific-heat capacity c or the heat transfer coefficient α') and to include mass transfer. The gauging function $G=0$. The product χu^n (in units of the temperature) equals $=-q^n/g^n$, where g^n is the overall thermal conductance at the stage n and q^n is the heat which drives the nth Carnot engine. The control u^n plays the role of the discrete rate of the temperature change of the fluid in time t. The nondimensional conductance $\theta^n/\chi=g^n/(cG)$ coincides with the so-called number of transfer units at the stage n, a well-known engineering quantity.

A generalization of the above equation includes the effect of mass transfer [25]. In this case the power intensity function f_0^n, which generalizes Eq. (51), has an involved form. Some redefinitions are suitable; molar quantities are used and the Lewis analogy is applied, which links the heat and mass transfer coefficients. In this case, the function f_0^n has units of a molar work, associated with nondimensional time τ, whose interval $\theta^n=g^n/G$. [A description based on the usual time requires applying $\chi=\rho c/(\alpha' a_v)$.] There are two state variables T and X (concentration), and two controls u and v. The first control is related to the heat flux, $q=-gcu$, where g is the mass transfer conductance in molar units. The second control is related to the molar mass flux, $m=-gv$. For each n, the intensity of power production per unit of τ is

$$f_0(T,X,u,v)=\frac{w}{g}=cu-cTv+\frac{g_2}{g}c^eT^e-\left(\frac{g_2}{g}c^e-c_pv\right)T^e\left\{\left(\frac{T+\left(c\frac{g_1}{g}+c_pv\right)^{-1}cu}{T+\frac{g_1}{g}\left(c\frac{g_1}{g}+c_pv\right)^{-1}cu}\right)\right.$$
$$\left.\times\left(\frac{(1+X)^{(1+X)}\left(X+\frac{gv}{g_1}\right)^{[X+(gv/g_1)]}}{X^X\left(1+X+\frac{gv}{g_1}\right)^{[1+X+(gv/g_1)]}}\right)^{(g_1R/g_2c^e)}\left(\frac{(1+X^e)^{(1+X^e)}\left(X^e-\frac{gv}{g_2}\right)^{[X^e-(gv/g_2)]}}{X^{eX^e}\left(1+X^e-\frac{gv}{g_2}\right)^{[1+X^e-(gv/g_2)]}}\right)^{(-g_2R/g_2c^e)}\right\}. \quad (52)$$

With this function, applied as f_0^n in the first sum of Eq. (51), we can find a maximum for the cumulative mechanical work when a finite-resource fluid changes its thermodynamic parameters in a finite time between two assumed states. The above power formula reduces exactly to that of pure heat transfer when the molar flux $m=0$ [25].

For an analytical result, i.e., for the problem of pure heat transfer whose function f_0^n appears in Eq. (51), Bellman's equation (25) with $P\equiv V$ has recently been solved [26]. The function of the optimal work production, V^N, is

$$V^N=-R^N=c(T^0-T^N)+cT^eN\left[1-\left(\frac{T^0}{T^N}\right)^{1/N}\right]$$
$$-cT^e\frac{\{N[1-(T^0/T^N)^{1/N}]\}^2}{\tau^N+N[1-(T^0/T^N)^{1/N}}. \quad (53)$$

This potential is associated with constant θ^n,u^n increasing linearly with T^n, and the optimal trajectory satisfying the rule $T^n=(T^{n-1}T^{n+1})^{1/2}$ for arbitrary stages $n-1$, n, and $n+1$. For the continuous limit we find

$$V=-R=c(T^i-T^f)-cT^e\ln\frac{T^i}{T^f}-cT^e\frac{[\ln(T^i/T^f)]^2}{\tau^f-\ln(T^i/T^f)}. \quad (54)$$

The last terms in Eqs. (53) and (54) are nonclassical; they are caused by finite rates which decrease work produced and increase work consumed.

For Eq. (52) only a numerical solution is possible. In this case a computer procedure generates tables of optimal controls and optimal costs through a direct extremizing procedure contained in the recurrence equation

$$R_*^n(T^n,X^n)=\min_{u^n,v^n,\theta^n}\{[-f_0(T^n,X^n,u^n,v^n)+h]\theta^n$$
$$+R_*^{n-1}(T^n-u^n\theta^n,X^n-v^n\theta^n)\}, \quad (55)$$

where the power function f_0 is given by Eq. (52) and the Hamiltonian constant h serves as the Lagrange multiplier of the time constraint to eliminate τ^n from the working set of original state variables. The X-free truncation of this equation serves to generate numerical generalizations of functions

(53) and (54) when both the transfer coefficients and the heat capacity vary along the process path, and an analytical solution cannot be obtained.

The classical thermodynamic work is recovered in a limit of a reversible process, for an infinite duration ($\tau^{\int} \Rightarrow \infty$). The classical work represents an exact evaluation of the maximum work production for infinite-size systems only, or for systems with excellent transfer conditions. This result proves that classical thermostatic limits are too low to be realistic, and finite-time limits should be more useful in practical evaluations.

VII. DRYING SEPARATION PROCESSES WITH COMPLICATED EQUILIBRIA

We now consider another group of processes, such as separation processes and chemical reactions which, as a rule, do not generate mechanical energy although they may yield valuable products. Here we are focused on optimization of complex processes of drying and adsorption which constitute an example of processes described by highly nonlinear state equations. These processes run frequently in cascades of ideally mixed fluidized beds, and are characterized by strong nonlinearities following from complex solid-gas equilibria (sigmoidal curves which do not approach straight lines even in limiting cases).

The performance criterion is usually the sum of the exploitation costs measured by the available energy (''exergy'') of the drying agent and the cascade cost understood as the investment cost of all stages. Neglecting fixed parts of these costs (which do not influence the basic result), the profit form of the performance index may be written as

$$S^N \equiv -\sum_{n=1}^{N} [eb_g^n(T_g^n, X_g^n) + h]\theta^n, \tag{56}$$

where b_g is the specific exergy of the drying gas and e is the economic value of the exergy unit. Economic considerations for fluidized beds link the numerical value of the time constraint multiplier, h, with the unit apparatus price. The h part of the optimization criterion represents the investment costs per mass unit of the dry solid product. An approximate expression for the criterion (56) is the quadratic objective with constant A, B, C, and h,

$$S^N = -\sum_{n=1}^{N} [\tfrac{1}{2}A(T_g^n - T^e)^2 + \tfrac{1}{2}B(X_g^n - X^e)^2 + C + h]\theta^n. \tag{57}$$

The state variables at the stage n are the outlet solid temperature T_s^n and outlet solid moisture content W_s^n. They appear in the discrete state equations

$$\frac{T_s^n - T_s^{n-1}}{\theta^n} = c_s^{-1}\{i_g^n(T_g^n, X_g^n) - i_s^n(W_s^n, T_s^n) - i_w^n(X_g^n - X_s^n(W_s^n, T_s^n))\} \tag{58}$$

and

$$\frac{W_s^n - W_s^{n-1}}{\theta^n} = X_g^n - X_s^n(W_s^n, I_s^n), \tag{59}$$

where i_w^n is the partial enthalpy of moisture in solid and $\theta^n = \Delta G^n/S$ is the gas mass flux through the stage n per unit solid mass flux S. The state equations contain the decision variables T_g^n and X_g^n, and the gas enthalpy function i_g^n which is evaluated in terms of these decisions. The state equations contain also complex state dependent equilibrium functions $i_s^n(W_s^n, T_s^n)$ and $X_s^n(W_s^n, T_s^n)$. They describe the enthalpy and humidity of gas in equilibrium with solid, and are given by semiempirical formulas [27].

The discrete maximum principle, Eqs. (35)–(39), is used to solve the problem of minimum cost (56). The Hamiltonian function is

$$\begin{aligned} H^{n-1}(W_s^n, T_s^n, z_1^{n-1}, z_2^{n-1}, T_g^n, X_g^n) &\equiv z_1^{n-1}c_s^{-1}\{i_g^n(T_g^n, X_g^n) - i_s^n(W_s^n, T_s^n) \\ &\quad - i_w^n(X_g^n - X_s^n(W_s^n, T_s^n))\} + z_2^{n-1}[X_g^n - X_s^n(W_s^n, T_s^n)] \\ &\quad - [eb_g^n(T_g^n, X_g^n) + h]. \end{aligned} \tag{60}$$

For this H the canonical set (36)–(39) is constructed and its numerical solution is obtained for optimal controls, optimal trajectories, and optimal costs. Drying of silicagel by air in the three-stage cascade of fluidized beds ($N=3$) is studied [11,28]. The initial state of solid and the final solid moisture content are prescribed, whereas the final solid temperature is free. The multiplier of the process duration, h, which is also an intensity index of the optimal process, is changed in the range 0.42–4.20 kJ/kg.

The optimal control data show the following properties: The optimal gas temperatures T_g^n decrease along the optimal path. The optimal gas humidites X_g^n decrease along the optimal path. For a very small h the values X_g^n attain the limiting environmental humidity ($X^e = 0.008$ kg/kg). The optimal dimensionless gas flows $\theta^n = \Delta G^n/S$ are unequal along the optimal path. The largest flows are at the first stage and the lowest at the last stage of the cascade. Each flow θ^n decreases when h increases, corresponding with the increase of the process intensity with h. Otherwise, for $h=0$, very large θ^n are obtained corresponding to drying of the solid by the environmental gas.

The optimal trajectories of the controlled drying process with a free final temperature of solid depend substantially on the factor h which is the constant of these paths. For small h (0.42 kJ/kg), the state transitions are through regimes of low temperatures of solid (with possible minima of T_s), consistent with the use of gas with the lower exergy potential (low T_g and large X_g, which are close to the ambient parameters, T^e and X^e). For large h, the state transitions are through higher temperatures of solid, with possible maxima of T_s. Such solutions apply to the drying of sugar, porous sorbents, and T-sensitive biological materials. These materials should be dried relatively fast, but otherwise their final temperature should not be too high. The results show that apparatuses of large unit cost should be designed for intensive optimal processes, to assure short process durations, so as to avoid basic mistakes in the design of new equipment.

VIII. TWO-PHASE SYSTEMS SPONTANEOUSLY RELAXING TO EQUILIBRIUM

Here we are dealing with relaxation processes in which state variables are linked by conservation laws for the energy, mass, and momentum. For processes of this sort, an approach which applies Lagrange multipliers to handle dependent rates is required. The system contains two phases δ and γ which relax to the mutual equilibrium. Applying the theorem of a minimum of entropy production to the relaxing system with heat and mass transfer between its two subsystems, we find the canonical (Hamilton's) structure of dynamics, and show a self-consistent way to derive this dynamics. The dependent variables, $\mathbf{x}=(\mathbf{n},e)-(\mathbf{n}^*,e^*)$, are deviations of mole numbers, $\mathbf{n}$, and energy, e, from their equilibrium values, $\mathbf{n}^*$ and e^*. In a forward DP algorithm we minimize the entropy production or maximize the entropy functional

$$S=S^f-\int_{t^0}^{t^f}[\tfrac{1}{2}\mathbf{R}^\gamma(\mathbf{x}):\mathbf{v}^\gamma\mathbf{v}^\gamma+\tfrac{1}{2}\mathbf{R}^\delta(\mathbf{x}):\mathbf{v}^\delta\mathbf{v}^\delta+\Psi(\mathbf{x}^\gamma,\mathbf{x}^\delta)+\mu\cdot(\mathbf{v}^\gamma+\mathbf{v}^\delta)]dt, \tag{61}$$

where the superscripts γ and δ refer to two phases, the superscript f to final states, Ψ is the second (state-dependent) dissipation function, and $\mathbf{R}^\gamma$ and $\mathbf{R}^\delta$ are $\mathbf{x}$-dependent resistances. The balance constraints are handled by the Lagrange multiplier μ'. The variables $\mathbf{x}=(\mathbf{x}^\gamma,\mathbf{x}^\delta)$ and $\mathbf{v}=(\mathbf{v}^\gamma,\mathbf{v}^\delta)$ satisfy the simple differential constraints

$$\dot{\mathbf{x}}^\gamma=\mathbf{v}^\gamma;\quad \dot{\mathbf{x}}^\delta=\mathbf{v}^\delta. \tag{62}$$

Our goal is to show that the quadratic approximation of the thermodynamic entropy

$$\mathcal{S}(\mathbf{x},\mathbf{n}^*,e^*)=\mathcal{S}^*(\mathbf{n}^{\gamma^*},e^{\gamma^*},\mathbf{n}^{\delta^*},e^{\gamma^*})+\mathbf{p}^*\cdot(\mathbf{x}^\gamma+\mathbf{x}^\delta)-\tfrac{1}{2}\Gamma^\gamma:\mathbf{x}^\gamma\mathbf{x}^\gamma-\tfrac{1}{2}\Gamma^\delta:\mathbf{x}^\delta\mathbf{x}^\delta, \tag{63}$$

where Γ is the Hessian matrix and the asterisk refers to the equilibrium, which is a suitable extremal function for the linear dynamics (with $\mathbf{x}$-independent $\mathbf{R}^\gamma$ and $\mathbf{R}^\delta$). Otherwise, the approximation will be insufficient for nonlinear dynamics with state-dependent resistances. The HJB theory along with Belman's equation (25) or the stage criterion (23) provide an efficient way to treat such nonlinear systems.

Defining the potential of integral entropy production $S_s\equiv\min(S^f-S)=S^f-P$, we arrive at the forward HJB equation (7) in the form

$$\max_{\mathbf{v}^\gamma,\mathbf{v}^\delta,\mu'}\left\{\frac{\partial S_\sigma}{\partial t}+\frac{\partial S_\sigma}{\partial\mathbf{x}^\gamma}\mathbf{v}^\gamma+\frac{\partial S_\sigma}{\partial\mathbf{x}^\delta}\mathbf{v}^\delta-\mathbf{R}^\gamma(\mathbf{x}^\gamma):\mathbf{v}^\gamma\mathbf{v}^\gamma-\tfrac{1}{2}\mathbf{R}^\delta(\mathbf{x}^\delta):\mathbf{v}^\delta\mathbf{v}^\delta-\Psi(\mathbf{x}^\gamma,\mathbf{x}^\delta)-\mu'\cdot(\mathbf{v}^\gamma+\mathbf{v}^\delta)\right\}=0, \tag{64}$$

where $\mathbf{v}^\gamma$ and $\mathbf{v}^\delta$ are the two dependent controls and the S_σ-free part represents the negative of the thermodynamic Lagrangian. The HJB formulation (64) is useful for an arbitrary dependence of resistance functions on the state $\mathbf{x}$. Of course, $\partial S_\sigma/\partial t=\partial\Psi/\partial t=0$ for adiabatic thermodynamics. In terms of the current nonequilibrium entropy $\mathcal{S}$ as the optimal function, the Hamilton-Jacobi equation of the dependent variable theory is a truncation of the general standard form

$$\frac{\partial\mathcal{S}}{\partial t}+\mathcal{H}_\sigma\left(\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\gamma},\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\delta},\mathbf{x}^\gamma,\mathbf{x}^\delta,t\right)=0, \tag{65}$$

with the functions $\mathcal{S}$ and $\mathcal{H}_\sigma$ explicitly independent of the time t. In linear adiabatic systems, with $\mathbf{x}$-independent resistances $\mathbf{R}^\gamma$ and $\mathbf{R}^\delta$, the Hamilton-Jacobi equation applies in a quadratic time-independent form

$$\tfrac{1}{2}\mathsf{L}:\left(\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\gamma}-\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\delta}\right)\left(\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\gamma}-\frac{\partial\mathcal{S}}{\partial\mathbf{x}^\delta}\right)-\tfrac{1}{2}\mathbf{W}^\gamma:\mathbf{x}^\gamma\mathbf{x}^\gamma-\tfrac{1}{2}\mathbf{W}^\delta:\mathbf{x}^\delta\mathbf{x}^\delta=\mathbf{0}, \tag{66}$$

where $\mathsf{L}\equiv(R^\gamma)^{-1}+R^\delta)^{-1}$ and $W^\gamma=\Gamma^\gamma(R^\gamma)^{-1}\Gamma^\gamma$. This is satisfied by the entropy potential, Eq. (63). In the phase space, for linear systems

$$\mathcal{H}_\sigma(\mathbf{p}^\gamma,\mathbf{p}^\delta,\mathbf{x}^\gamma,\mathbf{x}^\delta)\equiv\tfrac{1}{2}\mathsf{L}:(\mathbf{p}^\gamma-\mathbf{p}^\delta)(\mathbf{p}^\gamma-\mathbf{p}^\delta)-\tfrac{1}{2}\mathbf{W}^\gamma:\mathbf{x}^\gamma\mathbf{x}^\gamma-\tfrac{1}{2}\mathbf{W}^\delta:\mathbf{x}^\delta\mathbf{x}^\delta=\mathbf{0}. \tag{67}$$

This equation yields the canonical set in the form of dependent Hamilton's equations which are linear and satisfy the conservation laws identically.

In terms of the original state vector $\tilde{\mathbf{n}}=(\mathbf{n},e)$, and for Gibbs equation defining the nonequilibrium entropy as an additive quantity over the homogeneous subsystems

$$d\mathcal{S}\equiv d\mathcal{S}^\gamma+d\mathcal{S}^\delta=\mathbf{p}^\gamma\cdot d\tilde{\mathbf{n}}^\gamma+\mathbf{p}^\delta\cdot d\tilde{\mathbf{n}}^\delta, \tag{68}$$

the dynamics of phase γ has the canonical form

$$\frac{d\tilde{\mathbf{n}}^\gamma}{dt}=\frac{\partial\mathcal{H}_\sigma}{\partial\mathbf{p}^\gamma},\quad \frac{d\mathbf{p}^\gamma}{dt}=-\frac{\partial\mathcal{H}_\sigma}{\partial\tilde{\mathbf{n}}^\gamma}, \tag{69}$$

which, in the case of the linear dynamics, is governed by the extremum Hamiltonian of Eq. (67). (An analogous dynamics holds for the phase δ.) The canonical equations describe relaxation of mole numbers and energy and their thermodynamic adjoints p (temperature reciprocals and Planck potentials) to equilibrium. For the linear relaxation of the phase γ consistent with the quadratic entropy function, Eq. (63),

$$\frac{d\tilde{\mathbf{n}}^\gamma}{dt}=\mathbf{K}^\gamma(\tilde{\mathbf{n}}^{\gamma^*}-\tilde{\mathbf{n}}^\gamma),\quad \frac{d\mathbf{p}^\gamma}{dt}=\mathbf{K}^{\mathbf{T}^\gamma}(\mathbf{p}^*-\mathbf{p}^\gamma). \tag{70}$$

Thus the equations of motion for the state variables $\tilde{\mathbf{n}}$ and their thermodynamic adjoints $\mathbf{p}$ complement the canonical set (70). Our analysis shows that the linear relaxation of the state variables is governed by the transfer matrix $K^\gamma=(\mathbf{R}^\gamma)^{-1}\Gamma^\gamma$ and that of the thermodynamic adjoints by its transpose, $K^{T\gamma}=\Gamma^\gamma(\mathbf{R}^\gamma)^{-1}$. Only in the particular case when K is symmetric are relaxations of state variables and their thermodynamic adjoints governed by the same common matrix K. The analysis shows the coherence and elegance of the variational approach.

In nonlinear systems with $\mathbf{x}$-dependent $\mathbf{R}^\gamma$ and $\mathbf{R}^\delta$ in Eq. (61), forward recurrence equations (25) or (45) are applied to solve the quasilinear HJB equation (64) or the related

Hamilton-Jacobi equation (65). In terms of the optimal cost function $S_\sigma \equiv -V^n$, which represents the mimimum entropy production, the recurrence equation is

$$S_\sigma^n(\mathbf{x}^n) = \min_{\mathbf{v}^n,\theta^n,\mu^n} \{l_0^n(\mathbf{x}^n,\mathbf{u}^n,\mu'^n)\theta^n + S_\sigma^{n-1}(\mathbf{x}^n - \mathbf{v}^n\theta^n)\}, \tag{71}$$

where $\theta^n = t^n - t^{n-1}$ and $l_0^n \equiv -f_0^n$ is the thermodynamic Lagrangian at stage n. At each stage n,

$$l_0(\mathbf{x},\mathbf{v},\mu') \equiv \tfrac{1}{2}\mathbf{R}^\gamma(\mathbf{x}):\mathbf{v}^\gamma\mathbf{v}^\gamma + \tfrac{1}{2}\mathbf{R}^\delta(\mathbf{x}^\gamma):\mathbf{v}^\delta\mathbf{v}^\delta + \Psi(\mathbf{x}^\gamma,\mathbf{x}^\delta) + \mu'\cdot(\mathbf{v}^\gamma + \mathbf{v}^\delta). \tag{72}$$

Here the Lagrange multipliers μ' are extra coordinates of the control vector. To reduce the problem's dimensionality, the trivial conservation constraint is eliminated and the set of independent state variables $\alpha = \mathbf{x}^\gamma$ and controls $\mathbf{v}^\gamma$ is used. Note that $V^n = V_*^n$ whenever $H^n \equiv 0$; thus the potential functions S_σ^n and $S_{\sigma *}^n$ generated by Eq. (71) or its asterisk counterpart represent the same quantity which describes the minimum production of the classical entropy S_σ in the nonlinear case. This quantity should be subtracted from the reference final entropy S^f to get the actual entropy of the system [29].

IX. HEAT RAYS ALONG PATHS OF LEAST RESISTIVITY IN INHOMOGENEOUS MEDIA

When a thermal field in a rigid medium is imposed by fixing the thermal gradient, the flow of thermal energy can be described in terms of ''thermal rays,'' which are the paths of heat flow in the direction of temperature gradient. Their deviation from straight lines results from variable thermal conductivity [30,31]. The thermal rays travel along paths satisfying the principle of minimum of entropy production, which seems at first glance quite different from the well-known Fermat principle of minimum time for optical rays. However, the minimum of entropy production assures the minimum resistivity of the path, which causes the maximum of heat flux through the medium and makes the residence time of heat in this medium as short as possible. This, in fact, is very similar to the Fermat principle for propagation of light. Our purpose is to investigate this phenomenon by the method of dynamic programming.

We use the reference frame (x,y) in which the local resistivity of heat flow changes along the axis x, the axis y is tangent to a surface of constant specific resistivity ρ, and $u = dy/dx$ is the local direction of the gradient of temperature reciprocal T^{-1}. The shape of thermal rays can be described as an optimal control problem for a minimum of the resistivity integral,

$$(-S) = \int_{t_1}^{t_2} A_0^{-1}\rho(x)(1+u^2)dx, \tag{73}$$

subject to the control $u = dy/dx$. A_0 is the constant area of projection of the heat flux tube cross-sectional area on the surface of constant resistivity. The minimal resistance function of the problem defined as

$$R(x^i,y^i,x^f,y^f) \equiv \min \int_{t_1}^{t_2} A_0^{-1}\rho(x)(1+u^2)dx \tag{74}$$

satisfies the HJB equation

$$\frac{\partial R}{\partial x} + \max_u \left\{ \frac{\partial R}{\partial y}u - A_0^{-1}\rho(x)(1+u^2) \right\} = 0. \tag{75}$$

Extremizing the Hamiltonian in the above HJB equation yields as an optimal control

$$u = \frac{A_0}{2\rho(x)}\frac{\partial R}{\partial y}. \tag{76}$$

This optimality condition is written in the form of the tangent law of bending for a thermal ray,

$$\rho(x)\frac{dy}{dx} = \tfrac{1}{2}A_0\frac{\partial R}{\partial y} \equiv c, \tag{77}$$

where c is a constant which may be both positive or negative. The constancy of the partial derivative $\partial R/\partial y$ follows from an explicit independence of the model Lagrangian with respect to y. A suitable integral formula for the bending constant in terms of the deviation $y - y^0$ is

$$c = (y-y^0)\left(\int_{x^0}^{x} \rho^{-1}(x')dx' \right)^{-1}. \tag{78}$$

Expressing the optimal control u in the HJB equation (75) in terms of $p = \partial R/dy$ yields the Hamilton-Jacobi equation of the continuous problem

$$\frac{\partial R}{\partial x} + A_0^{-1}\rho(x)\left[\left(\frac{A_0}{2\rho(x)}\frac{\partial R}{\partial y} \right)^2 - 1 \right] = 0, \tag{79}$$

where the second term of the left-hand side expression is the optimal Hamiltonian. The solution to this equation can always be broken down to quadratures. However, if the function of specific resistivity $\rho(x)$ is too complicated, the integrals cannot be evaluated analytically. Hence the role of the discrete approach which solves numerically Bellman's recurrence equation of the problem

$$R^n(y^n,x^n) = \min_{\mathbf{u}^n,\theta^n} \{A_0^{-1}\rho(x^n)[1+(u^n)^2]\theta^n + R^{n-1}(y^n - u^n\theta^n, x^n - \theta^n)\}, \tag{80}$$

where $\theta^n = x^n - x^{n-1}$. This cannot be analytically solved for an arbitrary $\rho(x^n)$, thus the sequence of functions R^n must be generated numerically. Yet, in the limit of an infinite number of stages, an analysis shows that the potential function satisfying Eq. (80) takes the limiting form

$$R(x,y) = \int_{x^0}^{x} A_0^{-1}\rho(x')dx' + A_0^{-1}(y-y^0)^2\left(\int_{x^0}^{x} \rho^{-1}(x')dx' \right)^{-1}. \tag{81}$$

It may be verified that the above function satisfies both the HJB equation (75) and the Hamilton-Jacobi equation (79).

The numerical solution to Eq. (80) for a finite number of stages n represents the finite-stage generalization of the solution (81); this numerical solution automatically accomplishes the numerical integration required in Eq. (81).

X. PROPAGATING DIFFUSION-REACTION FRONTS IN ANNULAR MEMBRANES

Recent research shows that the propagation of the concentration fronts as (bio)chemical waves also satisfies the principle of minimum time. The dynamic programming approach leads to a HJB equation and its characteristic set for chemical waves. All these equations describe the link between the constrained wave fronts and associated ''rays.'' Usually, ''geodesic'' constraints caused by an obstacle influence the state changes and the entering (leaving) conditions of a ray as a tangentiality condition for rays that begin to slide over the boundary of an obstacle. Thus an analysis can determine complex shapes of rays in inhomogeneous media.

Self-propagating chemical fronts were discovered by experiments in reaction-diffusion systems occurring in fluids and porous solids. Autocatalytic chemical systems were shown to be responsible for the wave propagation, and autocatalytic models were applied to provide expressions for the wave propagation speed [32]. Excitability properties were recognized to be responsible for wave behavior. Spiral waves especially drew considerable attention because of analogous phenomena in biology [33]. A number of dynamical properties observed in experiments were substantiated in terms of interactions of the elementary wave properties with the chemical system geometry. It was Winfree [34] who suggested first that the shape of the spiral waves should be an involute of a small circle, the ''core'' of the spiral wave. An involute of a given curve C is a curve C^* which lies on the tangent surface of C (the surface generated by the tangent lines to C) and intersects the tangent lines orthogonally. The breakthrough was achieved when real open systems and the so-called continuously fed unstirred reactors (CFUR) appeared, which made of possible to study chemical waves under steady conditions. Noszticzius *et al.* [35] developed the first CFUR with a ring geometry using acrylamide gel and created chemical pinwheels in that reactor.

A chemical pinwheel system consists of a circular strip of gel which separates two concentric CSTR's. The wave motion can be understood as an interaction between diffusion and kinetics [36,37]. Chemical components diffuse into the gel, react, and create a medium of excitable properties. Concentrations of species in the outer and inner reservoirs usually differ, thus resulting in radial concentration gradients and inhomogeneous properties of the excitable medium [38]. The chemical species diffuse out of the front of the wave towards the area of lower concentration, the concentration of autocatalyst builds up, and after it crosses a threshold limit, kinetics takes over. In effect, the concentration increases strongly due to autocatalytic reactions, thus building the front of the wave. In inhomogeneous and (possibly) anisotropic media, the description of the propagation of the chemical wave is a very difficult task due to the obstacle constraints on the state coordinates. Our analysis of the wave motion [39] treats the chemical system as a constrained optimal control system which is analogous with a burning prairie. Due to the (nonrelativistic) causality, the real path of ignition is the one along which the fire first arrives at a point, as for all subsequent instants the grass will already be burned out at this point. This means that the system satisfies the Fermat principle of the least time [40].

The simplest approach requires that the propagation speed v is given as a known function of coordinates and directions; when this condition is satisfied, the simplest approach can be applied in its natural form, which deals with ordinary differential equations. For the lumped system, the speed v can be obtained from a basic approach which deals with the underlying autocatalytic model of reaction and diffusion described by partial differential equations of the type [37]

$$\partial_t \mathbf{u} = \mathbf{L}\mathbf{u} + \mathbf{N}(\mathbf{u}) + \mathbf{D}\nabla^2 \mathbf{u}. \tag{82}$$

In Eq. (82), $\mathbf{u}$ is the set of fields, $\mathbf{L}$ and $\mathbf{N}$ are, respectively, the linear and nonlinear reaction dynamics, and $\mathbf{D}$ is the transport (diffusion) matrix. The analysis proceeds by assuming that a constant wave profile emerges and propagates with a constant speed. Rectilinear, solitary wavefronts that propagate with a constant speed v_0 are one-dimensional solutions, $\mathbf{u}(\mathbf{x},t) = \mathbf{w}(x - v_0 t)$, of the ordinary differential equation

$$\mathbf{L}\mathbf{w} + \mathbf{N}(\mathbf{w}) + \mathbf{D}\mathbf{w}'' + v_0 \mathbf{w}' = 0, \tag{83}$$

obtained from Eq. (82) for $\mathbf{u} = \mathbf{w}(x - v_0 t)$, where the prime refers to differentiation with respect to the traveling wave coordinate $r = x - v_0 t$, and the rest state corresponds to $u = \mathbf{0}$. The solution to Eq. (83) represents a shape traveling with a speed v_0; diverse models yield a constant speed v_0 or a state-dependent v [37,41]. The physical propagation speed $v = dl/dt$ depends, in fact, on both the diffusion coefficient of the autocatalytic species and the rate constants of autocatalytic reactions; it is a function of the rest state. To apply the propagation speed in the framework of the minimum time approach, state coordinates must be assigned to each point of the physical space where the wave motion occurs.

When a function describing the propagation speed is known, a HJB equation can be formulated. For a constrained problem of minimum time in two-dimensional experimental systems, a HJB equation is

$$\max_{u\mu} \left\{ \frac{\partial T v(x,y,u)}{\partial x \sqrt{1+u^2}} + \frac{\partial T v(x,y,u) u}{\partial y \sqrt{1+u^2}} - [1 + \mu \phi(x,y)] \right\} = 0, \tag{84}$$

where $u = dy/dx$ and T is the function being sought, which describes the shortest transition time. The constraint $\phi(x,y) = 0$ was built in, operative when the ray slides over the surface of an obstacle; the corresponding Lagrange multiplier is μ. Note that the multipliers of the derivatives $\partial T/\partial x$ and $\partial T/\partial y$ in Eq. (84) represent the properly expressed rates dx/dt and dy/dt that satisfy identically the constraint $(dx/dt)^2 + (dy/dt)^2 = v^2(x,y,u)$. The numerical solution can be found with the aid of Bellman's equation for the minimum time $\Sigma \theta^n$,

$$T^n(y,x)=\min_{\mathbf{u}^n,\theta^n,\mu^n}\left\{[1+\mu^n\phi(x,y)]\theta^n + T^{n-1}\left(y-\frac{v(x,y,u^n)u^n\theta^n}{\sqrt{1+(u^n)^2}},x-\frac{v(x,y,u^n)\theta^n}{\sqrt{1+(u^n)^2}}\right)\right\}. \tag{85}$$

The solution describes straight rays in the simplest possible case of a homogeneous medium. In a complex chemical medium, the quantity T which describes the shortest transition time is a constrained generalization of the simplest transition function of a homogeneous and isotropic medium in which the wave motion is with the constant speed v,

$$T(x,y,x^0,y^0)=v^{-1}\sqrt{(x-x^0)^2+(y-y^0)^2}. \tag{86}$$

Equation (85) allows for numerical generation of the function $T(x,y)$ for the case of constrained wave motions in confined regions and in complex media. Experiments confirming the behavior of chemical fronts predicted by the theory are available [33].

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