Variational principles for functionals of the temperature T and for T itself in heat-transfer problems

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Given some functional $F(T)$ of interest in a heat-transfer problem, with T the true temperature, one often introduces a fictitious "alias" temperature θ and an associated functional $F(T,\theta)$. A variational principle (VP) for $F(T,\theta)$ provides estimates of $F(T)$ and of T. Such VP's have been derived on the basis of different physical principles and by means of different mathematical procedures. The unified formulation of the construction of VP's, used previously to derive VP's in a wide range of problems, can also be used in the present context. One introduces one Lagrange multiplier—which can be a constant, a function, an operator, etc.—for each of the constraints necessary to define T. While a VP $F_v(T_{tr},\theta)$ for a functional $F(T,\theta)$, with T_{tr} a trial function, can provide a systematic method for an estimation $T_{est}(\vec{r},t)$ of the temperature distribution $T(\vec{r},t)$ at a point $\vec{r}$ at the time t, it is only the estimate $F_v(T_{tr},\theta)$ of $F(T,\theta)$ which is stationary. The estimate T_{est} is not stationary; it contains first-order errors. Our main interest is in the development of a VP for T. Consideration of $F(T)=T$—we are no longer concerned with alias temperatures—provides a VP for $T(\vec{r},t)$ itself. $T(\vec{r},t)$ can be defined as the solution of linear or nonlinear differential equations, which can be homogeneous or inhomogeneous, and subject to a variety of boundary conditions. An almost identical procedure will provide a VP for the solution of any other equalization process such as the concentration $\Gamma(\vec{r},t)$ in a diffusion process. We also derive a VP for the temperature $T(r)$ and density $\rho(r)$, under specified quasiequilibrium conditions, of the coupled differential equations which characterize some stars. In addition, we consider variational identities. [It has often been stated, incorrectly, that one cannot obtain a VP for $T(\vec{r},t)$.]

I. INTRODUCTION

The variational principles (VP's) for different functionals of the temperature distribution $T(\vec{r},t)$ in heat-conduction and -transfer problems, with $\vec{r}$ a point in space and t the time, include those of Rosen,[1] of Glansdorff and Prigogine,[2–4] and of Biot.[5] Chapter 10 of the book by Finlayson[6] contains an excellent review and a penetrating analysis of these VP's. There is also a VP due to Chambers.[7] Variational principles are based on a variety of physical principles and their derivations involve a variety of mathematical approaches. Thus, the VP of Rosen for irreversible processes is based on Onsager's principle[8] of the minimum rate of entropy production, with the generalized currents varied and the generalized forces held fixed. The VP of Glansdorff and Prigogine utilizes the concept of the local potential, an extension of Onsager's approach, and is applicable to systems undergoing reversible or irreversible processes.[9] Biot's approach represents an extension of the concept of generalized coordinates and the corresponding Lagrangian equations of motion of classical mechanics to thermodynamic problems. It must be emphasized that the above VP's are not VP's for the functionals of physical interest. Rather, they are VP's for functionals which contain not only temperatures T_{tr} which are trial functions for the true temperature, but an alias temperature θ; we will elaborate on this point in Sec. II. Our first task will be to show that the VP's for the different functionals can be derived using the "unified formulation of the construction of VP's" approach of Gerjuoy, Rau, and Spruch,[10,11] an approach which has been shown to generate VP's readily in a wide range of fields. There have, of course, been many articles by many authors discussing a uniform procedure for the construction of VP's, but that of Ref. 11 is probably the most general, and it cites many of the other articles. We present here only the barest outline of the essential idea. In the present context of obtaining a variational principle $F_v(T_{tr})$ for a specified functional $F(T)$ of the unknown temperature distribution $T(\vec{r},t)$, we begin with

$$F_v(T_{tr})=F(T_{tr})+\sum_i \mathscr{L}_i B_i(T_{tr}) , \tag{1.1}$$

where $T_{tr}(\vec{r},t)$ is a (zeroth-order) trial estimate of $T(\vec{r},t)$, the $B_i(T)=0$ represent the constraints which define $T(\vec{r},t)$, and the $\mathscr{L}_i$ are Lagrange multipliers introduced to account for the constraints. The constraints $B_i(T)=0$ include the differential equation satisfied by $T(\vec{r},t)$ and can include the boundary conditions imposed on $T(\vec{r},t)$. The $\mathscr{L}_i$ can be constants, functions, operators, matrices, etc.; the form of an $\mathscr{L}_i$ depends upon the form of the constraint B_i being satisfied and on the functional under consideration. The requirement that $F_v(T_{tr})$ represent a VP imposes the condition

$$\delta F_v \equiv F_v(T_{tr}) - F(T) = 0 , \tag{1.2}$$

to first order, since the definition of a VP is that first-order errors vanish. Equation (1.2) provides the equations which define the $\mathscr{L}_i$. These latter equations need *not* be solved exactly, since a first-order error $\delta\mathscr{L}_i$ in the trial estimate $(\mathscr{L}_i)_{tr}$ of $\mathscr{L}_i$ leads to a second-order error in the estimate F_v of F. (One must be very careful in the discrete case, since then the equations defining some of the $\mathscr{L}_i$ are of the form $A\mathscr{L}_i = h_i$, with A^{-1} singular; the difficulty can be circumvented.[12]) We note that in the general problem of constructing a VP, the defining equations can be linear or nonlinear and homogeneous or inhomogeneous differential equations, or integral equations, integro-differential equations, or integro-difference equations.

Some but not all of the VP's to be considered can be easily derived if one utilizes the variational principle for the real inner product

$$M \equiv -(X,f) , \tag{1.3a}$$

where the function f is known and where the unknown function X is defined by

$$KX = f , \tag{1.3b}$$

where K is a known symmetric operator. A stationary expression $M_v = M_v(X_{tr})$ for the functional $M = M(X)$ is given by[13]

$$M_v(X_{tr}) = (X_{tr}, KX_{tr}) - 2(X_{tr}, f) , \tag{1.4}$$

with X_{tr} an estimate of the unknown X. Writing $X_{tr} = X + \delta X$, one readily finds that

$$M_v(X_{tr}) = M(X) + (\delta X,\ K\,\delta X) . \tag{1.5}$$

Equation (1.5) shows that, first, M_v differs from M by a second-order error and is therefore indeed a VP, and second, if K is non-negative (nonpositive), that M_v is not simply a VP but is a variational upper (lower) bound on M. If we use the VP of Eq. (1.4) to derive some of the F_v's and the uniform approach to derive the other F_v's, and if we wish to assert that all the F_v's are derivable by a uniform approach, it will be necessary to derive M_v by that uniform approach. (It may at the same time be instructive.) We start with

$$M_v(X_{tr}) \equiv -(X_{tr}, f) + (L_{tr},\ KX_{tr} - f) , \tag{1.6}$$

where the first term is simply a zeroth-order estimate of M and where the term in L_{tr} is introduced to account, to the relevant accuracy, for the only constraint, namely, Eq. (1.3b). Since M is a number, M_v must be a number, and the Lagrange multiplier must be a function. Following the notation of Ref. 11, it is therefore denoted by L, and its estimate by L_{tr}. ($\mathscr{L}$ is the generic form for a Lagrange multiplier.) If M_v is indeed to be a VP for M we must have

$$\delta M_v = -(f, \delta X) + (\delta L,\ KX - f) + (L,\ K\,\delta X) = 0 ,$$

second-order terms having been neglected. The term in δL vanishes by Eq. (1.3b), and using the symmetry of K we have

$$(KL - f,\ \delta X) = 0 ,$$

or, since δX is arbitrary,

$$KL = f .$$

It follows that $L = X$, and therefore that one can choose $L_{tr} = X_{tr}$. The insertion of this last relation into Eq. (1.6) gives the desired result, Eq. (1.4).

Given a variational estimate $F_v(T_{tr})$, one can introduce variational parameters in $T_{tr}(\vec{r},t)$ and determine these parameters by demanding that $\delta F_v = 0$. Thus, in the course of obtaining an estimate F_v of F, one obtains an estimate of $T(\vec{r},t)$. Experience has shown that this estimate can furnish a reasonably accurate estimate of $T(\vec{r},t)$. It should be clear, however, that whereas the estimate of F is stationary, the estimate of T in general is *not*. [Consider, for example, the very well-known Rayleigh-Ritz VP for the energy. The estimate

$$E_v = (\psi_{tr}, H\psi_{tr}) ,$$

with H the Hamiltonian and ψ_{tr} a normalized trial wave function, is stationary, that is, $E_v - E$ is of the order of some weighted average of $(\delta\psi)^2$, but ψ_{tr} itself is *not* stationary.] If one is interested in an estimate of T, a far more powerful result is obtained if one constructs a variational estimate $T_v(\vec{r},t)$ for $T(\vec{r},t)$ itself. We will do so in Sec. III. The approach is the same as that for the construction of any other VP.

We will also comment briefly on the construction of "variational identities,"[14] expressions of the form

$$F_v = F + \Delta F ,$$

in which the term ΔF, which contains errors of second order and higher, is given explicitly if formally. Variational identities are particularly useful in the development of variational bounds, which provide not only a VP but a knowledge of the sign of the error. A variational bound on $T(\vec{r},t)$ has been developed,[15] but will not concern us in the present paper.

It will be convenient to introduce the notation

$$Q(\vec{x}) \equiv Q(\vec{r},t) .$$

The differential equation for the heat-conduction problem is then

$$\vec{\nabla}\cdot\{k[\vec{x},\ T(\vec{x})]\vec{\nabla}T(\vec{x})\} + \beta[\vec{x},\ T(\vec{x})] - C[\vec{x},\ T(\vec{x})]\frac{\partial T(\vec{x})}{\partial t} = 0 , \tag{1.7}$$

where C is the heat capacity per unit volume, k is the thermal conductivity, and β is the heat generation per unit volume per unit time. We assume throughout that C and k are known real positive functions and that β is a known real function. [We have allowed C, k, and β to depend upon t through their dependence upon $T(\vec{r},t)$, and explicitly; physically, it is the former dependence which is of interest.] We also use the notation

$$d\vec{x}=d\vec{r}\,dt\ ,$$

$$\delta(\vec{x}-\vec{x}\,')=\delta(\vec{r}-\vec{r}\,')\delta(t-t')\ .$$

Having allowed k, C, and β to depend not only on $\vec{x}$ but on T, the heat equation is nonlinear in T; we sometimes limit ourselves to the linear case, for which k, C, and β depend upon $\vec{x}$ but not on $T(\vec{x})$. The most general boundary condition to be satisfied by $T(\vec{x})$ will be a boundary condition of the third kind imposed on the surface S surrounding the volume V of interest,

$$k[\vec{x},\ T(\vec{x})]\frac{\partial T(\vec{x})}{\partial n}+h[\vec{x},\ T(\vec{x})]T(\vec{x})=p[\vec{x},\ T(\vec{x})] \tag{1.8}$$

on S, for $t>0$, where $\partial/\partial n$ is the outward normal derivative at the surface S, h is the known heat-transfer coefficient, and p is a known function. Special cases of this boundary condition are, on S, for $t>0$,

$$h[\vec{x},\ T(\vec{x})]T(\vec{x})=p[\vec{x},\ T(\vec{x})]\ , \tag{1.9}$$

a boundary condition of the first kind, and

$$k[\vec{x},\ T(\vec{x})]\frac{\partial T(\vec{x})}{\partial n}=p[\vec{x},\ T(\vec{x})]\ , \tag{1.10}$$

a boundary condition of the second kind. We will also impose an initial condition

$$T(\vec{r},0)=T_{\rm in}(\vec{r})\ , \tag{1.11}$$

with $T_{\rm in}(\vec{r})$ a specified function.

We turn now to a consideration of a number of the functionals $F(T)$ for which VP's have been obtained for the associated $F(T,\theta)$. For the most part we will not be concerned with the physical significance of $F(T)$, nor with the physical principles nor mathematical techniques which were used to obtain $F_v(T_{\rm tr},\theta)$; our primary concern will be with the systematic derivation of the F_v's.

II. VARIATIONAL PRINCIPLES FOR SOME FUNCTIONALS OF THE TEMPERATURE

A. The functionals of Glansdorff and Prigogine

The objective should be to obtain a VP for some arbitrarily chosen functional $F(T)$. In fact, much of the work in heat-transfer problems has proceeded somewhat differently. One obtains a VP not for $F(T)$ itself but for a related functional $F(T,\theta)$. The interesting technique of Glansdorff and Prigogine of introducing an alias temperature θ, and a functional $F(T,\theta)$ related to $F(T)$, can simplify the analysis, but it must be made clear that one then obtains a VP not for $F(T)$ itself but for $F(T,\theta)$. The procedure is no more complicated computationally than the usual procedure for the development of a VP, but it does require a somewhat more elaborate notation. (The notation is largely ours, rather than theirs.) Given

$$T=T(\vec{x}),\ \ k=k(\vec{x},T),\ \ C=C(\vec{x},T)\ ,$$

they make the replacements

$$\frac{\partial T}{\partial T}\rightarrow\frac{\partial\theta}{\partial t},\ \ k\rightarrow k^*=k^*(\vec{x},\theta),\ \ C\rightarrow C^*=C^*(\vec{x},\theta)\ ,$$

where $\theta=\theta(\vec{x})$; where T appears explicitly in F (rather than as an argument of, say, k and C) it is not replaced. We denote by $F(T,\theta)$ the functional obtained by making the above replacements in $F(T)$. They then obtain a VP $F_v(T_{\rm tr},\theta)$ for $F(T,\theta)$. In obtaining the variation $\delta F_v(T_{\rm tr},\theta)$ of $F_v(T_{\rm tr},\theta)$ caused by a variation δT of T, they keep $\partial\theta/\partial t$, k^*, and C^* fixed. At *that* stage they make the further replacements

$$\partial\theta/\partial t\rightarrow\partial T_{\rm tr}/\partial t,\ \ k^*\rightarrow k_{\rm tr}=k(\vec{x},T_{\rm tr})\ ,$$

$$C^*\rightarrow C_{\rm tr}=C(\vec{x},T_{\rm tr})\ .$$

The procedure will become clear in the course of our analysis of the particular functional chosen by them. An example is worked out in some detail in the Appendix. A VP derived by holding certain quantities constant during an initial step in the calculation has been referred to[6,16] as a "restrictive VP."

For our first example of a rederivation of a VP we assume that there are no heat sources, that is, that $\beta=0$. Equation (1.7) then becomes

$$\vec{\nabla}\cdot[k\vec{\nabla}T(\vec{x})]-C\frac{\partial T}{\partial t}=0\ , \tag{2.1}$$

where $k=k(\vec{x},T)$ and $C=C(\vec{x},T)$. We further assume that the normal component of the heat flux vanishes on the surface S. By Fourier's law, the latter condition is

$$J_n(\vec{x})=-k(\vec{x},T)\frac{\partial T(\vec{x})}{\partial n}=0\ \ \text{on}\ S\ ,$$

or, simply,

$$\partial T(\vec{x})/\partial n=0\ . \tag{2.2}$$

The functional of interest is chosen to be

$$F(T)=\tfrac{1}{2}\int T(\vec{x})C(\vec{x},T)\frac{\partial T(\vec{x})}{\partial t}d\vec{x}=\tfrac{1}{2}\int TC\frac{\partial T}{\partial t}d\vec{x}\ , \tag{2.3}$$

where

$$\int d\vec{x}=\int_0^{t_0}dt\int_V d\vec{r}\ ; \tag{2.4}$$

t_0 is some fixed time and V is the spatial volume of integration. Before proceeding further, it will be useful to consider two consequences of restricting ourselves to trial functions $T_{\rm tr}(\vec{x})$ which satisfy the boundary condition imposed upon $T(\vec{x})$, that is, of demanding that

$$\frac{\partial T_{\rm tr}(\vec{x})}{\partial n}=0\ . \tag{2.5}$$

It follows, first, that

$$\frac{\partial\delta T(\vec{x})}{\partial n}=0\ , \tag{2.6}$$

and, second, that

$$\int T_{tr1}(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}T_{tr2}(\vec{x})]d\vec{x} = \int T_{tr2}(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}T_{tr1}(\vec{x})]d\vec{x}\ ,$$

that is, that $\vec{\nabla}\cdot k^*\vec{\nabla}$ is a symmetric operator; in the physical problem, we have $k=k(\vec{x},T)$ rather than $k^*=k^*(\vec{x},\theta)$, but it is the latter which is relevant in the following analysis of the functional now under consideration.

Now, in fact, Glansdorff and Prigogine do not seek a VP for $F(T)$ defined by Eq. (2.3), subject to Eqs. (2.1) and (2.2). Rather, they seek a VP for

$$F(T,\theta)=\tfrac{1}{2}\int T(\vec{x})C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t}d\vec{x}\ , \tag{2.7}$$

subject to

$$\vec{\nabla}\cdot[k^*\vec{\nabla}T]-C^*\frac{\partial\theta}{\partial t}=0 \tag{2.8}$$

and Eq. (2.2). Our rederivation will be based on Eqs. (1.3) and (1.4); to derive our VP we need merely make the appropriate identifications. We have

$$K=-\vec{\nabla}\cdot(k^*\vec{\nabla})\ .$$

With the further identifications

$$X(\vec{x})=T(\vec{x}),\quad \text{or } X=T$$

and

$$f(\vec{x},\theta)=-C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t},\quad \text{or } f=-C^*\frac{\partial\theta}{\partial t}$$

we see that $F(T,\theta)$ can be identified with $\frac{1}{2}M$, where M is defined by Eqs. (1.3) and (1.7), or rather by Eqs. (1.3) and (2.8), with the understanding that Eq. (2.2) is to be arbitrarily imposed. Using Eq. (1.4), the VP

$$F_v(T_{tr},\theta)=\int\left[-\tfrac{1}{2}T_{tr}(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}T_{tr}(\vec{x})] + T_{tr}(\vec{x})C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t}\right]d\vec{x}$$

follows immediately. An equivalent VP is obtained on integration by parts with respect to the spatial coordinates of the first term on the right-hand side. We thereby obtain

$$F_v(T_{tr},\theta)=\int\left[\tfrac{1}{2}k^*(\vec{x},\theta)[\vec{\nabla}T_{tr}(\vec{x})]^2 + C^*(\vec{x},\theta)T_{tr}(\vec{x})\frac{\partial\theta(\vec{x})}{\partial t}\right]d\vec{x}\ . \tag{2.9}$$

This is the VP given by Glansdorff and Prigogine.

It has been shown[5] that if T_{tr} is chosen to be a linear function of the variational parameters then the method of Glansdorff and Prigogine just described is equivalent to the Galerkin method. A Glansdorff-Prigogine VP is also given[6] for the same functional, that defined by Eq. (2.7), for the case for which, as above, $\beta=0$, but for which the boundary condition is more general. Consider, for example,

$$k(\vec{x},T)\frac{\partial T(\vec{x})}{\partial n}+h(\vec{x},T)T(\vec{x})=0,\quad \text{on } S\ . \tag{2.10}$$

We introduce the associated equation

$$k^*\frac{\partial T(\vec{x})}{\partial n}+h^*T(x)=0,\quad \text{on } S\ . \tag{2.11}$$

Rather than seeking a VP for $F(T)$ defined by Eq. (2.3) with T defined by Eqs. (2.1) and (2.10), we seek a VP for $F(T,\theta)$ defined by Eq. (2.7) with T defined by Eqs. (2.8) and (2.11).

With the boundary condition given by Eq. (2.11) rather than by Eq. (2.2), the operator $\vec{\nabla}\cdot(k^*\vec{\nabla})$ is no longer a symmetric operator, and we can no longer easily connect the equations defining F with the equations in Sec. I defining M. To obtain a VP for $F(T,\theta)$ for the present case, we will apply the very much more general uniform construction approach. We start with

$$F_v(T_{tr},\theta)=\tfrac{1}{2}\int T_{tr}(\vec{x})C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t}d\vec{x}+\tfrac{1}{2}\int L_{tr}(\vec{x})\left[-\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}T_{tr}(\vec{x})]+C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t}\right]d\vec{x}\ . \tag{2.12}$$

There is only one restriction on T (accounted for by the term with L_{tr}), for we restrict ourselves to trial functions which satisfy the boundary condition imposed on $T(\vec{x})$, that is, we demand that, on S,

$$k^*\frac{\partial T_{tr}}{\partial n}+h^*T_{tr}=0\ . \tag{2.13}$$

It follows that

$$k^*\frac{\partial\delta T}{\partial n}+h^*\delta T=0\ . \tag{2.14}$$

Setting $2\,\delta F_v=0$ gives

$$\int\delta T(\vec{x})C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t}d\vec{x}-\int L(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}\delta T(\vec{x})]d\vec{x}=0\ .$$

Integrating the second term twice by parts with respect to space gives

$$\int \delta T(\vec{x}) \left[C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t} - \vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}L] \right] d\vec{x} - \int \left[L(\vec{x})k^*(\vec{x},\theta)\frac{\partial\delta T(\vec{x})}{\partial n} - \frac{\partial L(\vec{x})}{\partial n}k^*(\vec{x},\theta)\delta T(\vec{x}) \right] dS\, dt = 0 .$$

This equation is satisfied by the choice

$$L = T ; \tag{2.15}$$

the volume integral then vanishes by Eq. (2.8), while the surface term vanishes on first using Eq. (2.14) and then using (2.11). Equation (2.15) strongly suggests the choice $L_{tr} = T_{tr}$ in Eq. (2.12). Using

$$-\int T_{tr}(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}T_{tr}(\vec{x})]d\vec{x}$$
$$= -\int T_{tr}(\vec{x})k^*(\vec{x},\theta)\frac{\partial T_{tr}(\vec{x})}{\partial n}dS\, dt$$
$$+ \int k^*(\vec{x},\theta)[\vec{\nabla}T_{tr}(\vec{x})]^2 d\vec{x}$$

and Eq. (2.13), we obtain

$$F_v(T_{tr},\theta) = \int \left[\tfrac{1}{2}k^*(\vec{x},\theta)[\vec{\nabla}T_{tr}(\vec{x})]^2 + T_{tr}(\vec{x})C^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial t} \right] d\vec{x} + \tfrac{1}{2}\int h^*(\vec{x},\theta)[T_{tr}(\vec{x})]^2 dS\, dt . \tag{2.16}$$

$F_v(T_{tr},\theta)$ is the local potential of Glansdorff and Prigogine, which is given by Eq. (10.45) of Finlayson,[6] except that our expression does not contain a T_S since we have assumed that the external temperature T_S is zero.

(One can easily show[6] that

$$\Delta F(T,\theta) \equiv F_v(T_{tr},\theta) - F(T,\theta)$$
$$= \tfrac{1}{2}\int k^*(\vec{x},\theta)[\vec{\nabla}\delta T(\vec{x})]^2 d\vec{x} + \tfrac{1}{2}\int h^*(\vec{x},\theta)[\delta T(\vec{x})]^2 dS\, dt \geq 0 .$$

It follows that $F_v(T_{tr},\theta)$ is not simply a variational principle for but a variational upper bound on $F(T,\theta)$. This is a formal result, since θ is defined only *after* one has introduced a T_{tr}. We will not examine its consequences, for our real interest lies not in the development of variational bounds (nor even of VP's) on $F(T,\theta)$, but rather of VP's on T, to be developed in Sec. III—if T_v is a VP for T, a VP for any functional $F(T)$ is immediately given by $F_v(T) = F(T_v)$—and of variational bounds[15] on T.)

In the Appendix we will apply the Glansdorff-Prigogine VP to a nonlinear (time-independent) heat-conduction problem, whose solution is known exactly, in order to bring out the salient points of their technique. The same problem will be solved by the VP for T itself, developed in Sec. III, and comparisons between the results of the two methods will be made in order to get some feeling for the sizes of the errors, and, more significantly, for the relative sizes of the errors.

Rosen's VP,[1]

$$F_v(T_{tr},\theta) = \int \left[\tfrac{1}{2}k^*(\vec{x},\theta)[\vec{\nabla}T_{tr}(\vec{x})]^2 + C^*(\vec{x},\theta)T_{tr}(\vec{x})\frac{\partial\theta(\vec{x})}{\partial t} \right] d\vec{r} , \tag{2.17}$$

is the same as the Glansdorff-Prigogine VP, with the boundary condition $\partial T(\vec{x})/\partial n = 0$ on S, except that the integration is over space *only*. If heat sources β are present the above VP's can be modified easily.

B. Chambers's VP

Chambers[7] derives a VP for the functional

$$F\left[\frac{\partial T}{\partial t},\theta\right] = -\tfrac{1}{2}\int C^*(\vec{x},\theta)\left[\frac{\partial T(\vec{x})}{\partial t}\right]^2 d\vec{r} . \tag{2.18}$$

$T(\vec{x})$ satisfies boundary conditions of the second kind. In the derivation $\partial T/\partial t$ is varied and T is kept fixed,

$$T = \theta , \tag{2.19}$$

as opposed to the Glansdorff-Prigogine approach where $\partial T/\partial t$ is kept fixed and T is varied;[4] the integration is over space only, and heat sources β are included. By our general method we write

$$F_v\left[\frac{\partial T_{tr}}{\partial t},\theta\right] = -\tfrac{1}{2}\int C^*(\vec{x},\theta)\left[\frac{\partial T_{tr}(\vec{x})}{\partial t}\right]^2 d\vec{r} + \tfrac{1}{2}\int L_{tr}(\vec{x})\left[-\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}\theta(\vec{x})] + C^*(\vec{x},\theta)\frac{\partial T_{tr}(\vec{x})}{\partial t} - \beta^*(\vec{x},\theta) \right] d\vec{r} . \tag{2.20}$$

Setting $\delta F_v = 0$ gives

$$-\int \left[C^*(\vec{x},\theta)\frac{\partial T(\vec{x})}{\partial t}\frac{\partial\delta T(\vec{x})}{\partial t} \right] d\vec{r} + \tfrac{1}{2}\int L(\vec{x})C^*(\vec{x},\theta)\frac{\partial\delta T(\vec{x})}{\partial t} d\vec{r} = 0 , \tag{2.21}$$

which is satisfied by

$$L=2\frac{\partial T}{\partial t}\ . \tag{2.22}$$

Replacing $L_{\rm tr}$ by $2\partial T_{\rm tr}/\partial t$ in Eq. (2.20) and integrating $-\int[\partial T_{\rm tr}(\vec{x})/\partial t]\vec{\nabla}\cdot[k^*(\vec{x},\theta)\vec{\nabla}\theta(\vec{x})]d\vec{r}$ by parts, one obtains the VP given by Chambers,

$$F_v\left[\frac{\partial T_{\rm tr}}{\partial t},\theta\right]=\int\left[\tfrac{1}{2}C^*(\vec{x},\theta)\left[\frac{\partial T_{\rm tr}(\vec{x})}{\partial t}\right]^2+[k^*(\vec{x},\theta)\vec{\nabla}\theta(\vec{x})]\cdot\vec{\nabla}\frac{\partial T_{\rm tr}(\vec{x})}{\partial t}-\beta^*\frac{\partial T_{\rm tr}(\vec{x})}{\partial t}\right]d\vec{r}$$
$$-\int\frac{\partial T_{\rm tr}(\vec{x})}{\partial t}k^*(\vec{x},\theta)\frac{\partial\theta(\vec{x})}{\partial n}dS\ . \tag{2.23}$$

[$F_v(\partial T_{\rm tr}/\partial t,\theta)$ is a variational upper bound on $F(\partial T/\partial t,\theta)$ since[7]

$$\Delta F\left[\frac{\partial T}{\partial t},\theta\right]=\int\tfrac{1}{2}C^*(\vec{x},\theta)\left[\frac{\partial\delta T(\vec{x})}{\partial t}\right]^2d\vec{r}\geq 0\ . \tag{2.24}$$

As for the variational bound given below Eq. (2.16), we will not consider the precise meaning of this result.]

It is interesting to observe that if the VP is given but the corresponding functional is not, as is often the case in the literature, the functional can always be found by converting the VP into a sum of constraint terms plus an extra term. The extra term is the functional. It is clear that the different VP's discussed in this section are just variations on the same theme. According to Finlayson,[6] "computations based on the principles of Rosen, Glansdorff and Prigogine, or Biot are equivalent to those based on Galerkin's method." (One could also add Chambers's VP to the list.)

III. A VARIATIONAL PRINCIPLE FOR THE TEMPERATURE ITSELF

A. The linear case

We will first assume that k, C, β, h, and p are independent of T. In Sec. I we wrote the heat equation in one of its more common forms. In order to facilitate some partial integrations, here it will be convenient to introduce

$$\lambda(\vec{x})\equiv C^{-1}(\vec{x}),\ \ \sigma(\vec{x})=\beta(\vec{x})C^{-1}(\vec{x})\ . \tag{3.1}$$

The heat-conduction equation of Eq. (1.7) is then given by the *linear* inhomogeneous form

$$B(\vec{x})=\lambda(\vec{x})\vec{\nabla}\cdot[k(\vec{x})\vec{\nabla}T(\vec{x})]+\sigma(\vec{x})-\frac{\partial T(\vec{x})}{\partial t}=0\ , \tag{3.2}$$

while the boundary condition, Eq. (1.8), becomes

$$k(\vec{x})\frac{\partial T(\vec{x})}{\partial n}+h(\vec{x})T(\vec{x})=p(\vec{x}),\ \text{on } S,\ \ \text{for } t>0\ . \tag{3.3}$$

We still have the initial condition

$$T(\vec{r},0)=T_{\rm in}(\vec{r})\ . \tag{3.4}$$

$T(\vec{x})$ is uniquely defined by Eqs. (3.2)–(3.4). One can proceed more generally, but we will assume that $T_{\rm tr}(\vec{x})$ is chosen to satisfy the boundary condition, Eq. (3.3), and the initial condition, Eq. (3.4). It follows that

$$k(\vec{x})\frac{\partial\delta T(x)}{\partial n}+h(\vec{x})\delta T(\vec{x})=0,\ \text{on } S,\ \ \text{for } t>0\ , \tag{3.5}$$

$$\delta T(\vec{r},0)=0\ , \tag{3.6}$$

and that Eq. (3.2) is the only constraint to be accounted for by the introduction of a Lagrange multiplier. The development of a VP for the function $T(\vec{x})$ will be somewhat more difficult than the development of a VP for the functionals considered previously, all of which were simply numbers. Our starting point in the development of a VP for $T(\vec{x})$ is

$$T_v(\vec{x})=T_{\rm tr}(\vec{x})+\int^{+}\Lambda_{\rm tr}(\vec{x},\vec{x}\,')\left[\lambda(\vec{x}\,')\vec{\nabla}\,'\cdot[k(\vec{x}\,')\vec{\nabla}\,'T_{\rm tr}(\vec{x}\,')]+\sigma(\vec{x}\,')-\frac{\partial}{\partial t'}T_{\rm tr}(\vec{x}\,')\right]d\vec{x}\,'\ , \tag{3.7}$$

where

$$\int^{+}d\vec{x}\,'\equiv\int_0^{t+0}dt'\int_V d\vec{r}\,'\ ,$$

with $t+0$ indicating that the upper limit t is to be approached from above. The Lagrange multiplier, which is to account for the constraint imposed by Eq. (3.2), is in this case a function of two sets of variables, $\vec{x}$ and $\vec{x}\,'$, and in line with the notation of Ref. 11 is therefore denoted by Λ, and its trial estimate by $\Lambda_{\rm tr}$. As always, we demand that the first-order variation, here of T_v, vanish. This gives

$$\delta T(\vec{x})+\int^{+}\Lambda(\vec{x},\vec{x}\,')\left[\lambda(\vec{x}\,')\vec{\nabla}\,'\cdot[k(\vec{x}\,')\vec{\nabla}\,']-\frac{\partial}{\partial t'}\right]\times\delta T(\vec{x}\,')d\vec{x}\,'=0\ . \tag{3.8}$$

We wish to rewrite this in a form which contains only $\delta T(\vec{x}')$—there is to be no $\delta T(\vec{x})$—and $\delta T(\vec{x}')$ is to appear in surface and volume integrals as a factor, *not* differentiated with respect to space or time. To do so, we begin by writing

$$\delta T(\vec{x}) = \int \delta T(\vec{x}')\delta(\vec{x}-\vec{x}')d\vec{x}' = \int^{+} \delta T(\vec{x}')\delta(\vec{x}-\vec{x}')d\vec{x}' . \tag{3.9}$$

Further, we integrate by parts with respect to time to give

$$-\int^{+} \Lambda(\vec{x},\vec{x}')\frac{\partial \delta T(\vec{x}')}{\partial t'}d\vec{x}' = -\int_V \Lambda(\vec{x},\vec{x}')\delta T(\vec{x}')d\vec{r}'\,\Big|_0^{t+0} + \int^{+} \delta T(\vec{x}')\frac{\partial \Lambda(\vec{x},\vec{x}')}{\partial t'}d\vec{x}' . \tag{3.10}$$

The term which is to be evaluated at $t'=0$ vanishes by Eq. (3.6). Finally, we integrate by parts twice with respect to space to give

$$\int^{+} \Lambda(\vec{x},\vec{x}')\lambda(\vec{x}')\vec{\nabla}'\cdot[k(\vec{x}')\vec{\nabla}'\delta T(\vec{x}')]d\vec{x}' = \int^{+} \delta T(\vec{x}')\vec{\nabla}'\cdot\{k(\vec{x}')\vec{\nabla}'[\Lambda(\vec{x},\vec{x}')\lambda(\vec{x}')d\vec{x}'\} - \int_0^{t+0} dt' \int_S dS'\delta T(\vec{x}')\left[\lambda(\vec{x}')\Lambda(\vec{x},\vec{x}')h(\vec{x}')+k(\vec{x}')\frac{\partial[\Lambda(\vec{x},\vec{x}')\lambda(\vec{x}')]}{\partial n'}\right] . \tag{3.11}$$

In arriving at Eq. (3.11), we used Eq. (3.5) to replace a term containing a derivative of δT by a term containing δT. We now insert Eqs. (3.9)–(3.11) in Eq. (3.8) and equate to zero the coefficients of $\delta T(\vec{x}')$ in integrals of the form

$$\int^{+} d\vec{x}' ,$$

$$\int_0^{t+0} dt' \int_S dS' ,$$

and

$$\int d\vec{r}'\,\Big|_{t'=0}^{t'=t+0} .$$

We thereby obtain

$$\vec{\nabla}'\cdot\{k(\vec{x}')\vec{\nabla}'[\Lambda(\vec{x},\vec{x}')\lambda(\vec{x}')]\} + \frac{\partial \Lambda(\vec{x},\vec{x}')}{\partial t'} = -\delta(\vec{x}-\vec{x}') , \tag{3.12}$$

$$\left[k(\vec{x}')\frac{\partial}{\partial n'}+h(\vec{x}')\right][\Lambda(\vec{x},\vec{x}')\lambda(\vec{x}')]=0 , \tag{3.13}$$

and

$$\Lambda(\vec{x},\vec{x}')=0, \quad t'>t \tag{3.14}$$

respectively. The insertion into Eq. (3.7) of an approximation Λ_{tr} to Λ, the Green's function defined by Eqs. (3.12)–(3.14), gives the sought-after VP for $T(\vec{x})$. (Λ_{tr} might, for example, be the known Green's function for some simpler, roughly similar problem. We often write G for Λ and G_{tr} for Λ_{tr}.)

At least in principle, one can iterate and obtain an improved estimate of $T(\vec{x})$. (A brief discussion of this "super VP" approach has been presented.[14]) Thus, having obtained $T_v(T_{tr})$, one could use this estimate of T as a new trial function,

$$T_{tr\,tr} \equiv T_v(T_{tr})$$

to obtain an improved estimate

$$T_{vv} \equiv T_v(T_{tr\,tr}) ,$$

with an error which is of order

$$(T-T_{tr})^4 .$$

It is interesting to observe that a variational identity for $T(\vec{x})$ follows readily from Eq. (3.8). Thus, writing $\delta T = T_{tr} - T$, and using Eq. (3.2) to eliminate $T(x')$ under the integral, we find

$$T(\vec{x}) = T_{tr}(\vec{x}) + \int^{+} \Lambda(\vec{x},\vec{x}')\left[\left[\lambda(\vec{x}')\vec{\nabla}'\cdot[k(\vec{x}')\vec{\nabla}'] - \frac{\partial}{\partial t'}\right]T_{tr}(\vec{x}')+\sigma(\vec{x}')\right]d\vec{x}' . \tag{3.15}$$

Equation (3.15) is an identity, valid for any T_{tr}. If, in particular, we choose T_{tr} to be T_{hom}, the solution of the homogeneous heat-conduction equation,

$$\lambda(\vec{x})\vec{\nabla}\cdot[k(\vec{x})\vec{\nabla}T_{hom}(\vec{x})] - \frac{\partial T_{hom}(\vec{x})}{\partial t} = 0 , \tag{3.16}$$

subject to the boundary conditions satisfied by $T(\vec{x})$, Eq. (3.15) reduces to an integral equation of standard form[17]

$$T(\vec{x}) = T_{hom}(\vec{x}) + \int^{+} \Lambda(\vec{x},\vec{x}')\sigma(\vec{x}')d\vec{x}' .$$

B. The nonlinear case

We now allow λ, k, σ, h, and p to depend upon T as well as upon $\vec{x}$. T in $\lambda, k, \ldots$ will *not* be held fixed during the variations to be considered. The heat-conduction equation then has the (nonlinear) form

$$B^*(\vec{x}) \equiv \left[\lambda^*(\vec{x})\vec{\nabla}\cdot[k^*(\vec{x})\vec{\nabla}] - \frac{\partial}{\partial t}\right]T(\vec{x}) + \sigma^*(\vec{x}) = 0 , \tag{3.17}$$

where for an arbitrary function Q, we use

$$Q^*(\vec{x}) \equiv Q[\vec{x},\ T(\vec{x})] \ . \tag{3.18}$$

[The notation here differs slightly from that of Sec. II, where k^* represented $k^*(x,\theta)$.] Not having specified the precise T dependence of $\lambda, k, \ldots$, our derivation of a VP for T will necessarily involve some formal operations. Our starting point is now

$$T_v(\vec{x}) = T_{\rm tr}(\vec{x}) + \int^{+} \Lambda_{\rm tr}(\vec{x},\vec{x}\,')B^*_{\rm tr}(\vec{x}\,')d\vec{x}\,' \ , \tag{3.19}$$

where, replacing T by $T_{\rm tr}$ in Eq. (3.17),

$$B^*_{\rm tr}(\vec{x}) \equiv B[\vec{x},\ T_{\rm tr}(\vec{x})] \ . \tag{3.20}$$

(The T dependence of $\Lambda_{\rm tr}$, and of the Λ to appear shortly, will not be indicated explicitly.) Ignoring terms of second order and higher in $T - T_{\rm tr}$, we have, expanding about $B^*(\vec{x}) = 0$,

$$B^*_{\rm tr}(\vec{x}) = B^{*\prime}(\vec{x})[T_{\rm tr}(\vec{x}) - T(\vec{x})] \ , \tag{3.21}$$

where

$$B^{*\prime}(\vec{x}) \equiv \delta B^*(\vec{x})/\delta T$$

is the Fréchet functional derivative.[18] [If $B^*(\vec{x})$ is linear in T as it was in Sec. III A, but which we do not assume to be the case here, $B^{*\prime}(\vec{x})$ is independent of T and the analysis simplifies considerably.] The requirement that the first-order variation δT_v vanish gives

$$\delta T(\vec{x}) + \int^{+} \Lambda(\vec{x},\vec{x}\,')B^{*\prime}(\vec{x}\,')\delta T(\vec{x}\,')d\vec{x}\,' = 0 \ . \tag{3.22}$$

It is now *assumed* that there exists an adjoint operator $(B^{*\prime})^\dagger$ such that

$$\int^{+} \Lambda B^{*\prime}\delta T\, d\vec{x}\,' = \int^{+} \delta T (B^{*\prime})^\dagger \Lambda\, d\vec{x}\,' \ . \tag{3.23}$$

In a concrete case, with the T dependence of λ, k, etc. specified, one will be able to determine whether or not the adjoint of $B^{*\prime}$ exists. In general, one would expect it to exist. In other words, we assume (and expect) it to be possible to impose boundary conditions on Λ such that all surface terms vanish. (For example, assume that in B^*, we have $\sigma = 0$, $\lambda = \lambda_0$, and $k = k_0 + k_1 T$, where λ_0, k_0, and k_1 are constants, that T and $T_{\rm tr}$ satisfy boundary conditions of the first kind, and that Λ satisfies the corresponding homogeneous boundary condition on S. We then have

$$B^{*\prime} = \lambda_0 k_0 \vec{\nabla}^2 + \lambda_0 k_1 [2(\vec{\nabla} T)\cdot\vec{\nabla} + (\vec{\nabla}^2 T) + T\vec{\nabla}^2] - \frac{\partial}{\partial t}$$

and we find that

$$(B^{*\prime})^\dagger = \lambda_0(k_0 + k_1 T)\nabla^2 + \frac{\partial}{\partial t} \ ,$$

so that $(B^{*\prime})^\dagger$ does indeed exist in this case.) Equations (3.22) and (3.23) give

$$[B^{*\prime}(\vec{x})]^\dagger \Lambda(\vec{x},\vec{x}\,') = -\delta(\vec{x} - \vec{x}\,') \ . \tag{3.24}$$

With $\Lambda_{\rm tr}$ an approximation to Λ, uniquely defined by Eq. (3.24) and the boundary conditions, we can then use our VP for $T(\vec{x})$, Eq. (3.19).

A variational identity for the nonlinear case is obtained in a fashion analogous to that used for the linear case. Setting $\delta T = T_{\rm tr} - T$ in Eq. (3.22), we find

$$T(\vec{x}) = T_{\rm tr}(\vec{x}) + \int^{+} \Lambda(\vec{x},\vec{x}\,')B^{*\prime}(\vec{x}\,') \times [T_{\rm tr}(\vec{x}\,') - T(\vec{x}\,')]d\vec{x}\,' \ . \tag{3.25}$$

That this is indeed a variational identity is easily seen. One need merely bring $B^{*\prime}$ to the left of Λ, as $(B^{*\prime})^\dagger$, and use Eq. (3.24). Note, however,that as opposed to the variational identity for the linear case, the variational identity given by Eq. (3.26) contains T under the integral sign.

IV. A VARIATIONAL PRINCIPLE FOR THE TEMPERATURE AND DENSITY DISTRIBUTIONS IN A STAR

As our final example involving heat flow, we obtain a VP for the temperature and density distributions, $T(r)$ and $\rho(r)$, in a spherically symmetric star of radius R under quasiequilibrium conditions, where r is the distance from the origin. This problem is, of course, not only extremely important but very complicated, involving nonlinear coupled differential equations. We let $P(r)$ be the pressure, M_r the mass within a sphere of radius r, L_r the energy flux through the surface of radius r, $\epsilon(r)$ the energy release per unit mass per unit time from nuclear processes, and $\kappa(r)$ the opacity. We also use G for the gravitational constant, c for the speed of light, and α for the Stefan-Boltzmann constant. We follow Schwarzschild[19] in outlining the problem. (L_r is a standard notation for energy flux and should not be confused with the Lagrangians.) Hydrostatic equilibrium, the relationship between mass and density, energy conservation, and radiative equilibrium are described by the differential equations

$$\frac{dP}{dr} = -\frac{G\rho M_r}{r^2} \ , \tag{4.1}$$

$$\frac{dM_r}{dr} = 4\pi r^2 \rho \ , \tag{4.2}$$

$$\frac{dL_r}{dr} = 4\pi r^2 \rho\epsilon \ , \tag{4.3}$$

and

$$\frac{dT}{dr} = -\frac{3}{4\alpha c}\frac{\kappa\rho}{T^3}\frac{L_r}{4\pi r^2} \ , \tag{4.4}$$

respectively. [Limiting our discussion to a bare outline of the problem, we ignore the many modifications of the above equations which may be required; if, for example, there is no radiative equilibrium, an equation for convective energy equilibrium replaces Eq. (4.4), and Eq. (4.7b) below must be replaced.] In addition, we need some explicit relations to characterize the interior of the star. We will not give the relations explicitly—our approach is therefore necessarily a formal one—but it is to be understood that the explicit forms are known. These relations include the equation of state,

$$P = P(\rho, T) \ , \tag{4.5a}$$

the form of the opacity

$$\kappa=\kappa(\rho,T)\ , \tag{4.5b}$$

and the equation for energy generation,

$$\epsilon=\epsilon(\rho,T)\ . \tag{4.5c}$$

Equations (4.5) also depend upon the abundances of hydrogen, helium, and the heavy elements; for simplicity, we assume these abundances to be constant for the time interval under consideration.

Four coupled first-order differential equations require four boundary conditions. Two are at the origin. These are clearly

$$M_r=0 \text{ and } L_r=0,\ \ r=0\ .$$

Since $\rho(r)$, $\kappa(r)$, and $\epsilon(r)$ are finite at $r=0$, these are equivalent, by Eqs. (4.1) through (4.4), to

$$dP/dr=0 \text{ and } dT/dr=0,\ \ r=0\ .$$

Since we prefer to work with $T(r)$ and $\rho(r)$, we rewrite the boundary condition in still a different equivalent form,

$$dT/dr=0 \text{ and } d\rho/dr=0,\ \ r=0\ . \tag{4.6a}$$

Since ρ and T at $r=R$, the surface of the star, are many orders of magnitude smaller than characteristic values of ρ and T in the interior of the star, the two boundary conditions at the surface can be taken to be

$$T(R)=0,\ \ \rho(R)=0\ . \tag{4.6b}$$

We now replace our four first-order differential equations by two second-order differential equations. Eliminating M_r from Eqs. (4.1) and (4.2) gives

$$B_1^*(r)\equiv\frac{d}{dr}\left[\frac{r^2}{\rho}\frac{dP^*(r)}{dr}\right]+4\pi G r^2\rho=0\ , \tag{4.7a}$$

while eliminating $L(r)$ between Eqs. (4.3) and (4.4) gives

$$B_2^*(r)=\frac{4ac}{3}\frac{d}{dr}\left[\frac{r^2T^3}{\kappa\rho}\frac{dT}{dr}\right]+\rho\epsilon r^2=0\ . \tag{4.7b}$$

In Eq. (4.7a),

$$P^*(r)\equiv P[r,T(r),\rho(r)]\ , \tag{4.8a}$$

and, more generally, for an arbitrary function Q, we let

$$Q^*(r)\equiv Q[r,T(r),\rho(r)]\ . \tag{4.8b}$$

Equations (4.7) represent coupled differential equations for $T(r)$ and $\rho(r)$. We now set $X_1(r)=T(r)$ and $X_2(r)=\rho(r)$, and introduce the column vector $X(r)$ with elements $X_1(r)$ and $X_2(r)$. Further, we introduce the column vector $B^*(r)$ with elements $B_1^*(r)$ and $B_2^*(r)$. At this stage, our objective is to determine a VP for $X(r)$, defined by the differential equation $B^*(r)=0$ and by the boundary conditions

$$\frac{dX}{dr}=0 \text{ at } r=0,\ \ X(R)=0\ .$$

We assume that the boundary conditions at $r=0$ and at $r=R$ are satisfied by $X_{\rm tr}(r)$. We then start with

$$X_v(r)=X_{\rm tr}(r)+\int\Lambda_{\rm tr}(r,r')B_{\rm tr}^*(r')dr'\ , \tag{4.9}$$

where $0\le r,\ r'\le R$, where

$$B_{\rm tr}^*(r)\equiv B[r,T_{\rm tr}(r),\rho_{\rm tr}(r)]\ ,$$

and where $\Lambda_{\rm tr}$ is a two-by-two matrix whose elements are functions of r and r' and which satisfies the boundary conditions

$$\frac{\partial\Lambda_{\rm tr}(r,r')}{\partial r}=0 \text{ at } r=0,\ \ \Lambda(R,r')=0\ . \tag{4.10}$$

Setting $\delta X_v=0$ gives

$$\delta X(r)+\int\Lambda(r,r')\delta B^*(r')dr'=0\ . \tag{4.11}$$

We now write

$$\delta X(r)=\int\delta(r-r')\delta X(r')dr'$$

and

$$\begin{aligned}\delta B^*(r')&=\begin{bmatrix}\delta B_1^*(r')\\ \delta B_2^*(r')\end{bmatrix}\\ &=\begin{bmatrix}\dfrac{\partial B_1^*(r')}{\partial X_1} & \dfrac{\partial B_1^*(r')}{\partial X_2}\\ \dfrac{\partial B_2^*(r')}{\partial X_1} & \dfrac{\partial B_2^*(r')}{\partial X_2}\end{bmatrix}\begin{bmatrix}\delta X_1(r')\\ \delta X_2(r')\end{bmatrix}\\ &\equiv\mathscr{B}^{*\prime}(r')\delta X(r')\ ,\end{aligned} \tag{4.12}$$

where the derivatives are Fréchet functional derivatives. Equation (4.11) therefore becomes

$$\int[\delta(r-r')1+\Lambda(r,r')\mathscr{B}^{*\prime}(r')]\delta X(r')dr'=0\ , \tag{4.13}$$

where 1 is the two-by-two unit matrix. Though $\delta X(r')$ is arbitrary, we cannot equate the term in square brackets to zero. Rather, we must assume that the imposition of boundary conditions on Λ identical in form to those imposed above on $\Lambda_{\rm tr}$ enables us to rewrite Eq. (4.13) as

$$\int\delta X(r')[\delta(r-r')1+\mathscr{B}^{*\prime\dagger}(r')\Lambda(r,r')]dr'=0\ . \tag{4.14}$$

Λ is then a Green's function, defined by boundary conditions and by

$$\mathscr{B}^{*\prime\dagger}(r')\Lambda(r,r')=-\delta(r-r')1\ . \tag{4.15}$$

We are now in a position to determine an approximation $\Lambda_{\rm tr}(r,r')$ to $\Lambda(r,r')$ and then to use Eq. (4.9) as our VP.

We close with the observation that it has often been stated, incorrectly, that one cannot obtain a VP for a characteristic, such as $T(\vec{r},t)$, of a system which is not time reversible.[20]

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APPENDIX: A CONCRETE EXAMPLE

We remarked in the Introduction that whereas the estimate $F_v(T_{\rm tr},\theta)$ of $F(T,\theta)$ obtained by the Glansdorff-

Prigogine procedure is stationary, the estimate of T obtained in the course of the analysis in general is not stationary. We emphasize again that $F_v(T_{tr},\theta)$ is a variational principle for $F(T,\theta)$ but not for the functional $F(T)$ of the actual problem. It has already been stated by Finlayson and Scrivens (Ref. 4, p. 293) and by Finlayson[6] that the fact that δF_v vanishes and that ΔF is non-negative does not imply that F_v is a minimum principle when θ is kept fixed during the variation; more precisely, $F_v(T_{tr},\theta)$ is not a minimum principle for the functional $F(T)$ of the actual problem. The Glansdorff-Prigogine principle will be illustrated with a concrete example.[6] Consider one-dimensional steady-state conduction across a slab of width d. For later convenience we denote the coordinates and temperatures by x' and $T'(x')$. The endpoints $x'=0$ and $x'=d$ have the temperatures

$$T'(0)=T'_0,\quad T'(d)=T'_1 \;. \tag{A1}$$

The heat-conduction equation is

$$\frac{d}{dx'}\left[k(T')\frac{dT'}{dx'}\right]=0 \;, \tag{A2}$$

where we assume that

$$k(T')=k_0+k_1(T'-T'_0) \;, \tag{A3}$$

with k_0 and k_1 constants. The equations are made dimensionless by choosing

$$T(x)=[T'(x')-T'_0]/(T'_1-T'_0)$$

and

$$x=x'/d \;.$$

For simplicity, we make the particular choice

$$(k_1/k_0)(T'_1-T'_0)=1 \;.$$

We then have

$$k(T')/k_0=1+(k_1/k_0)[T'(x')-T'_0]=1+T(x) \;,$$

and the problem reduces to the solution of

$$\frac{d}{dx}\left[[1+T(x)]\frac{dT(x)}{dx}\right]=0,\quad T(0)=0,\quad T(1)=1 \;. \tag{A4}$$

The exact solution of Eq. (A4),

$$T(x)=-1+(1+3x)^{1/2} \;, \tag{A5}$$

will serve as a basis of comparison for any estimate of $T(x)$. We will now obtain an estimate of $T(x)$ in the course of developing a VP, namely, $F_v(T_{tr},\theta)$ for the $F(T,\theta)$ associated with

$$F(T)=\tfrac{1}{2}\int_0^1 k(T)\left[\frac{dT(\vec{x})}{dx}\right]^2 dx \;, \tag{A6}$$

where

$$k(T)\equiv k(T')/k_0=1+T(x) \;.$$

The associated $F(T,\theta)$ is

$$F(T,\theta)=\tfrac{1}{2}\int_0^1 (1+\theta)\left[\frac{dT}{dx}\right]^2 dx \;, \tag{A7}$$

and the VP for $F(T,\theta)$, which follows from Eq. (2.9), is

$$F_v(T_{tr},\theta)=\tfrac{1}{2}\int_0^1 (1+\theta)\left[\frac{dT_{tr}}{dx}\right]^2 dx \;, \tag{A8}$$

where we demand that $T_{tr}(0)=0$ and $T_{tr}(1)=1$. We restrict the trial function $T_{tr}(x)$ to be a simple quadratic form in x. We then have

$$T_{tr}(x)=x+a(x^2-x) \;, \tag{A9}$$

where a is a variational parameter. Equating $\partial F_v/\partial a$ to zero and *then* setting $\theta=T_{tr}=x+a(x^2-x)$, we obtain $a^2-15a-5=0$, which allows $a=-0.326$ or 15.326. The value $a=15.326$ is not an acceptable physical solution since the direction of the heat flow, and therefore the sign of dT/dx must be the same at $x=0$ and 1. The estimate of T is thus

$$T_{est}=1.326x-0.326x^2 \;. \tag{A10}$$

The same result was obtained by Finlayson using the Galerkin method.[6] The results are given in Table I. The estimate of T is quite good. It differs from the exact T by

TABLE I. Exact T vs T_{est}, obtained from F_v of Glansdorff and Prigogine, and vs T_v. p_{est} represents the percentage error in T_{est}, namely, $100(T_{est}-T)/T$, while p_v represents the percentage error in T_v, namely, $100(T_v-T)/T$, for various values of the parameter ϵ.

				$\epsilon=0.01$		$\epsilon=0.05$		$\epsilon=0.2$		$\epsilon=0.4$	
x	T	T_{est}	p_{est}	T_v	p_v	T_v	p_v	T_v	p_v	T_v	p_v
0	0	0	0	0	0	0	0	0	0	0	0
$\ll 1$	$\approx 1.50x$	$\approx 1.33x$	11.1			$T_v\approx[1.5-(\epsilon/8)+O(\epsilon^2)]x$					
0.05	0.07238	0.0655	9.5	0.07233	0.069	0.07218	0.276	0.07164	1.02	0.07105	1.84
0.10	0.1402	0.129	7.9	0.1401	0.071	0.1398	0.285	0.1389	0.93	0.1378	1.71
0.20	0.2649	0.252	4.9	0.2647	0.076	0.2644	0.189	0.2629	0.76	0.2612	1.4
0.30	0.3784	0.368	2.6	0.3783	0.026	0.3778	0.159	0.3760	0.63	0.3740	1.2
0.40	0.4832	0.478	1.0	0.4831	0.021	0.4826	0.124	0.4807	0.52	0.4787	0.93
0.50	0.5811	0.582	0.17	0.5810	0.017	0.5805	0.103	0.5787	0.41	0.5767	0.76
0.60	0.6733	0.678	0.74	0.6732	0.015	0.6727	0.089	0.6712	0.31	0.6694	0.58
0.70	0.7607	0.768	0.92	0.7606	0.013	0.7602	0.066	0.7589	0.24	0.7574	0.43
0.80	0.8439	0.852	0.95	0.8438	0.012	0.8436	0.036	0.8426	0.15	0.8416	0.27
0.90	0.9235	0.929	0.54	0.9235	0.00	0.9234	0.011	0.9228	0.076	0.9223	0.13
1.00	1	1	0	1	0	1	0	1	0	1	0

about 10% near $x=0$ and by less than 1% for $x=0.4-1$.

From Eq. (A5) it follows that

$$F(T)=\tfrac{1}{2}\int_0^1 (1+T)\left[\frac{dT}{dx}\right]^2 dx$$

is given by

$$F(T)=\tfrac{3}{4}\int_0^1 dT=\tfrac{3}{4}T\,|_0^1=\tfrac{3}{4}\ . \tag{A11}$$

For trial functions of the form

$$T_{tr}=x+af(x),\quad f(0)=f(1)=0\ ,$$

Eq. (A8) gives

$$F_v(T_{tr},\theta)=\tfrac{1}{2}\int_0^1 (1+\theta)(1+2af_x+a^2f_x^2)dx\ , \tag{A12}$$

where $f_x \equiv df/dx$. We then have

$$\delta F_v=\int_0^1 (1+\theta)(f_x+af_x^2)dx=0\ .$$

The use of this last relationship in Eq. (A12) gives

$$F_v(T_{tr},\theta)=\tfrac{1}{2}\int_0^1 (1+\theta)(1+af_x)dx\ .$$

Now replacing θ by T_{tr}, and noting that $1+af_x=d(1+T_{tr})/dx$, we obtain, without ever having specified $f(x)$ other than its endpoint values,

$$F_v(T_{tr})=\tfrac{1}{4}(T_{tr}+1)^2\,|_0^1=\tfrac{3}{4}\ . \tag{A13}$$

It is interesting to observe that $F_v(T_{tr})$ has exactly the same numerical value as $F(T)$; on the other hand, the forms in Eqs. (A11) and (A13), namely $3T/4$ and $(T_{tr}+1)^2/4$, are different. Of course, it will not always be the case that $F_v(T_{tr})$ is equal to $F(T)$. For the trial function $T_{tr}=x^2+a(x^2-x)$, F_v differs markedly from F. Also, for the linear problem ($k=1$), for which $T=x$, the choice $T_{tr}=\sin(\pi x/2)+a(x^2-x)$ gives an $F_v(T_{tr})$ which differs from $F(T)$. Finally, we have

$$F(T,T_{est})=\tfrac{1}{2}\int_0^1 (1+1.326-0.326x^2)\times\left[\frac{d}{dx}(-1+\sqrt{1+3x}\,)\right]^2 dx=0.748\ ,$$

which differs from F_v by 0.27%. Note that $(F_v-F)/F$ is of the order of some weighted average of $[(T_{est}-T)/T]^2$ and is positive, where F here is $F(T,T_{est})$.

By comparing it with the exact solution, Thomaes (Ref. 4, p. 305) showed that the solution obtained by means of F_v for a specific steady-state problem, with k an exponential function of the temperature, converges. Glansdorff and Prigogine obtained a general proof of convergence.[21]

The nonlinear problem, Eq. (A4), will now be solved using the variational expression for T itself, Eq. (3.19);

$$T_v(x)=T_{tr}(x)+\int_0^1 G_{tr}(x,x')\frac{d}{dx'}\times\left[[1+T_{tr}(x')]\frac{d}{dx'}\right]T_{tr}(x')dx'$$

$$\equiv T_{tr}(x)+I(x)\ . \tag{A14}$$

The requirement that $\delta T_v(x)=0$ leads, in a fashion similar to that used in Sec. III, to the requirement that

$$[1+T(x')]\frac{d^2}{dx'^2}G(x,x')=-\delta(x-x')\ ;$$

note that the operator on the left is the adjoint (with x replaced by x') of the Frechét functional derivative of the left-hand side of Eq. (A4). (We have not indicated the dependence of G and G_{tr} on T.) We must also impose boundary conditions

$$G(0,x')=0,\quad G(1,x')=0\ . \tag{A15}$$

G is given by

$$G(x,x')=x_<(1-x_>)[1+T(x)]^{-1}=x_<(1-x_>)/(1+3x)^{1/2}\ . \tag{A16}$$

We do not, of course, want to use the exact G since the exact G will not normally be known. Introducing a parameter ϵ, we choose

$$G_{tr}(x,x')=Dx_<^{1+\epsilon}(1-x_>^{1+\epsilon})\ , \tag{A17}$$

where D is a variational parameter and, as before, we choose

$$T_{tr}=x+a(x^2-x)\ .$$

Equating $\partial T_v/\partial D$ to zero is equivalent to the requirement that $I=0$, so our variational approach in the present case is the analog of that used by Hulthén.[22] We find

$$I=(1+\epsilon)(x-1)\left[a^2\left[\frac{1}{2+\epsilon}-\frac{3}{3+\epsilon}(x+1)+\frac{2}{4+\epsilon}(x^2+x+1)\right]+a\left[\frac{3}{3+\epsilon}(x+1)\right]+\frac{1}{2+\epsilon}\right]=0\ .$$

When ϵ is set equal to zero, T_v reduces to T. This is to be expected since the choice $\epsilon=0$ leads to

$$G_{tr}=D(1+3x)^{1/2}G\ . \tag{A18}$$

The x'-independent factor $D(1+3x)^{1/2}$ plays the role of a multiplicative factor in the evaluation of I; since I vanishes for the correct Green's function, it therefore also vanishes for G_{tr} given by Eq. (A18). The results for T_v for different choices of ϵ are presented in Table I. One notes from the results in Table I that the values of T_v, for all values of x and ϵ considered, are not only very close to but below T. We have developed[15] quite general upper and lower variational bounds on T, but the generality was obtained at a cost, the variational bounds being rather cumbersome. We suspect, but have not shown, that there are many particular cases for which an upper or lower variational bound on T is obtainable in a simpler form. For the present problem, an expansion of F_v through terms of order ϵ^2 shows that T_v provides a lower (upper) variational bound if ϵ is positive (negative), but we caution the reader that for the problem at hand G_{tr} reduces to G for $\epsilon=0$.

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