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Maximum and minimum free energies and the concept of a minimal state

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RIASSUNTO: Vengono presentati alcuni risultati riguardanti l'energia libera dei materiali con memoria sia nel caso generale sia in quello della teoria lineare della viscoelasticità. Viene sviluppato un nuovo metodo variazionale nel dominio del tempo o in quello della frequenza. In quest'ultimo caso viene assegnata una famiglia di forme esplicite per l'energia libera asspociata a un dato stato di un materiale viscoelastico a spettro discreto. Tale famiglia comprende l'energia libera massima e quella minima.

ABSTRACT: Certain results about free energies of materials with memory are presented, both in the general case and within the theory of linear viscoelasticity. A new variational method is developed in both the time and frequency domains. In the latter case, explicit forms of a family of free energies, associated with a given state of a discrete spectrum viscoelastic material, are given, including both maximum and minimum free energies.

1-Introduction

The objective of this paper is to summarize recent work [1] on isothermal free energies of viscoelastic materials, highlighting the main results but omitting most detailed proofs. Certain results about free energies of materials with memory are presented, both for the abstract development of thermodynamics and for its formulation within the theory of

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linear viscoelasticity. These developments build on results of FABRIZIO, GIORGI and MORRO [4]. Also, explicit forms of a family of free energies associated with a given state (in the sense of [2]) of a linear viscoelastic material are given on the frequency domain, based on a generalisation of the variational approach of GOLDEN [5], who derived a general expression for the isothermal minimum free energy of a linear viscoelastic material in the case of a scalar constitutive relation. A generalization of the developments reported in [5] to the full tensorial case has been given recently by DESERI, GENTILI and GOLDEN [6], the results of which are also useful in the present work. The paper is in two parts, A and B.

In Part A, following the point of view of FICHERA [7], [8], [9], [10], a definition of a fading memory material, without the use of any topology, is proposed. Then a general definition of the minimum free energy is given, using the concept of maximum recoverable work (see also DAY [11], [12]). The concept of a *minimal state* is introduced, which coincides with the definition of a state in Noll's theory [2], see also [13], [14]. It is shown that the minimum free energy is independent of the definition of state, and in particular can be represented as a functional of the minimal state. A definition of state adopted, though, with appropriate restrictions, it is a function of the minimal state.

Also, for a linear constitutive relation, the Wiener-Hopf equation [15] for the strain continuation associated with the maximum recoverable work from a given state is studied. A uniqueness and existence theorem is proved for this equation. It is solved directly, using the Wiener-Hopf technique, leading to an explicit formula for the minimum free energy in the full tensorial case, which generalises the scalar result in [5] and agrees with the formula given in [6].

In Part B, a new variational approach is developed in both the time and frequency domain, the latter being essentially a generalization of the method of [5]. Explicit expressions are derived for a partially ordered family of free energies associated with a minimal state, in the case of discrete spectrum materials (those with a relaxation function given by a finite sum of decaying exponentials). Included in this family is the minimum free energy, already known, and the maximum free energy.

The following notation will be used. Vectors are indicated by boldface characters. Tensors and matrices are denoted by boldface capitals. Sym

is the set of all symmetric second order tensors. Lin(Sym) is the set of all linear transformations from Sym to Sym. If $\mathbf{L}, \mathbf{M} \in \text{Lin}$, then $\mathbf{L} \cdot \mathbf{M}$ stands for $tr(\mathbf{L}\mathbf{M})$. Also, $|\mathbf{L}|^2 = \mathbf{L} \cdot \mathbf{L}$.

The reals are denoted by \mathbb{R} , the non-negative reals by \mathbb{R}^+ and the strictly positive reals by \mathbb{R}^{++} ; also \mathbb{R}^- , \mathbb{R}^{--} denote the non-positive and strictly negative reals.

– Part A: General theorems

2 – Fading Memory

Consider a continuous body \mathcal{B} , undergoing deformation such that a material point at \mathbf{X} in the reference configuration, is at position $\mathbf{x} = \mathbf{p}(\mathbf{X}, t)$ at time t. The deformation of the body is characterized by $\mathbf{F}(\mathbf{X}, t) = \nabla_{\mathbf{X}} \mathbf{p}(\mathbf{X}, t)$. The tensor field $\mathbf{L}(\mathbf{X}, t) = \nabla_{\mathbf{x}} \dot{\mathbf{p}}(\mathbf{X}, t)$ is the velocity gradient. The superimposed dot indicates a material time derivative. We have the identity

$$\mathbf{F}(\mathbf{X},t) = \mathbf{L}(\mathbf{X},t)\mathbf{F}(\mathbf{X},t) \,.$$

In the context of linear theories, we will use the (symmetric) strain tensor \mathbf{E} defined as $2\mathbf{E}(\mathbf{X},t) = \mathbf{F}^T(\mathbf{X},t)\mathbf{F}(\mathbf{X},t) - \mathbf{I}$ where \mathbf{I} is the unit tensor.

Let us denote by \mathbf{T} the *Cauchy stress tensor*. Our constitutive assumption is that the symmetric tensor $\mathbf{T}(\mathbf{X},t)$ is a specified functional on a suitable set of histories $\mathbf{F}^t \mathbf{X}$), defined as:

$$\mathbf{F}^t(\mathbf{X}, s) = \mathbf{F}(\mathbf{X}, t-s), \quad s \in \mathbb{R}^+.$$

The stress tensor is given by the functional:

(2.1)
$$\mathbf{T}(\mathbf{X},t) = \mathbf{\tilde{T}}(\mathbf{F}^t(\mathbf{X}))$$

In order to give a more precise definition of this property of fading memory at a material point $\mathbf{X} \in \mathcal{B}$, it is necessary to consider the set \mathcal{D} of the histories which make up the domain of definition of the functional (2.1). We suppose this set \mathcal{D} be such that if $\mathbf{F}^t(\mathbf{X}) \in \mathcal{D}$, then the partly static history \mathbf{F}_{τ}^t , associated with $\mathbf{F}^t(\mathbf{X})$, belongs to \mathcal{D} , where:

$$\mathbf{F}_{\tau}^{t}(\mathbf{X},s) = \begin{cases} \mathbf{F}(\mathbf{X},t) & s \in [0,\tau) \\ \mathbf{F}^{t}(\mathbf{X},t-s) & s \in [\tau,\infty) \,. \end{cases}$$

Thus τ is the duration of the static part of the history.

DEFINITION 2.1. A viscoelastic material is characterized by the constitutive equation (2.1), where $\mathbf{F}^t \in \mathcal{D}$ and there exists a constitutive equation $\mathbf{T}(\mathbf{X},t) = \mathbf{\tilde{T}}(\mathbf{F}(\mathbf{X},t))$ of an elastic material, such that:

$$\lim_{\tau \to \infty} \mathbf{\hat{T}}(\mathbf{F}_{\tau}^{t}(\mathbf{X})) = \mathbf{\tilde{T}}(\mathbf{F}(\mathbf{X}, t)).$$

Moreover $(\mathbf{\hat{T}}(\mathbf{F}_{\tau}^{t}(\mathbf{X})) - \mathbf{\tilde{T}}(\mathbf{F}(\mathbf{X},t)))$ belongs to $L^{2}(\mathbb{R}^{+})$ as a function of τ .

This definition was inspired by the work of FICHERA [7], [8], [9], [10].

3 – Simple material systems and dissipation principles

In this section, we consider certain dissipation principles and state some theorems, adopting for greater generality the axiomatic formulation of the thermodynamics of simple material systems [2], [3].

A map $P : [0, d_p) \to \text{Lin}_2$, piecewise continuous on the time interval $[0, d_p)$ defined as: $P(\tau) = \mathbf{L}(\tau), \tau \in [0, d_p)$, is said to be a *kinetic process* of duration $d_p \in \mathbb{R}^+$. The set Π of all *accessible* processes P satisfies the following properties:

i) if $P \in \Pi$, then its restriction $P_{[t_1,t_2)}$ to the interval $[t_1,t_2) \subset [0,\infty)$ belongs to Π

ii) if $P_1, P_2 \in \Pi$, then $P_1 * P_2 \in \Pi$, where

$$P_1 * P_2(\tau) = \begin{cases} P_1(\tau) & \tau \in [0, d_{p_1}) \\ P_2(\tau - d_{p_1}) & \tau \in [d_{p_1}, d_{p_1} + d_{p_2}). \end{cases}$$

The restriction $P_{[0,t)}$ will be denoted by P_t . The process P_0 of zero duration is referred to as the zero process.

We introduce the notion of state by means of the definition of a simple material element [2], [3].

DEFINITION 3.1. A simple solid material element at any point is a set $\{\Pi, \Sigma, \hat{C}, \hat{\rho}, \hat{W}\}$ such that:

- a: Π is the family of all accessible kinetic processes,
- b: Σ the state space is the set of states σ of the system,
- c: \hat{C} : $\Sigma \to \text{Lin}_2$ maps any state σ onto the current value of the *deformation gradient* \mathbf{F} ,

d: the map $\hat{\rho} : \Sigma \times \Pi \to \Sigma$ is the evolution function, which transforms the state σ_1 , under the process P into $\sigma_2 = \hat{\rho}(\sigma_1, P)$. Moreover, the mapping is such that:

(3.1)
$$\hat{\rho}(\sigma, P_1 * P_2) = \hat{\rho}(\hat{\rho}(\sigma, P_1), P_2), \quad \forall P_1, P_2 \in \Pi \quad \sigma \in \Sigma$$
$$\hat{\rho}(\sigma, P_0) = \sigma,$$

- e: the map $\hat{W}: \Sigma \times \Pi \to \mathbb{R}$ is the *work response*, which to each state σ and process *P* assigns the corresponding work,
- f: finally, there exists a function $\hat{\mathbf{T}} : \Sigma \times \Pi \to \text{Sym}$, the stress response, in terms of which the work can be written as:⁽¹⁾

$$\hat{W}(\sigma, P) = \int_0^{d_p} \hat{\mathbf{T}}(\sigma, P_t) \cdot \mathbf{L}(t) \, dt.$$

For materials with fading memory the state at time t will be defined as the current value and the past history of the deformation gradient, or the strain in the linear case.

Now we can introduce an equivalence relation on the space state Σ by means of the following:

DEFINITION 3.2. Two states $\sigma_1, \sigma_2 \in \Sigma$ are equivalent if

$$\hat{C}_1(\sigma_1) = \hat{C}_2(\sigma_2)$$
$$\hat{\mathbf{T}}(\sigma_1, P) = \hat{\mathbf{T}}(\sigma_2, P)$$

for all $P \in \Pi$.

Definition 3.2 satisfies the requirements for an equivalence relation, which we denote by \mathcal{R} . If the space state Σ of a simple material contains equivalent states, then it is possible to build a new state space Σ_R , for the given material element, as the quotient of Σ on \mathcal{R} . The elements σ_R of Σ_R will be called *minimal states*. It is not however necessary to use, for the given material element, the minimal state space Σ_R . It is correct also to use any notion of state, which satisfies the Definition 3.1. It is easy to prove:

⁽¹⁾Strictly, this applies only to incompressible materials since we have omitted the density. However, this is irrelevant in the linear approximation, which is of primary interest here.

PROPOSITION 3.1. If σ_1 and σ_2 are two equivalent states then

$$W(\sigma_1, P) = W(\sigma_2, P), \quad \forall P \in \Pi.$$

The converse is also true if $\hat{C}_1(\sigma_1) = \hat{C}_2(\sigma_2)$.

DEFINITION 3.3. A pair (σ, P) is called a cyclic process if $\hat{\rho}(\sigma, P) = \sigma$.

In this work, we are interested only in isothermal processes. For such processes the Second Law of Thermodynamics can be written (see [3]) as:

The Dissipation Principle: For every cyclic process (σ, P) we have:

(3.2)
$$W(\sigma, P) = \int_0^{d_p} \hat{\mathbf{T}}(\sigma, P_t) \cdot \mathbf{L}(t) \, dt \ge 0$$

DEFINITION 3.4. A set $S \subset \Sigma$ is *invariant under* $\hat{\rho}$, if for every $\sigma_1 \in S$, and $P \in \Pi$, the state $\sigma = \hat{\rho}(\sigma_1, P) \in S$.

DEFINITION 3.5. A function $\psi : S_{\psi} \to \mathbb{R}^+$ is a free energy if:

- i) the domain S_{ψ} is invariant under $\hat{\rho}$,
- ii) for any pair $\sigma_1, \sigma_2 \in S_{\psi}$ and $P \in \Pi$, such that $\hat{\rho}(\sigma_1, P) = \sigma_2$ we have

(3.3)
$$\psi(\sigma_2) - \psi(\sigma_1) \le W(\sigma_1, P).$$

In the following, the set of all free energies of the simple material element under consideration be denoted by Ψ .

We define

(3.4)
$$\mathcal{W}(\sigma) = \{W(\sigma, P); P \in \Pi\}.$$

The Strong Dissipation Principle: The set $\mathcal{W}(\sigma)$ is bounded below for all $\sigma \in \Sigma$. Furthermore, there is a state σ^{\dagger} , which we refer to as the zero state, such that

(3.5)
$$\inf \mathcal{W}(\sigma^{\dagger}) = 0.$$

REMARK 3.1. For a fading memory material, the zero state is $\sigma^{\dagger} = \mathbf{0}^{\dagger}$, where $\mathbf{0}^{\dagger}$ is the zero history.

DEFINITION 3.6. A state $\sigma \in \Sigma$ is *attainable* from all of Σ if, for any initial state $\sigma^i \in \Sigma$, there exists a process $P \in \Pi$ such that $\hat{\rho}(\sigma^i, P) = \sigma$. A simple material system is attainable if any state σ is attainable from every other state $\sigma' \in \Sigma$.

It is proved in [4] that the Dissipation Principle follows from the Strong Dissipation Principle; also the converse proposition holds if the system is attainable. However, for a simple material system with fading memory not all states are attainable. For this reason, in the following we adopt the Strong Dissipation Principle.

Let us define the set

(3.6)
$$\Phi := \{ \phi : \Sigma \to \mathbb{R}^+; \phi(\sigma) \le \psi(\sigma) \; \forall \psi \in \Psi, \; \forall \sigma \in \mathcal{S}_{\psi}; \phi(\sigma^{\dagger}) = 0 \}$$

and the function $\phi_M : \Sigma \to \mathbb{R}^+$ where

(3.7)
$$\phi_M(\sigma) = \sup\{\phi(\sigma); \phi \in \Phi\}.$$

Thus ϕ_M is the largest functional with the property that it is less than or equal to any free energy for all states

We define $\mathcal{W}(\sigma)$ as

(3.8)
$$\mathcal{W}(\sigma) := \{ W(\sigma, P) - \phi_M(\hat{\rho}(\sigma, P)) ; P \in \Pi \}.$$

4 – Minimum and maximum free energies

DEFINITION 4.1. A functional ψ_m is called the *minimum free energy* if:

i) ψ_m is a free energy with domain $\mathcal{S}_{\psi} = \Sigma$.

ii) the zero state $\sigma^{\dagger} \in \Sigma$ is such that $\psi_m(\sigma^{\dagger}) = 0$

iii) for any free energy $\psi : S_{\psi} \to \mathbb{R}^+$ such that $\sigma^{\dagger} \in S_{\psi}$, and $\psi(\sigma^{\dagger}) = 0$, we have:

(4.1)
$$\psi(\sigma) \ge \psi_m(\sigma) \quad \forall \ \sigma \in \mathcal{S}_{\psi}.$$

REMARK 4.1. The minimum free energy (if it exists) is unique. The proof follows easily from the inequality (4.1).

THEOREM 4.1. The functional

$$\psi_m(\sigma) := -\inf \mathcal{W}(\sigma)$$

is the minimum free energy.

The proof of this theorem is given in [4].

THEOREM 4.2. The functional

(4.2)
$$\tilde{\psi}_m(\sigma) := -\inf \widetilde{\mathcal{W}}(\sigma) = \sup\{-W(\sigma, P) + \phi_M(\hat{\rho}(\sigma, P)); P \in \Pi\}$$

is a free energy such that $\tilde{\psi}_m(\sigma) = \psi_m(\sigma) \; \forall \; \sigma \in \Sigma$.

This result is proved in [1]. It follows from (4.2) that, given $\sigma \in S_{\psi}$, for every $\varepsilon > 0$, there is a process P_{ε} such that

(4.3)
$$\tilde{\psi}_m(\sigma) < -W(\sigma, P_{\varepsilon}) + \phi_M(\hat{\rho}(\sigma, P_{\varepsilon})) + \varepsilon$$

REMARK 4.2. A similar result holds for any choice of $\phi \in \Phi$ defined by (3.6). We can in fact weaken considerably the constraint on the functions $\phi \in \Phi$ that they be less than or equal to all free energies for all states.

(4.4) COROLLARY 4.3. If $\exists \varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$ $\phi_M(\hat{\rho}(\sigma, P_{\varepsilon})) \le \psi(\hat{\rho}(\sigma, P_{\varepsilon})) \ \forall \ \psi \in \Psi, \ \sigma \in \mathcal{S}_{\psi}$

where P_{ε} is defined by (4.3), then Theorem 4.2 holds with $W(\sigma)$ defined by (3.8), though now ϕ_M is constrained only by (4.4) rather than by (3.7).

Thus, in fact, the property must hold only for the final states of processes in the vicinity of the optimal process.

REMARK 4.3. It is always possible to represent the minimum free energy as a function of the minimal state σ_R . It is clear from the definition of $\mathcal{W}(\sigma)$, given by (3.4) and from the fact that $W(\sigma, P) = W(\sigma_R, P)$ for all $P \in \Pi$, that $\inf \mathcal{W}(\sigma) = \inf \mathcal{W}(\sigma_R)$. Therefore, if $\sigma \in \sigma_R$

(4.5)
$$\psi_m(\sigma) = \psi_m(\sigma_R) \,.$$

Hence the minimum free energy is independent of the definition of state that is used.

Let us denote by Σ_{σ} the set of all $\sigma' \in \Sigma$ attainable from σ , viz.

$$\Sigma_{\sigma} = \{ \sigma' \in \Sigma; \exists P \in \Pi; \sigma' = \hat{\rho}(\sigma, P) \}.$$

For any pair σ_{0} , $\sigma \in \Sigma$, such that $\sigma \in \Sigma_{\sigma_{0}}$, we can consider the set:

(4.6)
$$N(\sigma_0, \sigma) = \{ W(\sigma_0, P), \forall P \in \Pi; \hat{\rho}(\sigma_0, P) = \sigma \}.$$

From the Strong Dissipation Principle, this set is bounded below. We state a further theorem proved in [1]:

THEOREM 4.4. For any fixed σ^i , the functional $\psi_M^{\sigma^i} : \Sigma_{\sigma^i} \to \mathbb{R}^+$ defined by

$$\psi_M^{\sigma^i}(\sigma) = \inf N(\sigma^i; \sigma) + \psi_m(\sigma^i)$$

is a free energy, called a maximal free energy. For any free energy ψ : $S_{\psi} \to \mathbb{R}^+$, such that $S_{\psi} \supset \Sigma_{\sigma^i}$, and $\psi(\sigma^i) = \psi_m(\sigma^i)$, we have

(4.7)
$$\psi(\sigma) \le \psi_M^{\sigma^i}(\sigma), \quad \forall \ \sigma \in \Sigma_{\sigma^i}.$$

REMARK 4.4. Of course for any $\sigma^i \in \Sigma$ we may obtain a different free energy. Moreover, for a fixed $\sigma^i \in \Sigma$ the definition of maximum free energy may depend on the definition of state. We can however construct a maximum free energy that is defined on the space of minimal states. In other words, if we consider the definition of minimal state, then (4.6) is replaced by

$$N(\sigma_{0R}, \sigma_R) = \{ W(\sigma_{0R}, P), \forall P \in \Pi; \hat{\rho}(\sigma_{0R}, P) = \sigma_R \}.$$

This set is generally larger than $N(\sigma_0, \sigma)$, if $\sigma_0 \in \sigma_{0R}$, and $\sigma \in \sigma_R$. For this reason the maximum free energy defined on Σ_R as

$$\psi_M^{\sigma_R^i}(\sigma_R) = \inf N(\sigma_R^i; \sigma_R) + \psi_m(\sigma_R^i)$$

satisfies the inequality

$$\psi_M^{\sigma_R^i}(\sigma_R) \leq \psi_M^{\sigma^i}(\sigma)\,, \ \ \sigma^i \in \sigma_R^i, \ \ \sigma \in \sigma_R\,.$$

Relation (4.7) will apply to any free energy $\psi(\sigma_R)$ defined on Σ_R provided $\psi(\sigma_R^i) = \psi_m(\sigma_R^i)$. We shall give the form of the maximum free energy $\psi_M^{\sigma_R^i}(\sigma_R)$ on Σ_R for a particular linear model in Section 10.

5 – Linear viscoelasticity.

For the remainder of this paper, we shall be dealing with the case of a linear viscoelastic solid, characterized by the stress-strain relation

(5.1)
$$\mathbf{T}(t) = \mathbf{G}_0 \mathbf{E}(t) + \int_0^\infty \mathbf{G}'(s) \mathbf{E}^t(s) \, ds$$

where we assume that $\mathbf{G}'(\cdot) \in L^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+)$ and also $(\mathbf{G}(\cdot) - \mathbf{G}_{\infty}) \in L^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+)$. The relaxation function:

$$\mathbf{G}(s) = \mathbf{G}_0 + \int_0^s \mathbf{G}'(t) \, ds$$

is well defined. We have $\mathbf{G}_0 = \mathbf{G}(0)$. Also, $\mathbf{G}_{\infty} = \mathbf{G}(\infty) = \lim_{s \to \infty} (\mathbf{G}_0 + \int_0^s \mathbf{G}'(s) ds)$ is positive and well-defined as a consequence of the fading memory property [1]. Thermodynamics implies the symmetry of \mathbf{G}_0 and \mathbf{G}_{∞} [12], but not the symmetry of $\mathbf{G}(s), s \in \mathbb{R}^{++}$. However, in the following, we assume that $\mathbf{G}(s)$ is a fourth order symmetric tensor. There is the further property [1] that $\mathbf{G}_0 > \mathbf{G}_{\infty}$.

For any $f \in L^2(\mathbb{R})$, we denote its Fourier transform by

(5.2)
$$f_F(\omega) = \int_{-\infty}^{\infty} f(\xi) e^{-i\omega\xi} d\xi = f_+(\omega) + f_-(\omega)$$
$$f_+(\omega) = \int_0^{\infty} f(\xi) e^{-i\omega\xi} d\xi$$
$$f_-(\omega) = \int_{-\infty}^0 f(\xi) e^{-i\omega\xi} d\xi .$$

Only real valued functions f will be considered so that $\bar{f}_F(\omega) = f_F(-\omega)$ where the bar denotes the complex conjugate. Functions defined on \mathbb{R}^+ are identified with functions on \mathbb{R} which vanish identically on \mathbb{R}^{--} . For such functions, $f_F = f_c - if_s$, where f_c , f_s are respectively the Fourier cosine and sine transforms. In this notation

$$\mathbf{G}_F'(\omega) = \mathbf{G}_c'(\omega) - i \quad \mathbf{G}_s'(\omega) \,.$$

It is a consequence of the Second Law that [16]

$$\mathbf{G}'_s(\omega) < 0$$
, $\forall \, \omega \in \mathbb{R}^{++}$

As a consequence of $\mathbf{G}' \in L^2(\mathbb{R}^+)$ and of Plancherel theorem, the constitutive equation (5.1) can be written as [4]

(5.3)
$$\mathbf{T}(t) = \mathbf{G}_0 \mathbf{E}(t) + \frac{2}{\pi} \int_0^\infty \mathbf{G}'_s(\omega) \mathbf{E}^t_s(\omega) \, d\omega$$

for any $\mathbf{E}^t \in L^2(\mathbb{R}^+)$. It is possible to generalize (5.3) so that it holds for a much larger class of histories [1].

6 – Maximum recoverable work

We denote by $\mathbf{G}(|s|)$ the extension of $\mathbf{G}(s)$ to an even function on \mathbb{R} . Also, we suppose any process $P \in \Pi$ is defined over \mathbb{R}^+ by means of the trivial extension

(6.1)
$$P(t) = \begin{cases} P(t), & t \in [0, d_p) \\ 0, & t \in [d_p, \infty). \end{cases}$$

Now let us evaluate the work $W(\sigma_0, P)$, where $\sigma_0 = \mathbf{E}^0$ is the history at t = 0. We consider states at t = 0 in this section and the next, for convenience. There is no loss of generality in doing so. In later sections, the discussion is based on states at time t, not necessarily zero. Also, $P \in \Pi$ is a process such that $P(t) = \dot{\mathbf{E}}(t), t \in [0, d_p)$. We have $\mathbf{E}^t = \hat{\rho}(\mathbf{E}^0, P_t)$ and the stress is given by

$$\mathbf{T}(\mathbf{E}^t) = \mathbf{G}_0 \mathbf{E}(t) + \int_0^t \mathbf{G}'(s) \mathbf{E}^t(s) \, ds - \mathbf{I}_0(t, \mathbf{E}^0)$$

where

(6.2)
$$\mathbf{I}_0(t, \mathbf{E}^0) = -\int_0^\infty \mathbf{G}'(t+\tau)\mathbf{E}^0(\tau) \, d\tau, \ t \ge 0.$$

Moreover, from (6.1) it follows that there exists the limit $\mathbf{E}(\infty) = \lim_{t \to +\infty} \mathbf{E}(t)$. We have, after some manipulation

(6.3)
$$W(\sigma, P) = \frac{1}{2} \int_0^\infty \int_0^\infty \mathbf{G}(|t-\tau|) \dot{\mathbf{E}}(\tau) \cdot \dot{\mathbf{E}}(t) d\tau dt - \int_0^\infty \tilde{\mathbf{I}}_0(t, \mathbf{E}^0) \cdot \dot{\mathbf{E}}(t) dt$$

where

(6.4)
$$\tilde{\mathbf{I}}_0(t, \mathbf{E}^0) = -\mathbf{G}(t)\mathbf{E}(0) + \mathbf{I}_0(t, \mathbf{E}^0).$$

In order to obtain the maximum recoverable work from state $\sigma_0 = \mathbf{E}^0$, we consider the maximum of $-W(\sigma_0, P)$ with respect to the set of functions given by

$$\mathbf{E}(t) = \mathbf{E}^{(m)}(t) + \varepsilon \mathbf{e}(t) \qquad t \in \mathbb{R}^+$$

where ε is a real parameter and \mathbf{e} is a arbitrary smooth function such that $\mathbf{e}(0) = 0$. If $\mathbf{E}^{(m)}$ is the process from which we obtain the maximum recoverable work, then differentiating $W(\sigma, P)$ with respect to ε and using the fact that $\dot{\mathbf{e}}(t)$ is arbitrary, we obtain for $t \in \mathbb{R}^+$

(6.5)
$$\int_0^\infty \mathbf{G}(|t-\tau|)\dot{\mathbf{E}}^{(m)}(\tau)\,d\tau = \tilde{\mathbf{I}}_0(t,\mathbf{E}^0)\,.$$

Equation (6.5) is an integral equation of the Wiener-Hopf type, the solution of which gives the process $\mathbf{E}^{(m)}$ which yields the maximum recoverable work. We have from Theorem 4.1 and relations (6.3), (6.5)

$$\psi_m(\mathbf{E}^0) = \frac{1}{2} \int_0^\infty \int_0^\infty \mathbf{G}(|t-\tau|) \dot{\mathbf{E}}^{(m)}(\tau) \cdot \dot{\mathbf{E}}^{(m)}(t) d\tau dt$$

where $\dot{\mathbf{E}}^{(m)}$ is now the solution of the Wiener-Hopf equation (6.5).

It is important to prove the existence and uniqueness of the solution of (6.5). Let us assume that the kernel $\mathbf{G}(|t|)$ is a positive operator. We denote by \mathcal{G} the set

$$\mathcal{G} = \left\{ \dot{\mathbf{E}} : [0, \infty) \to \text{Sym}; \int_0^\infty \int_0^\infty \mathbf{G}(|t - \tau|) \dot{\mathbf{E}}(t) \cdot \dot{\mathbf{E}}(\tau) d\tau dt < \infty \right\}.$$

We can introduce an inner product on \mathcal{G} by

(6.6)
$$(\dot{\mathbf{E}}_1, \cdot \dot{\mathbf{E}}_2) = \int_0^\infty \int_0^\infty \mathbf{G}(t-\tau|) \dot{\mathbf{E}}_1(\tau) \cdot \dot{\mathbf{E}}_2(t) d\tau dt$$

to make \mathcal{G} a Hilbert space.

Equation (6.5) can be written as

$$\mathcal{A}\dot{\mathbf{E}} = \mathbf{I}_0$$

where \mathcal{A} is an operator from \mathcal{G} to its dual \mathcal{G}' . It is bounded and coercive. Then, from the Lax-Milgram theorem, we have the following result:

THEOREM 6.1. For any $\tilde{\mathbf{I}}_0 \in \mathcal{G}'$, the equation (6.5) has a unique solution $\dot{\mathbf{E}} \in \mathcal{G}$ such that

$$\|\dot{\mathbf{E}}\|_{\mathcal{G}} \leq K \|\tilde{\mathbf{I}}_0\|_{\mathcal{G}'}$$
.

In other words, there exists an isomorphism between \mathcal{G} and \mathcal{G}' .

PROPOSITION 6.2. Two histories \mathbf{E}_1^0 , \mathbf{E}_2^0 correspond to two equivalent states if and only if

(6.7)
$$\tilde{\mathbf{I}}_0(t, \mathbf{E}_1^0) = \tilde{\mathbf{I}}_0(t, \mathbf{E}_2^0) \quad \forall t \in \mathbb{R}^+$$

PROOF. If (6.7) holds for any $t \in \mathbb{R}^+$, then for $t \to \infty$ we have

(6.8)
$$\mathbf{E}_1^0(0) = \mathbf{E}_2^0(0).$$

Equation (6.7) and (6.8) imply equivalence according to Definition 3.2. The converse is trivial.

REMARK 6.1. Proposition 6.2 yields a bijective map between \mathcal{G}' and the set Σ_R . In other words it is possible to identify any class of equivalent histories with a function $\tilde{\mathbf{I}}_0$.

This result allows us to represent the minimum free energy as a function defined on the set Σ_R of equivalent histories which will be done explicitly for a particular class of materials in Section 10.

Let us now consider the implications of Theorem 4.2 and in particular Corollary 4.3. Motivated by the latter result and the fact, stated formally in Section 8, that the elastic free energy is less than or equal to any viscoelastic free energy, we take ϕ_M to be $\phi(\infty)$ where $\phi(t)$ is the elastic free energy corresponding to strain $\mathbf{E}(t)$, given by

(6.9)
$$\phi(t) = \frac{1}{2} \mathbf{G}_{\infty} \mathbf{E}(t) \cdot \mathbf{E}(t) \,.$$

This choice will be justified more clearly later. If we seek the history which maximizes the functional

$$W(\sigma, P) - \phi(\infty) =$$
(6.10)
$$= \frac{1}{2} \int_0^\infty \int_0^\infty \mathbf{G}(|t - \tau|) \dot{\mathbf{E}}(\tau) \cdot \dot{\mathbf{E}}(t) d\tau dt - \int_0^\infty \tilde{\mathbf{I}}_0(t, \mathbf{E}^0) \cdot \dot{\mathbf{E}}(t) dt - \phi(\infty)$$

where $\tilde{\mathbf{I}}_0(t, \mathbf{E}^0)$ is defined by (6.4) then, instead of (6.5), we obtain

(6.11)
$$\int_0^\infty \mathbf{G}(|t-\tau|)\dot{\mathbf{E}}^{(m)}(\tau)\,d\tau = \tilde{\mathbf{I}}_0(t,\mathbf{E}^0) + \mathbf{G}_\infty \mathbf{E}^{(m)}(\infty)$$

noting that $\mathbf{e}(\infty) = \int_0^\infty \dot{\mathbf{e}}(t) dt$.

Let us express the solution of (6.5), namely $\dot{\mathbf{E}}^{(m)}$, as the sum

(6.12)
$$\dot{\mathbf{E}}^{(m)} = \dot{\mathbf{E}}^{(m_1)} + \dot{\mathbf{E}}^{(m_2)}$$

where $\dot{\mathbf{E}}^{(m_1)}$ is the solution of (6.11) and $\dot{\mathbf{E}}^{(m_2)}$ satisfies the equation obtained by subtracting (6.11) from (6.5), namely

(6.13)
$$\int_{0}^{\infty} \mathbf{G}(|t-\tau|) \dot{\mathbf{E}}^{(m_{2})}(\tau) d\tau = -\mathbf{G}_{\infty} \mathbf{E}^{(m_{1})}(\infty) = = -\mathbf{G}_{\infty} \Big(\mathbf{E}^{(m_{1})}(0) + \int_{0}^{\infty} \dot{\mathbf{E}}^{(m_{1})}(\tau) d\tau \Big)$$

As a consequence of Theorem 6.1, equation (6.13) has a unique solution $\dot{\mathbf{E}}^{(m_2)} \in \mathcal{G}$, which we denote formally by

$$\dot{\mathbf{E}}^{(m_2)}(t) = -\mathbf{E}^{(m_1)}(\infty)\delta(t-\infty).$$

This function can be expressed as the limit of a sequence [1]. Note that (6.12) corresponds to continuations given formally by

(6.14)
$$\mathbf{E}^{(m)}(t) = \mathbf{E}^{(m_1)}(t) - \mathbf{E}^{(m_1)}(\infty)H(t-\infty)$$

where H(s) is the Heaviside step-function.

REMARK 6.2. As a consequence of Theorem 4.2, the maximum recoverable work, which we obtain using the functional $W(\sigma, P)$ or $(W(\sigma, P) - \phi_M(\hat{\rho}(\sigma, P)))$ is the same, but the processes from which we obtain this maximum recoverable work are different. If we use $W(\sigma, P)$, the optimal process is $\dot{\mathbf{E}}^{(m)}$ which satisfies (6.5); while if we use $(W(\sigma, P) - \phi_M(\hat{\rho}(\sigma, P)))$, the optimal process is $\dot{\mathbf{E}}^{(m_1)}$ which satisfies (6.11).

We have from Theorem 4.2 and Corollary 4.3, (6.10) and (6.11)

$$\psi_m(\mathbf{E}^0) = \frac{1}{2} \int_0^\infty \int_0^\infty \mathbf{G}(|t-\tau|) \dot{\mathbf{E}}^{(m_1)}(\tau) \cdot \dot{\mathbf{E}}^{(m_1)}(t) d\tau dt - \phi(\infty) + \mathbf{G}_\infty \mathbf{E}(\infty) \mathbf{E}(0)$$

where $\dot{\mathbf{E}}^{(m_1)}$ is now the solution of equation (6.11). Carrying out partial integrations and using (6.11), we find that

(6.15)
$$\psi_m(\mathbf{E}^0) = S(0) + \frac{1}{2} \int_0^\infty \int_0^\infty \frac{\partial^2}{\partial t \partial \tau} \mathbf{G}(|t-\tau|) \mathbf{E}^{(m_1)}(\tau) \cdot \mathbf{E}^{(m_1)}(t) d\tau dt$$
$$S(t) = \mathbf{T}(t) \cdot \mathbf{E}(t) - \frac{1}{2} \mathbf{G}_0 \mathbf{E}(t) \cdot \mathbf{E}(t) .$$

The form (6.15) is shown in Section 8 (Proposition 8.1) to have the characteristic properties of a free energy, one of which eliminates the freedom of an additive constant. This justifies the inclusion of $\phi(\infty)$ in (6.10).

7 – Minimum Free Energy

We begin with some preliminary results and definitions. Following [5], we will be considering frequency space quantities, defined by analytic continuation from integral definitions, as functions on the complex ω plane, denoted by Ω , where

(7.1)
$$\Omega^{+} = \{ \omega \in \Omega \mid \Im \omega \in \mathbb{R}^{+} \}$$
$$\Omega^{(+)} = \{ \omega \in \Omega \mid \Im \omega \in \mathbb{R}^{++} \}.$$

Similarly, Ω^{-} and $\Omega^{(-)}$ are the lower half-planes including and excluding the real axis, respectively. The quantities f_{\pm} , defined by (5.2), are analytic in $\Omega^{(\mp)}$ respectively.

The function \mathbf{G}'_F is analytic on $\Omega^{(-)}$. This follows from its integral definition over \mathbb{R}^+ . It will be assumed further that \mathbf{G}'_F is analytic on \mathbb{R} and thus on Ω^- . It is defined by analytic continuation in regions of Ω^+ where the Fourier integral does not converge.

The quantity \mathbf{G}'_s has singularities in both $\Omega^{(+)}$ and $\Omega^{(-)}$ that are mirror images of each other. It goes to zero at the origin and must also be analytic there. Thus, it vanishes as ω^n where the integer $n \ge 1$. It is assumed that n = 1.

A quantity central to our considerations is defined by

(7.2)
$$\mathbf{H}(\omega) := -\omega \mathbf{G}'_s(\omega) \,.$$

It is a positive, even function of the frequency. We have [1]

(7.3)
$$\mathbf{G}'(0) = -\mathbf{H}(\infty) \,.$$

If $\mathbf{G}(s)$, $s \in \mathbb{R}^+$ is extended to the even function $\mathbf{G}(|s|)$ on \mathbb{R} then $\mathbf{G}'(|s|)$ is an odd function with Fourier transform given by

(7.4)
$$\mathbf{G}'_F(\omega) = -2i\mathbf{G}'_s(\omega) \,.$$

We will be using the Fourier transforms of the strain history and continuation defined by

(7.5)
$$\mathbf{E}_{+}^{t}(\omega) = \int_{0}^{\infty} e^{-i\omega s} \mathbf{E}^{t}(s) ds$$
$$\mathbf{E}_{-}^{t}(\omega) = \int_{-\infty}^{0} e^{-i\omega s} \mathbf{E}^{t}(s) ds$$

It is necessary to include cases where the histories and continuations do not belong to L^2 , as outlined in [1]. The quantity \mathbf{E}^t_+ is analytic on $\Omega^{(-)}$ and \mathbf{E}^t_- is analytic on $\Omega^{(+)}$. Both are assumed to be analytic on IR. It is further assumed that they are analytic at infinity, so that if $\mathbf{E}^t(0)$ is finite, which is of course assumed, \mathbf{E}^t_\pm go to zero at large ω as ω^{-1} in all directions. We will require the derivative of \mathbf{E}^t_+ with respect to t. Assuming that the strain history has a derivative which is continuous and belongs to $L^1(\mathbb{R}^+)$, then

(7.6)
$$\frac{d}{dt}\mathbf{E}_{+}^{t}(\omega) = -i\omega\mathbf{E}_{+}^{t}(\omega) + \mathbf{E}(t).$$

We can write (5.3) in the form

(7.7)
$$\mathbf{T}(t) = \mathbf{G}_0 \mathbf{E}(t) + \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{\mathbf{H}(\omega)}{\omega} \mathbf{E}_+^t(\omega) d\omega$$

where the oddness of $\mathbf{H}(\omega)/\omega$ has been used.

Let us now solve the Wiener-Hopf equation (6.11). It can be written in the form [1]

(7.8)
$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t} \mathbf{G}(|t-\tau|) \mathbf{E}^{0}(\tau) d\tau = \mathbf{R}(t)$$
$$\mathbf{E}^{0}(\tau) = \mathbf{E}^{(m_{1})}(-\tau), \quad \tau \in \mathbb{R}^{-1}$$
$$\mathbf{R}(t) = 0, \quad t \in \mathbb{R}^{-1}$$

while on \mathbb{R}^+ , the quantity \mathbf{E}^0 is the given history. This relation defines \mathbf{R} on \mathbb{R}^+ . Taking Fourier transforms and multiplying across by ω , we obtain, with the aid of (7.4) and (7.2),

(7.9)
$$2i\mathbf{H}(\omega)(\mathbf{E}^{0}_{+}(\omega) + \mathbf{E}^{(m)}(\omega)) = \omega\mathbf{R}_{+}(\omega)$$

where $\mathbf{E}^{(m)}(\omega)$ is the Fourier transform of $\mathbf{E}^{0}(\tau)$ defined by (7.8) on \mathbb{R}^{--} and is the quantity we wish to determine. Also, $\mathbf{R}_{+}(\omega)$ is analytic on $\Omega^{(-)}$ and by assumption also on \mathbb{R} .

Now [6], the tensor **H** (which is isomorphic to a matrix in $\mathbb{R}_6 \times \mathbb{R}_6$) can be factorized as follows: $\mathbf{H}(\omega) = \mathbf{H}_+(\omega)\mathbf{H}_-(\omega)$, where \mathbf{H}_{\pm} is analytic,

with no zeros in its determinant, on Ω^{\mp} . We multiply (7.9) by $[\mathbf{H}_{+}(\omega)]^{-1}$ to obtain

(7.10)
$$\mathbf{H}_{-}(\omega)(\mathbf{E}^{0}_{+}(\omega) + \mathbf{E}^{(m)}(\omega)) = \frac{\omega}{2i}[\mathbf{H}_{+}(\omega)]^{-1}\mathbf{R}_{+}(\omega).$$

With the aid of the Plemelj formulae [17], we write

(7.11)

$$\mathbf{Q}(\omega) := \mathbf{H}_{-}(\omega)\mathbf{E}_{+}^{0}(\omega) = \mathbf{q}_{-}(\omega) - \mathbf{q}_{+}(\omega)$$

$$\mathbf{q}_{\pm}(\omega) = \lim_{z \to \omega^{\mp}} \mathbf{q}(z)$$

$$\mathbf{q}(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\mathbf{Q}(\omega')}{\omega' - z} d\omega'$$

where \mathbf{q}_{-} is analytic on $\Omega^{(+)}$ and \mathbf{q}_{+} is analytic on $\Omega^{(-)}$. In fact, they are given by $\mathbf{q}(z)$ for $z \in \Omega^{(+)}$ and $\Omega^{(-)}$ respectively. With earlier assumptions giving that $\mathbf{H}_{-}(\omega)\mathbf{E}_{+}^{0}(\omega)$ is analytic on \mathbb{R} , it can be deduced that \mathbf{q}_{\pm} are analytic on \mathbb{R} [5]. In $\Omega^{(-)}$, \mathbf{q}_{-} is defined by analytic continuation from Ω^{+} , while \mathbf{q}_{+} is correspondingly defined in $\Omega^{(+)}$. Substituting (7.11) into (7.10) we obtain

(7.12)
$$\mathbf{K}(\omega) = \mathbf{q}_{-}(\omega) + \mathbf{H}_{-}(\omega)\mathbf{E}^{(m)}(\omega) = \mathbf{q}_{+}(\omega) + \frac{\omega}{2i}[\mathbf{H}_{+}(\omega)]^{-1}\mathbf{R}_{+}(\omega).$$

The function $\mathbf{K}(\omega)$ is analytic on Ω^- by virtue of the first relation and analytic on Ω^+ by virtue of the second. It is therefore analytic over the entire complex plane. By Liouville's theorem it must be a polynomial. However, for $|\omega| \to \infty$, $\mathbf{K}(\omega) \to 0$ as $1/\omega$ since \mathbf{q}_- and $\mathbf{E}^{(m)}$ have this property. Hence, it must vanish everywhere so that

(7.13)
$$\mathbf{H}_{-}(\omega)\mathbf{E}^{(m)}(\omega) + \mathbf{q}_{-}(\omega) = 0$$

and the minimum free energy (6.15) may be represented in the form

(7.14)
$$\psi_m(\mathbf{E}^0) = S(0) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{H}(\omega) \mathbf{E}^{(m)}(\omega) \cdot \bar{\mathbf{E}}^{(m)}(\omega) d\omega$$
$$= S(0) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{q}(\omega) \cdot \bar{\mathbf{q}}(\omega) d\omega$$

The above solution can be extended to a much wider class of histories [1].

– Part B: A new variational method

8 – Certain time-domain relationships

In this first section of Part B, we shall present certain observations and demonstrations, the object of which is to elucidate the content of the developments of later sections in the frequency domain, by pointing to equivalent developments, as far as possible, in the time domain.

We understand throughout this section that $\mathbf{G}(s)$ refers to its even extension $\mathbf{G}(|s|)$, $s \in \mathbb{R}$. The work function

(8.1)
$$W(t) = \phi(-\infty) + \int_{-\infty}^{t} \mathbf{T}(s) \cdot \dot{\mathbf{E}}(s) ds$$

can be expressed in the form [1]

(8.2)
$$W(t) = S(t) + \frac{1}{2} \int_{-\infty}^{t} \int_{-\infty}^{t} \mathbf{G}_{12}(s-u) \mathbf{E}(u) \cdot \mathbf{E}(s) du ds$$
$$\mathbf{G}_{12}(s-u) = \frac{\partial^2}{\partial u \partial s} \mathbf{G}(s-u) \,.$$

It may be written as

(8.3)
$$W(t) = S(t) + \frac{1}{2} \int_0^\infty \int_0^\infty \mathbf{G}_{12}(s-u) \mathbf{E}^t(u) \cdot \mathbf{E}^t(s) du \, ds \, .$$

A frequency representation can also be given as in (7.14):

(8.4)
$$W(t) = S(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{H}(\omega) \mathbf{E}_{+}^{t}(\omega) \cdot \bar{\mathbf{E}}_{+}^{t}(\omega) d\omega$$

where **H** is defined by (7.2) and \mathbf{E}_{+}^{t} by (7.5). Note that, in frequency space, the integral term is clearly non-negative since **H** is positive-definite.

We define the scalar product of $\mathbf{E}_1, \mathbf{E}_2 : \mathbb{R} \to \text{Sym}$ (differing from, though related to (6.6) if $\mathbf{E}_1, \mathbf{E}_2$ are zero on \mathbb{R}^{--})

(8.5)
$$(\mathbf{E}_{1}, \mathbf{E}_{2}) = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{G}_{12}(s-u) \mathbf{E}_{1}^{t}(u) \cdot \mathbf{E}_{2}^{t}(s) du ds =$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{H}(\omega) \mathbf{E}_{1F}^{t}(\omega) \cdot \bar{\mathbf{E}}_{2F}^{t}(\omega) d\omega =$$
$$= (\mathbf{E}_{2}, \mathbf{E}_{1})$$

where

(8.6)
$$\mathbf{E}_{F}^{t}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega s} \mathbf{E}^{t}(s) ds = \mathbf{E}_{+}^{t}(\omega) + \mathbf{E}_{-}^{t}(\omega).$$

The last relation of (8.5) follows by virtue of the symmetry of the tensor \mathbf{G}_{12} . If quantities defined in frequency space are in the brackets, it is understood that the second form of (8.5) is to be used. The norm of \mathbf{E} is defined by

$$\|\mathbf{E}\|^2 = (\mathbf{E}, \mathbf{E}) \ge 0$$
$$= \|\mathbf{E}_F\|^2 = (\mathbf{E}_F, \mathbf{E}_F).$$

This corresponds to the integral terms in (8.3) and (8.4) if \mathbf{E}^t vanishes on \mathbb{R}^- , or equivalently, if $\mathbf{E}^t_{-}(\omega)$ vanishes. Note that for such a history

(8.7)
$$(\mathbf{T}(t) - \mathbf{G}_0 \mathbf{E}(t)) \cdot \mathbf{E}_a = -2(\mathbf{E}_h, \mathbf{E}^t)$$

for arbitrary $\mathbf{E}_a \in \text{Sym}$, where \mathbf{E}_h is a constant history equal to \mathbf{E}_a and $(\mathbf{E}(t), \mathbf{E}^t)$ is the state resulting in stress $\mathbf{T}(t)^{(2)}$. Its Fourier transform (see (7.5)) is $\mathbf{E}_a(i\omega^-)^{-1}$, which yields (7.7).

Let \mathbf{E}^t be a given history with zero continuation, i.e. $\mathbf{E}^t(s), s \in \mathbb{R}^{--}$ vanishes. Also, let $\mathbf{E}(-\infty) = 0$. We have $\mathbf{E}^t(0^+) = \mathbf{E}(t)$, a specified quantity. Let

$$\mathbf{E}_1^t = \mathbf{E}^t + \mathbf{E}_d^t$$

⁽²⁾The bracket notation for scalar product and state may be distinguished by the fact that, in the latter case, the argument of $\mathbf{E}(t)$ is explicitly included.

where in general $\mathbf{E}_{1}^{t}, \mathbf{E}_{d}^{t}$ are not assumed to vanish on \mathbb{R}^{--} . The constraint

(8.9)
$$\int_{-\infty}^{\infty} \mathbf{G}_2(s-u) \mathbf{E}_d^t(u) du = 0, \quad s \in \mathbb{R}^-$$

is imposed, where the subscript "2" indicates differentiation with respect to u, giving a discontinuous function. It implies that

(8.10)
$$\int_{-\infty}^{\infty} \mathbf{G}_{12}(s-u) \mathbf{E}_d^t(u) du = 0, \quad s \in \mathbb{R}^{--}.$$

Note that we exclude the point zero from this relation. It will be dealt with later, in the light of a further assumption of a discontinuity in \mathbf{E}_d^t . In fact, (8.10) also implies (8.9) on \mathbb{R}^{--} by virtue of the fact that \mathbf{G}_2 vanishes at large times. The variational principle involves seeking a choice of \mathbf{E}_1^t which minimizes $\|\mathbf{E}_1^t\|^2$ under specified variations subject to (8.10). Two cases were considered in [1], corresponding to the minimum and maximum free energy, using a generalisation of the Lagrange multiplier technique

We now show how in general free energies emerge from the above considerations. The discussion will based on the orthogonality condition

(8.11)
$$(\mathbf{E}_d^t, \mathbf{E}_1^t) = 0, \quad \mathbf{E}_d^t = \mathbf{E}_1^t - \mathbf{E}^t$$

from which it follows that

(8.12)
$$\|\mathbf{E}^t\|^2 = \|\mathbf{E}_1^t\|^2 + \|\mathbf{E}_d^t\|^2$$

This orthogonality can be shown to hold for the two cases considered in [1]. It also applies to the solutions that emerge from the more general variational scheme introduced in Section 10.

Let us first state the characteristic properties of an isothermal free energy, provable within a general framework [18], [19], [12]:

P1:

(8.13)
$$\frac{\partial \psi(t)}{\partial \mathbf{E}(t)} = \mathbf{T}(t) \,.$$

P2: Let \mathbf{E}^{\dagger} be a static history equal to \mathbf{E}_0 at all past times. Then

$$\psi(\mathbf{E}^{\dagger})=\phi(\mathbf{E}_{0})$$
 .

where $\phi(\mathbf{E}_0)$ is the elastic free energy defined by (6.9).

P3: For any history \mathbf{E}_a^t

$$\psi(\mathbf{E}_a^t) \ge \phi(\mathbf{E}_a(t))$$
.

P4: Condition (3.3) holds. For ψ differentiable, this will be true if

$$\dot{\psi}(t) = \mathbf{T}(t) \cdot \dot{\mathbf{E}}(t) - D(t)$$

where $D(t) \ge 0$.

The discussion is restricted to differentiable histories and continuations, except at the current time t where finite discontinuities in \mathbf{E}_1^t and \mathbf{E}_m^t must be allowed.

Note that P2 eliminates the freedom of an additive constant in ψ , provided ϕ is taken to be uniquely defined.

PROPOSITION 8.1. The quantity

(8.14)
$$\psi(t) = S(t) + \|\mathbf{E}_1^t\|^2$$

where \mathbf{E}_1^t is defined by (8.8) and constrained by (8.9), (8.11), obeys properties P1-P4 of a free energy if \mathbf{E}_1^t has a finite discontinuity at the origin.

PROOF. Property P1 follows from (8.14) on noting that

$$\frac{\partial S(t)}{\partial \mathbf{E}(t)} = \mathbf{T}(t) \,.$$

We can write (8.14) in the form

(8.15)
$$\psi(t) = \phi(t) + \|\mathbf{E}_1^t - \mathbf{E}_1^\dagger\|^2$$

where \mathbf{E}_1^{\dagger} is the static history that \mathbf{E}_1^t becomes if \mathbf{E}^t is the static history equal to $\mathbf{E}(t)$ at each time [1]. The quantity $\phi(t)$ is the elastic free energy

for strain $\mathbf{E}(t)$. This follows with the aid of (8.7) and (8.10). Note that (8.15) is an explicitly positive form of the free energy. Properties P2, P3 follow immediately.

We may replace $\|\mathbf{E}_1^t\|^2$ by $\|\mathbf{E}^t\|^2 - \|\mathbf{E}_d^t\|^2$ in (8.14) by virtue of (8.12). Differentiating and using the fact that $S(t) + \|\mathbf{E}^t\|^2 = W(t)$ as given by (8.3) is also given by (8.1), we obtain

$$\dot{\psi}(t) = \mathbf{T}(\mathbf{E}^t) \cdot \dot{\mathbf{E}}(t) - D(t)$$
$$D(t) = \frac{d}{dt} \|\mathbf{E}_d^t\|^2$$

so that if P4 is to hold, D(t) must be non-negative. It is convenient to use \mathbf{E}_d rather than \mathbf{E}_d^t at this point, the former quantity having a discontinuity at time t. Thus

$$\|\mathbf{E}_d\|^2 = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{G}_{12}(s-u) \mathbf{E}_d(u) \cdot \mathbf{E}_d(s) du ds$$

and

$$\frac{d}{dt} \|\mathbf{E}_d\|^2 = \int_{-\infty}^{\infty} \mathbf{G}_{12}(t-u) \mathbf{E}_d(u) du \cdot (\mathbf{E}_d(t^-) - \mathbf{E}_d(t^+))$$

where the symmetry of **G** has been used. At s = 0, (8.10) has the form

$$\int_{-\infty}^{\infty} \mathbf{G}_{12}(t-u) \mathbf{E}_d(u) du = \mathbf{G}'(0) (\mathbf{E}_d(t^+) - \mathbf{E}_d(t^-))$$

so that

(8.16)
$$\frac{d}{dt} \|\mathbf{E}_d^t\|^2 = -\mathbf{G}'(0)|\mathbf{E}_d(t^-) - \mathbf{E}_d(t^+)|^2 \ge 0.$$

In particular, if \mathbf{E}_d^t vanishes on \mathbb{R}^{--} then $\mathbf{E}_d(t^+) = \mathbf{E}_d^t(0^-) = 0$.

The connection between the discontinuity in the history at the current time and the rate of dissipation is interesting from a physical point of view.

[23]

9-The discrete spectrum model

In the remaining sections, we derive explicit forms of various free energies associated with a discrete spectrum material. Only the scalar case will be considered.

The stress function T(t) and the current value and strain history $(E(t), E^t)$ are scalars related by

(9.1)
$$T(t) = G(0)E(t) + \int_0^\infty G'(s)E^t(s)ds$$

where G_0 and G' are also scalar quantities. The relaxation function

$$G(t) = G_0 + \int_0^t G'(u) du, \quad G_0 = G(0)$$

is given by the explicit form

$$G(t) = G_{\infty} + \sum_{i=1}^{n} G_i e^{-\alpha_i t}; \quad G_{\infty} = G_0 - \sum_{i=1}^{n} G_i$$

where *n* is a positive integer, the inverse decay times $\alpha_i : \in : \mathbb{R}^+$, i = 1, 2, ..., n and the coefficients G_i are also generally assumed to be positive. Let $\alpha_1 < \alpha_2 < \alpha_3 \ldots$ We have

(9.2)
$$G'(t) = \sum_{i=1}^{n} g_i e^{-\alpha_i t}, \quad g_i = -\alpha_i G_i < 0.$$

The scalar quantity $H(\omega)$ corresponding to (7.2) has the form [5]

(9.3)
$$H(\omega) = H_{\infty} \prod_{i=1}^{n} \left\{ \frac{\gamma_i^2 + \omega^2}{\alpha_i^2 + \omega^2} \right\}$$

where $H_{\infty} = H(\infty)$, defined by the scalar form of (7.3) to be $H_{\infty} = -G'(0) = -\sum_{i=1}^{n} g_i > 0$. In (9.3), $\gamma_1 = 0$ and $(-\gamma_i^2), i = 2, 3, \ldots n$ are the zeros of $H_1(\omega^2) = H(\omega)$ which occur such that $\alpha_1^2 < \gamma_2^2 < \alpha_2^2 < \gamma_3^2 \ldots$

The factorization of H as specified by (9.3) may be established by inspection to be

$$H_{+}(\omega) = h_{\infty} \prod_{i=1}^{n} \left\{ \frac{\omega - i\gamma_{i}}{\omega - i\alpha_{i}} \right\}$$
$$H_{-}(\omega) = h_{\infty} \prod_{i=1}^{n} \left\{ \frac{\omega + i\gamma_{i}}{\omega + i\alpha_{i}} \right\} =$$
$$= \bar{H}_{+}(\omega) = H_{+}(-\omega); \quad h_{\infty} = H_{\infty}^{1/2}$$

In this paper, we consider a much larger class of factorizations of H obtained by interchanging the zeros of H_+ and H_- , but leaving the singularity structure unchanged. There are $N = 2^{n-1}$ distinct factorizations of this kind which we distinguish by the label f = 0, 1, 2, ... N. The case f = 0 is where no zeros are interchanged and f = N where all zeros are interchanged. These can be written as

(9.4)

$$H(\omega) = H_{+}^{f}(\omega)H_{-}^{f}(\omega)$$

$$H_{+}^{f}(\omega) = h_{\infty}\prod_{i=1}^{n} \left\{\frac{\omega - i\rho_{i}}{\omega - i\alpha_{i}}\right\}$$

$$H_{-}^{f}(\omega) = h_{\infty}\prod_{i=1}^{n} \left\{\frac{\omega + i\rho_{i}}{\omega + \alpha_{i}}\right\} =$$

$$= \bar{H}_{+}^{f}(\omega) = H_{+}^{f}(-\omega)$$

$$\rho_{i} = \varepsilon_{i}\gamma_{i}, \quad \varepsilon_{1} = 1, \quad \varepsilon_{i} = \pm 1, \quad i = 2, 3, \dots n.$$

The superscript f is omitted on ρ_i and is to be understood from context. Most of the relations derived in [5] do not depend on the location of the zeros of H_+ and H_- , but do depend crucially on the location of the singularities. We note here certain results to be used later which can be proved in a manner identical to that given in [5].

The quantity

(9.5)
$$Q^{(ft)}(\omega) = H^f_{-}(\omega)E^t_{+}(\omega) = q^{(ft)}_{-}(\omega) - q^{(ft)}_{+}(\omega)$$

where $q_{-}^{(ft)}(\omega)$ is analytic in Ω^+ , going to zero at large ω as ω^{-1} , while $q_{+}^{(ft)}(\omega)$ is analytic in Ω^- with similar large ω behaviour. They are given

by the limit $z \to \omega \in \mathbb{R}$ of

(9.6)
$$q^{(ft)}(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{Q^{(ft)}(\omega)}{\omega - z} d\omega$$

from above and below the real axis respectively. The analyticity of these quantities on \mathbb{R} follows from the assumed analyticity of G'_F and E^t_+ on \mathbb{R} [5]. They are defined over the entire complex plane by analytic continuation.

It can be shown that [5]

(9.7)
$$\frac{d}{dt}q_{+}^{(ft)}(\omega) = -i\omega q_{+}^{(ft)}(\omega) - K_{f}(t)$$
$$\frac{d}{dt}q_{-}^{(ft)}(\omega) = -i\omega q_{-}^{(ft)}(\omega) - K_{f}(t) + H_{-}^{f}(\omega)E(t)$$
$$K_{f}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} H_{-}^{f}(\omega) \Big[E_{+}^{t}(\omega) - \frac{E(t)}{i\omega^{-}} \Big] d\omega$$

using the notation of (7.5). Also

(9.8)
$$\frac{1}{2\pi} \int_{-\infty}^{\infty} q_{+}^{(ft)}(-\omega) d\omega = -\frac{1}{2} K_f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} q_{+}^{(ft)}(\omega) d\omega \frac{1}{2\pi} \int_{-\infty}^{\infty} q_{-}^{(ft)}(-\omega) d\omega = \frac{1}{2} (K_f(t) - h_{\infty} E(t)) = \frac{1}{2\pi} \int_{-\infty}^{\infty} q_{-}^{(ft)}(\omega) d\omega.$$

We also consider a generalization of (9.5) where the strain is defined over \mathbb{R} , with Fourier transforms given by (8.6). With a view to future applications, the relevant relations will be written for E_d^t , the scalar version of the quantity introduced in (8.8):

(9.9)
$$U^{(ft)}(\omega) = H^{f}_{-}(\omega)E^{t}_{dF}(\omega) = H^{f}_{-}(\omega)(E^{t}_{d+}(\omega) + E^{t}_{d-}(\omega)) = u^{(ft)}_{-}(\omega) - u^{(ft)}_{+}(\omega)$$

where

(9.10)
$$u_{\pm}^{(ft)}(\omega) = \lim_{z \to \omega^{\mp}} u^{(ft)}(z)$$
$$u^{(ft)}(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{U^{(ft)}(\omega)}{\omega - z} d\omega$$

The quantities $u_{\pm}^{(ft)}$ have the same analyticity properties as $q_{\pm}^{(ft)}$. It is clear that

(9.11)
$$\begin{aligned} u_{-}^{(ft)}(\omega) &= q_{d-}^{(ft)} + H_{-}^{f}(\omega)E_{d-}^{t}(\omega) = q_{d+}^{(ft)} + H_{-}^{f}(\omega)E_{dF}^{t}(\omega) \\ u_{+}^{(ft)}(\omega) &= q_{d+}^{(ft)} \end{aligned}$$

where $q_{d\pm}^{(ft)}$ are defined by (9.5) and (9.6) with $E_{d\pm}^t$ replacing E_{\pm}^t .

We will now state a result, proved in [1], which is not confined to a discrete spectrum material. It relies upon the fact that $H(\omega)$ is factorizable into quantities analytic on Ω^+ and Ω^- , with zeros that may be interchanged. Analyticity excludes non-isolated as well as isolated singularities, of course. It relies also on the analyticity of the various quantities on the real axis

PROPOSITION 9.1. The strain history and continuation E_d^t obeys (8.9) if $u_{-}^{(ft)}$ vanishes. Relation (8.9) implies that $u_{-}^{(ft)}$ vanishes in two cases: (i) where no exchange of zeros in H_{\pm} takes place (f = 0); and (ii) where E_{d-}^t vanishes.

The first case (f = 0) corresponds to the minimum free energy, while case (ii) corresponds to the maximum free energy (f = N). In fact we see from (9.11) that E_{d-}^t vanishing yields $q_{d-}^{(Nt)} = 0$ so that Proposition 9.1 is stating that condition (8.9) implies that $q_{d-}^{(Nt)}$ vanishes. Recalling that (8.9) in this case is the condition for equivalence of states E_1^t and E^t , we conclude that $q_{1-}^{(Nt)}$ defined by (9.5), for a given history E_1^t , is a state variable on the space of minimal states Σ_R .

In Section 10, we shall adopt the condition $u_{-}^{(\tilde{f}t)} = 0$ as the constraint on our variational scheme in all cases, not just in the two described in Proposition 9.1. This condition implies (8.9) but is a stronger assumption in general (except in the two cases), which is in effect the content of Proposition 9.1.

It is proved in [6], for general materials and in the full tensorial case, that (stated for scalars) $q_{-}^{(ft)}$ is a state variable for f = 0. The argument used in that reference can easily be extended to all f. Thus, we state

COROLLARY 9.2. The quantity $q_{-}^{(ft)}$ is a function of state for all permutations f.

An implication of this result is that all the free energies given in the following sections are functions of state. If $q_{-}^{(ft)}$ is a function of state, then in general $q_{+}^{(ft)} = q_{-}^{(ft)} - H_{-}^{f}E_{+}^{t}$ will not be, because of the occurance of the transformed history.

It is convenient to introduce a conventional scalar product

(9.12)
$$\langle f,g\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{f}(\omega)g(\omega)d\omega$$

as well as (8.5). Observe that f and g are orthogonal in this scalar product if f is analytic in Ω^+ and g in Ω^- or vica versa and both vanish at infinity at least as strongly as ω^{-1} . We write

$$\langle f, f \rangle = \|f\|_L$$

indicating the Lesbeque L^2 norm.

10 – A family of free energies in Σ_R

We will now derive an expression for a free energy corresponding to each permutation f and a given state $\sigma = (E(t), E^t)$, which are functionals only of the equivalence class σ_R rather than σ . This family includes the minimum free energy derived in [5], a maximum free energy defined on Σ_R and intermediate functionals. No clear ordering emerges from the general treatment. However, in Section 11, we present explicit forms for these free energies and establish a partial ordering within the family.

These developments are the frequency domain generalization of the theory presented in Section 8. In frequency space, we shall see that it is possible to obtain explicit results with relative ease.

The following constrained optimization problem is considered. For a given state $(E(t), E^t)$, we seek E_d^t which minimizes $||E_1^t||^2$, where $E_1^t = E^t + E_d^t$, subject not to (8.9) but to the stronger condition (except in two cases; see Proposition 9.1)

(10.1)
$$u_{-}^{(ft)}(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{H_{-}^{f}(\omega') E_{dF}^{t}(\omega')}{\omega' - \omega^{+}} d\omega' = 0.$$

Note that in general E_1^t, E_d^t are defined on IR. It follows from (9.11) that

(10.2)
$$E_{dF}^{t}(\omega) = -\frac{q_{d+}^{(ft)}(\omega)}{H_{-}^{f}(\omega)} = -\frac{1}{2\pi i H_{-}^{f}(\omega)} \int_{-\infty}^{\infty} \frac{H_{-}^{f}(\omega') E_{dF}^{t}(\omega')}{\omega' - \omega^{-}} d\omega'.$$

Using the factorization (9.4), we see that the quantity to be minimized has the form

$$M(t) = \|H_{-}^{f}(E_{+}^{t} + E_{dF}^{t})\|_{L}^{2}.$$

Now

(10.3)
$$U^{(ft)}(\omega) = H^{f}_{-}(\omega)E^{t}_{dF}(\omega) = -u^{(ft)}_{+}(\omega)$$

by virtue of (10.1). Using (9.5), we see that

(10.4)
$$M(t) = \|q_{-}^{(ft)} - q_{+}^{(ft)} - u_{+}^{(ft)}\|_{L}^{2}.$$

Let us vary $u_{+}^{(ft)}(\omega)$, replacing it by $u_{+}^{(ft)}(\omega) + k(\omega)$ where $k(\omega)$ is arbitrary except for the constraint that it has the same analytic structure as $u_{+}^{(ft)}(\omega)$ - namely that it is analytic in Ω^{-} and goes to zero at infinity as ω^{-1} . The minimization condition is

$$\langle k, q_{-}^{(ft)} - q_{+}^{(ft)} - u_{+}^{(ft)} \rangle = 0$$

for all allowable k. The $q_{-}^{(ft)}$ term drops out by virtue of the comment after (9.12). Application of the corresponding argument in [5] yields that $u_{+}^{(ft)} = -q_{+}^{(ft)}$ or from (9.5), (9.6) and (10.3)

(10.5)
$$E_{dF}^{(ft)}(\omega) = \frac{q_{+}^{(ft)}(\omega)}{H_{-}^{f}(\omega)} = \frac{1}{2\pi i H_{-}^{f}(\omega)} \int_{-\infty}^{\infty} \frac{H_{-}^{f}(\omega') E_{+}^{t}(\omega')}{\omega' - \omega^{-}} d\omega' = E_{dm}^{(ft)}(\omega)$$

which is the optimal choice. From (10.2) it follows that

$$q_{1+}^{(ft)}(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{H_{-}^{f}(\omega') E_{1}^{t}(\omega')}{\omega' - \omega^{-}} d\omega' = 0.$$

The resulting free energy follows by inserting (10.5) (in the form $u_{+}^{(ft)} = -q_{+}^{(ft)}$) into (10.4) and recalling (8.14):

(10.6)
$$\psi_f(t) = S(t) + \|q_-^{(ft)}\|_L^2 = S(t) + \|E_f^t\|^2$$

where E_f^t is the optimal choice of E_1^t (denoted by E_{fo}^t in this context), here given by

(10.7)
$$E_{f}^{t}(\omega) = \frac{q_{-}^{(ft)}(\omega)}{H_{-}^{f}(\omega)} = \frac{1}{2\pi i H_{-}^{f}(\omega)} \int_{-\infty}^{\infty} \frac{H_{-}^{(f)}(\omega') E_{+}^{t}(\omega')}{\omega' - \omega^{+}} d\omega'.$$

We write

(10.8)
$$E_f^t(\omega) = E_{f+}^t(\omega) + E_{f-}^t(\omega)$$

where $E_{f+}^t(\omega)$ is analytic in Ω^- and corresponds to a history before time t, while $E_{f-}^t(\omega)$ is analytic in Ω^+ and corresponds to a continuation after time t.

If the zeros in H_{-}^{f} are not permuted (f = 0) then E_{f+}^{t} vanishes. This case is readily identified as the minimum free energy derived in [5] with E_{f}^{t} identified as the negative of the optimal continuation given in that paper. If all the zeros are permuted (f = N) then E_{f-}^{t} vanishes [1], corresponding to the maximum free energy. If some zeros are permuted, we have an intermediate situation where neither E_{f+}^{t} nor E_{f-}^{t} vanish.

For a static history (see (7.5)), $E_{+}^{t}(\omega) = E_{s}^{t}(\omega) = E(t)/(i\omega)$, we have from (10.7), closing on $\Omega^{(+)}$, that [5]

(10.9)
$$E_{fs}^t(\omega) = \frac{E(t)}{i\omega}$$

One can write (10.6) in the form (see (8.15))

(10.10)
$$\psi_f(t) = \phi(t) + \|E_f^t - E_{fs}^t\|^2$$

on using the scalar form of relation (8.7) and

$$(l, E_{+}^{t} - E_{f}^{t}) = \frac{1}{2} \langle h, q_{+}^{(ft)} \rangle = 0; \quad h = 2i \frac{H_{-}^{(f)}(\omega)}{\omega}$$

where $l = 1/i\omega$. The orthogonality follows from the remark after (9.12).

It is clear that properties P1-P3 of a free energy follow from (10.6) and (10.10). All that remains is to show that

(10.11)
$$T(t)\dot{E}(t) = \dot{W}(t) = \dot{\psi}_f(t) + D_f(t); \quad D_f(t) \ge 0.$$

Using (9.5) and the scalar form of (8.4), we can write

(10.12)
$$W(t) = S(t) + \|q_{-}^{(ft)} - q_{+}^{(ft)}\|_{L}^{2} = S(t) + \|q_{-}^{(ft)}\|_{L}^{2} + \|q_{+}^{(ft)}\|_{L}^{2}$$

where the orthogonality of $q_{-}^{(ft)}$, $q_{+}^{(ft)}$ follows from the remark after (9.12). We note in passing here that this orthogonality is that expressed by (8.11) as may be seen from (10.5) and (10.7). Comparing (10.11) and (10.12), we see with the help of (10.6) that

(10.13)
$$D_f(t) = \frac{d}{dt} ||q_+^{(ft)}||^2 = K_f^2(t)$$
$$K_f(t) = \langle H_+^{(f)}, E_+^t - E_s^t \rangle$$

where E_s^t is the static history $E(t)/(i\omega)$. We have used (9.7) and (9.8) in writing (10.13). The quantity K_f is real and D_f is clearly non-negative.

It is shown in [1] that the time domain history and continuation with minimum norm are in general non-zero for large positive and negative times and have a discontinuity at time t. The magnitude of this discontinuity is related to (10.13) in such a manner as to give agreement with (8.16). In intermediate cases, the history and continuation are arbitrary to within an additive constant. This freedom allows us to make a particular choice of E_{fs}^t in (10.10), as pointed out after (8.15).

Finally, observe that (10.10) can be written in the form

$$\psi_f(t) = \phi(t) + \|p_f\|_L^2$$

$$p_f(\omega) = q_-^{(ft)}(\omega) - \frac{H_-^f(\omega)E(t)}{i\omega}.$$

It now manifestly depends only on the couple $(E(t), q_{-}^{(ft)})$ and is therefore a state variable.

11 – Explicit forms

Detailed expressions for these free energies are now presented, in terms of the viscoelastic parameters of the discrete spectrum model. Also, a ranking will be given among subsequences of these forms. It is furthermore pointed out that linear combinations of the free energy, with positivity restrictions on the coefficients, are also free energies. The results quoted are obtained as described in [5] with minor modifications.

The quantities $q_{\pm}^{(ft)}(\omega)$ defined by (9.5) and (9.6) have the form

$$q_{-}^{(ft)}(\omega) = ih_{\infty} \sum_{i=1}^{n} \frac{R_{i}^{f} E_{+}^{t}(-i\alpha_{i})}{\omega + i\alpha_{i}}$$

$$q_{+}^{(ft)}(\omega) = q_{-}^{(ft)}(\omega) - H_{-}^{f}(\omega) E_{+}^{t}(\omega) =$$

$$= ih_{\infty} \sum_{i=1}^{n} \frac{R_{i}^{f} [E_{+}^{t}(-i\alpha_{i}) - E_{+}^{t}(\omega)]}{\omega + i\alpha_{i}} - h_{\infty} E_{+}^{t}(\omega)$$

$$R_{i}^{f} = (\rho_{i} - \alpha_{i}) \prod_{\substack{j=1\\ j \neq i}}^{n} \left\{ \frac{\rho_{j} - \alpha_{i}}{\alpha_{j} - \alpha_{i}} \right\}$$

where the ρ_i are defined in (9.4). Explicit expressions may also be given for the optimal histories/continuations [1].

The quantity $K_f(t)$, given by (9.7), has the form

(11.2)
$$K_f(t) = -h_\infty \sum_{i=1}^n \frac{R_i^f}{\alpha_i} e_i(t)$$

where $e_i(t) = E(t) - \alpha_i E_+^t(-i\alpha_i)$.

Using (11.1), we find that the free energy $\psi_f(t)$, given by (10.6), has the form [5]

$$\begin{split} \psi_f(t) &= S(t) + H_{\infty} \sum_{i,j=1}^n \frac{R_i^f R_j^f}{\alpha_i + \alpha_j} E_+^t (-i\alpha_i) E_+^t (-i\alpha_j) = \\ &= S(t) + \frac{1}{2} \int_0^\infty ds_1 \int_0^\infty ds_2 E^t(s_1) F_f(s_1, s_2) E^t(s_2) \\ F_f(s_1, s_2) &= 2H_{\infty} \sum_{i,j=1}^n \frac{R_i^f R_j^f}{\alpha_i + \alpha_j} e^{-\alpha_i s_1 - \alpha_j s_2} \,. \end{split}$$

A particular ranking among the free energies was established in [1]. Start from the minimum energy $\psi_m(t)$ which corresponds to $\varepsilon_i = 1, i = 1, 2, \ldots n$. Interchanging a zero $\gamma_l, l \neq 1$ and denoting the resulting free energy by $\psi^{(1)}(t)$, it can be shown that

$$\psi^{(1)}(t) \ge \psi^{(0)}(t)$$
.

If another zero is interchanged, one can show by the same argument that $\psi^{(2)}(t) \geq \psi^{(1)}(t)$ and so on. There are (n-1)! pathways starting with $\psi_m(t)$ and ending with $\psi^{(M)}(t)$ with all zeros interchanged, where, on each step, a zero untouched in previous steps, is interchanged. Along a particular pathway, we have

(11.3)
$$\psi^{(M)}(t) = \psi^{(n)}(t) \ge \psi^{(n-1)}(t) \ge \dots \ge \psi^{(1)}(t) \ge \psi^{(0)}(t) = \psi_m(t)$$
.

The superscripts n, n - 1 etc. will have quite different meanings on different pathways. The minimum and maximum free energies in each sequence (11.3) are unique however. Thus, $\psi_m, \psi^{(M)}$ are respectively the minimum and maximum free energies corresponding to the element $\sigma_R \in \Sigma_R$ defined by $(E(t), E^t)$.

The dissipation function corresponding to $\psi_f(t)$ is given by

(11.4)
$$D_f(t) = K_f^2(t)$$

where $K_f(t)$ is defined by (11.2).

The N free energies defined by different factorizations are all in the set S_{σ} of free energies associated with the equivalence class σ_R . They are in fact on the boundary of this convex set, in a sense that is discussed in [1]. The convexity of S_{σ} means that we can form a family of free energies given by

$$\psi(t) = \sum_{f} a_f^2 \psi^f(t), \qquad \sum_{f} a_f^2 = 1$$

where the sum is in general over all 2^{n-1} factorizations and each a_f can take all real values. Clearly $\psi_m(t) \leq \psi(t) \leq \psi^{(M)}(t)$.

For n = 1, the set S_{σ} reduces to a singleton - as demonstrated for a very general exponential form in [14]. For n = 2, the range of allowable

free energies can be determined by elementary considerations. This was done by Breuer and ONAT [20].

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