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GENERAL DISSIPATIVE MATERIALS FOR SIMPLE HISTORIES

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ABSTRACT. A material with memory typically has a set of many free energy functionals associated with it, all members of which yield the same constitutive relations. An alternative interpretation of this set is explored in the present work.

Explicit formulae are derived for the free energy and total dissipation of an arbitrary material in the cases of step function and sinusoidal/exponential histories. Expressions for the fraction of stored and dissipated energy are deduced. Also, various formulae are given for discrete spectrum materials.

For materials with relaxation function containing one decaying exponential, the associated Day functional is the physical free energy. For more general materials, we seek a best fit of the relaxation function with one decaying exponential to that chosen for the general case. The free energy, total dissipation and fractions of stored and dissipated energies relating to the Day material are derived for the various histories. Similar data, in the case of the general material, are explored for the minimum and maximum free energies and also for a centrally located free energy given in the literature. Various plots of aspects of this data, including comparisons between the behaviour for general and Day materials, are presented and discussed.

1. INTRODUCTION.

In this work, we consider completely linear materials with memory, where the stress is given by a linear functional of strain¹. For such materials, free energies and associated rates of dissipation are quadratic functionals of strain characterized by

¹We consider for definiteness here isothermal mechanical problems, indeed those for solid viscoelastic materials. Also, only the scalar case is considered, which simplifies the algebra and allows us to focus on the essential structure of the arguments. It must be emphasized however that similar results can be given with little extra difficulty, for viscoelastic fluids, certain non-isothermal problems, electromagnetism, non-simple materials etc. as presented in the references noted above, and also for the general tensor cases relating to all these materials. Indeed, it is shown in [2], page 135 how tensor equations correspond to a series of scalar relations in each eigenspace of the tensor relaxation function.

kernels defined on $\mathbb{R}^+ \times \mathbb{R}^+$. Various results for classical free energy functionals of this kind are presented in [7, 8]. Developments over the last two decades relating to free energies for these materials may be found in for example [17, 9, 12, 13, 18, 10, 19, 2, 1, 20, 21, 22]. These deal mainly with the minimum, maximum and other extremal free energies. An exception is the free energy proposed in [10] (see also [2, 21]) and denoted by $\psi_F(t)$. Numerical examples are included in [3, 23] and the present work.

Let us identify a particular material with memory, which will be referred to as material I. It is assumed to exhibit linear behaviour. The stress-strain relation of this material is known, in other words, its relaxation function is given. There are generally many free energies and corresponding dissipation functionals associated with material I. All of these generate the same stress and therefore have the same relaxation function. They form a convex set with a minimum and a maximum element ([11] for example). We denote this set by \mathcal{F} , which is of course dependent on the choice of strain history. The physical free energy for material I, yielding the observed rate of dissipation, is a member of \mathcal{F} , as well as all free energies with the given stress.

Remark 1.1. In recent papers [20, 22], it was shown that any material with memory can be uniquely characterized by specifying the kernel of its physical rate of dissipation functional. This quantity determines the relaxation function, which in turn yields the stress-strain or constitutive relation, for a given strain history. The work function can be deduced from these quantities. However, the dissipation kernel determines also the amount of dissipation under deformation, and indeed the associated free energy. We will consider the set of all such kernels associated with materials with a specified constitutive relation; this set will be denoted by \mathcal{K} . For a given choice of strain history, \mathcal{K} generates a set of free energies \mathcal{F} , corresponding to our chosen constitutive relation. It will emerge that the boundaries of \mathcal{K} and \mathcal{F} are at least roughly determined by the relaxation function of the constitutive relation.

The following alternative viewpoint will be discussed in the present work. We interpret the set of kernels \mathcal{K} as specifying all the distinct linear materials with the same constitutive relation but different dissipation rates as a result of deformation. These can be labeled by individual members of \mathcal{K} . One of them yields the physical free energy in \mathcal{F} for material I. Other members of \mathcal{F} would traditionally be regarded as approximations to or bounds on (notably the minimum and maximum free energy) this physical free energy. Instead, we now regard these, or more specifically the corresponding kernels in \mathcal{K} , as describing different actual materials with the same constitutive relation, but different dissipation properties. For the material labeled by a particular kernel, the relevant member of \mathcal{F} for a given strain history is the physical free energy for that material. Particular examples may not currently exist as real materials but it seems reasonable to assume that they could be manufactured, to a close approximation, now or in the future.

It is not a new prediction that materials with a particular constitutive relation may have different rates of dissipation, but it is interesting to see how it emerges in this way.

Both of the above viewpoints are valid and can be adopted as context demands. We will refer to the more traditional viewpoint, where \mathcal{K} is the set of kernels producing the physical free energy of material I as well as approximations to and bounds on this quantity, as Interpretation 1 or II. The viewpoint that each $K(s, u) \in \mathcal{K}$

fully describes a separate material, each equally of interest, will be referred to as I2.

Under I2, the set \mathcal{K} is defined not by the choice of material I but by the constitutive equation of the materials. If we replace material I by another material with the same stress-strain relation, the set \mathcal{K} remains unchanged. We do not focus on one specific example but rather treat all materials labeled by members of \mathcal{K} on an equal footing.

Free energy functionals, generalized to three dimensions, are useful in defining the topology of the space of states, when studying stability and related problems for the integro-differential equations describing the evolution of materials with memory (for example [14]); these evolution equations are of course derived from the constitutive equations of the material.

Another use for free energies is in modeling dissipation of energy in a material with memory, for example material I. To do this accurately requires knowledge of the physical rate of dissipation kernel which may be difficult to determine. This in turn yields the physical free energy kernel of material I and a complete description of the thermodynamic behaviour of this material under load.

Even without exact knowledge of thermodynamic behaviour, we can explore the dissipation behaviour for the minimum and maximum free energies, together with a centrally (in \mathcal{F}) located functional [18, 2] (referred to below as the central free energy). Detailed formulae for these free energies are given, with corresponding total (and rate of) dissipation and the work function, for step function and sinusoidal/exponential (abbreviated to SE) histories. This latter category includes semi-infinite sinusoidal/exponential (abbreviated to SSE) histories and SE histories, where the strain vanishes for $t < 0$. Also, fractions of stored and dissipated energies are defined and discussed. Various relevant quantities are plotted.

As noted earlier, the minimum and maximum free energies together with associated total dissipations provide bounds on energy storage and dissipation in material I. They are also descriptive of valid materials in their own right, according to viewpoint I2 outlined in remark 1.1.

For semi-infinite sinusoidal histories, the work function and the total dissipation are infinite, while the free energy and rate of dissipation are finite. It is therefore not possible to give fractions of stored and dissipated energies in this case. However, free energy and rate of dissipation formulae are given for general rate of dissipation kernels. These are compared with previously obtained results for specific kernels.

Remark 1.2. We will deal only with free energies that are functionals of the minimal state, as defined in [2], page 151 and in many other papers, most recently [20, 21, 22, 23].

The Day free energy for a discrete spectrum material with one decay time is the only free energy that is a functional of the minimal state. It is therefore the unique physical free energy for that material. This quantity and the associated dissipation are explored for a choice of relaxation function approximately equal to that for the more general set of materials under consideration.

Regarding the notational convention for referring to equations, we adopt the following rule. A group of relations with a single equation number (***) will be individually labeled by counting “=” signs or “<”, “>”, “≥” and “≤”. Thus, (***)₅ refers to the fifth “=” sign, if all the relations are equalities. Relations with “∈” are ignored for this purpose.

For notational conventions in general and for many basic results, we refer to [2] and indeed to a variety of other publications, such as [18, 20, 21]. Such basic formulae and many derivations of results are omitted here.

The numerical work was carried out using mainly Matlab R2015b; one aspect involved the use of Maple 2017.

2. STRAIN HISTORY, STRESS AND FREE ENERGIES

The current value of the strain function is $E(t)$ while the strain history and relative history are given by

$$E^t(s) = E(t-s), \quad E_r^t(s) = E^t(s) - E(t), \quad s \in \mathbb{R}^+, \quad (2.1)$$

where \mathbb{R} is the real line, while \mathbb{R}^+ is $[0, \infty)$. It is generally assumed here that

$$\lim_{s \rightarrow \infty} E^t(s) = \lim_{u \rightarrow -\infty} E(u) = 0, \quad (2.2)$$

which simplifies certain formulae. However, for strictly sinusoidal histories, relation (2.2) does not hold.

There are generally three equivalent forms of the constitutive equations and free energy/rate of dissipation functionals (for example, [20, 21]). We shall confine ourselves to one of these here.

Let $T(t) = \tilde{T}(E^t, E(t))$ be the stress at time t , where \tilde{T} is understood to be a functional of E^t and a function of $E(t)$. Then the constitutive relation with a linear memory term has the form

$$\begin{aligned} T(t) &= G_\infty E(t) + \int_0^\infty \tilde{G}(u) \dot{E}^t(u) du, \\ \tilde{G}(u) &= G(u) - G_\infty, \quad \dot{E}^t(u) = \frac{\partial}{\partial t} E^t(u), \end{aligned} \quad (2.3)$$

where the quantity $G(\cdot) : \mathbb{R}^+ \mapsto \mathbb{R}^+$ is the relaxation function of the material. The functional dependence on \dot{E}^t is easily transformed into a dependence on E^t with the aid of an integration by parts. We have

$$G_\infty = G(\infty), \quad G_0 = G(0), \quad G_0 - G_\infty > 0. \quad (2.4)$$

The assumption is made that

$$\tilde{G}(\cdot) \in L^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+), \quad (2.5)$$

which will be relevant in the context of taking Fourier transforms.

For linear materials, the constitutive relation is characterized by the relaxation function $G(u)$.

A free energy at time t is denoted by $\psi(t) = \tilde{\psi}(E^t, E(t)) \in \mathcal{F}$, where $\tilde{\psi}$, as for \tilde{T} above, is a functional of E^t and a function of $E(t)$. The basic properties of free energies [4, 25] are given as follows. All required derivatives of $\tilde{\psi}(E^t, E(t))$ are assumed to exist. The relation

$$\frac{\partial}{\partial E(t)} \tilde{\psi}(E^t, E(t)) = \frac{\partial}{\partial E(t)} \psi(t) = T(t) \quad (2.6)$$

must hold for all $\psi(t) \in \mathcal{F}$. For linear materials, this is the constitutive relation (2.3), which, as we shall see, at least roughly determines the boundary of \mathcal{F} . For any history E^t ,

$$\tilde{\psi}(E^t, E(t)) \geq \tilde{\phi}(E(t)) \quad \text{or} \quad \psi(t) \geq \phi(t), \quad (2.7)$$

where $\phi(t)$ is the equilibrium value of the free energy $\psi(t)$ which, for a completely linear material, is given by

$$\tilde{\phi}(E(t)) = \frac{1}{2}G_\infty E^2(t). \quad (2.8)$$

For any $(E^t, E(t))$ we have the first law (balance of energy)

$$\dot{\psi}(t) + D(t) = T(t)\dot{E}(t), \quad D(t) \geq 0, \quad (2.9)$$

where $D(t)$ is the rate of dissipation of energy associated with $\psi(t)$. This non-negativity requirement on $D(t)$ is an expression of the second law.

Integrating (2.9) over $(-\infty, t]$ yields that

$$\psi(t) + \mathcal{D}(t) = W(t), \quad \mathcal{D}(t) \geq 0, \quad (2.10)$$

where

$$W(t) = \int_{-\infty}^t T(u)\dot{E}(u)du, \quad \mathcal{D}(t) = \int_{-\infty}^t D(u)du \geq 0. \quad (2.11)$$

We assume that these integrals are finite, except for purely periodic histories. The quantity $W(t)$ is the work function, while $\mathcal{D}(t)$ is the total dissipation resulting from the entire history of deformation of the body. Note that $\dot{\mathcal{D}}(t) = D(t)$.

Under I2 defined in remark 1.1, the functional $\psi(t) \in \mathcal{F}$ is the physical free energy for a particular material with a physically observed rate of dissipation $D(t)$ and constitutive relation given by (2.6) or (2.3).

The fraction of energy stored and dissipated, respectively, for any given history, can be determined from (2.10), according to the formulae

$$F_s(t) = \frac{\psi(t)}{W(t)}, \quad F_d(t) = \frac{\mathcal{D}(t)}{W(t)}, \quad F_s(t) + F_d(t) = 1. \quad (2.12)$$

Remark 2.1. The implied description of a free energy for the material as a measure of the stored energy is a convenient intuitive shorthand, which will be used in this work. However, there are various complexities surrounding this issue. For one thing, any stored energy in the material can be only partially transformed into useful work, since in particular the deformation necessary for this transformation will itself generate dissipation.

Also, there is the more general question regarding whether the definition of the free energy functional for a given history justifies this identification with stored energy. A particular choice of free energy is in general intermediate between the minimum and the maximum free energies for the material, or equal to one or other of these quantities (see remark 1.1, relating to I1). Now, the minimum free energy at time t is defined as the maximum recoverable work from that time, while the maximum free energy at time t is the minimum work required to achieve this state from the initial state, obtained by searching among histories in the same minimal state as the given history ([5, 2], for example). Both of these are related to stored energy but are, in the case of dissipative materials, quite different from each other. Intermediate free energy functionals are linear combinations of these and other functionals, as we shall see later. Thus, a clear, simple definition is not generally available in every case, though our characterization of such functionals as energy storage measures has validity.

Remark 2.2. The variation of $\psi(t)$, $\mathcal{D}(t)$ and the ratios in (2.12) over time is of interest. It would be useful also to pick a particular time, for example, $t \rightarrow \infty$, or average over times, in the case of oscillatory behaviour, yielding constant quantities

which characterize storage and dissipation occurring in the material. Such quantities will be determined where possible.

3. THE GENERAL FORM OF A FREE ENERGY FUNCTIONAL

For a scalar theory with a linear memory constitutive relation for the stress, the most general form of a free energy is

$$\psi(t) = \phi(t) + \frac{1}{2} \int_0^\infty \int_0^\infty \dot{E}^t(s) \tilde{G}(s, u) \dot{E}^t(u) ds du \in \mathcal{F}, \quad (3.1)$$

$$\tilde{G}(s, u) = G(s, u) - G_\infty, \quad G_\infty = G(\infty, u) = G(s, \infty), \quad s, u \in \mathbb{R}^+.$$

The kernel $\tilde{G}(s, u)$ must be such that the integral term in (3.1) is non-negative. The relaxation function $G(u)$, introduced in (2.3), is given by

$$G(u) = G(0, u) = G(u, 0) \quad \forall u \in \mathbb{R}^+. \quad (3.2)$$

It follows from (2.4) and (3.2) that

$$G_0 = G(0) = G(0, 0), \quad (3.3)$$

and also that G_∞ in (2.4) and (3.1)₃ are the same quantity. There is no loss of generality in taking

$$\tilde{G}(s, u) = \tilde{G}(u, s). \quad (3.4)$$

The set of all $\tilde{G}(s, u)$ with the non-negativity property will be denoted by \mathcal{G} . The rate of dissipation can be deduced from (2.9) to be

$$D(t) = -\frac{1}{2} \int_0^\infty \int_0^\infty \dot{E}^t(s) K(s, u) \dot{E}^t(u) ds du, \quad (3.5)$$

where

$$K(s, u) = G_1(s, u) + G_2(s, u) \in \mathcal{K}. \quad (3.6)$$

The integral in (3.5) must be non-positive. This requirement on $K(\cdot, \cdot)$ is central to the definition of the set \mathcal{K} . It can be assured, for example, by adopting sums of products forms for the kernel, as in [20]. For any given $\tilde{G}(s, u) \in \mathcal{G}$, relation (3.6) is a mapping $\mathcal{G} \mapsto \mathcal{K}$.

The quantity $K(s, u)$ is defined on $\mathbb{R}^+ \times \mathbb{R}^+$. It can also be taken to be symmetric in its arguments, just as in (3.4). The non-negativity requirements on \tilde{G} , $-K$ imply in particular that ([2], page 127)

$$\tilde{G}(s, s) \geq 0, \quad K(s, s) \leq 0, \quad s \in \mathbb{R}^+. \quad (3.7)$$

The assumption is made that (cf. (2.5))

$$\tilde{G}(\cdot, \cdot), K(\cdot, \cdot) \in L^1(\mathbb{R}^+ \times \mathbb{R}^+) \cap L^2(\mathbb{R}^+ \times \mathbb{R}^+) \quad (3.8)$$

which will also be relevant in the context of taking the Fourier transform of these quantities.

The work function, given by (2.11)₁, can be expressed as ([2], page 153 and earlier references cited therein):

$$W(t) = \phi(t) + \frac{1}{2} \int_0^\infty \int_0^\infty \dot{E}^t(s) \tilde{G}(|s - u|) \dot{E}^t(u) ds du. \quad (3.9)$$

We see that it can be cast in the form (3.1) by putting $\tilde{G}(s, u) = \tilde{G}(|s - u|)$. The quantity $W(t)$ has some but not all the properties [23] of a free energy, though with

zero dissipation, which is clear from (2.10). It also follows from (2.10), for any free energy $\psi(t)$, that

$$\psi(t) \leq W(t). \quad (3.10)$$

It is shown in [20, 22] that the material can be uniquely characterized by choosing the correct physical kernel $K(s, u)$, yielding a non-negative rate of dissipation. This may be achieved either by experimental measurement or by appealing to a theoretical model, or perhaps a combination of both approaches. Thus, $K(s, u)$ is the fundamental quantity determining a particular material. The set of all such kernels \mathcal{K} will generate a set of free energies \mathcal{F} for each choice of strain history.

A free energy functional of the form (3.1) with the correct non-negativity properties is uniquely generated by the kernel

$$\tilde{G}(s, u) = - \int_0^\infty K(z + s, z + u) dz, \quad (3.11)$$

which is a mapping $\mathcal{K} \mapsto \mathcal{G}$. Relation (3.2) gives

$$G(s) = G(s, 0) = G_\infty - \int_0^\infty K(z + s, z) dz = G_\infty - \int_0^\infty K(z, z + s) dz. \quad (3.12)$$

It follows that

$$G_0 = G_\infty - \int_0^\infty K(z, z) dz, \quad (3.13)$$

using the notation of (2.4).

Each $K(s, u)$ in \mathcal{K} yields the same relaxation function through (3.12). This is part of the definition of \mathcal{K} . However, there are usually many different $K(s, u)$ in \mathcal{K} , generating different rates of dissipation through (3.5) for any specified history.

We shall see later that the minimum, maximum and various intermediate free energies along the boundary of \mathcal{F} are determined from the form of the relaxation function; similarly for the associated rates of dissipation. Thus, $G(s)$ determines the boundaries of \mathcal{F} and \mathcal{K} , at least in an approximate sense.

Two important dimensionless parameters are

$$\beta = \frac{G_\infty}{G_0}, \quad \chi = \frac{G_0 - G_\infty}{G_0} = 1 - \beta = -\frac{1}{G_0} \int_0^\infty K(z, z) dz, \quad \beta, \chi \in [0, 1]. \quad (3.14)$$

Remark 3.1. These provide simple measures of the memory contribution and therefore, the amount of energy loss due to material deformation. The smaller the quantity β or the larger the parameter χ , the greater the energy loss. These parameters will prove important in the context of detailed forms of the fractions given by (2.12).

Remark 3.2. Expressions for the free energy, total dissipation and the ratios $F_s(t)$, $F_d(t)$ will be given in the case of a general rate of dissipation kernel $K(s, u)$, and three different types of strain history. These quantities are important characteristic properties of the material described by this kernel. The fractions $F_s(t)$, $F_d(t)$ represent, in a normalized fashion, the physical content of (2.10). Any choice of $K(s, u) \in \mathcal{K}$ will describe the stress-strain and energy behaviour of one specific material.

Matters are more difficult when we seek to reverse this process and determine the kernel $K(s, u)$ which describe a pre-chosen material, earlier referred to as material I.

4. FREQUENCY DOMAIN QUANTITIES

Let Ω be the complex ω plane and

$$\begin{aligned}\Omega^+ &= \{\omega \in \Omega \mid \text{Im}(\omega) \in \mathbb{R}^+\}, \\ \Omega^{(+)} &= \{\omega \in \Omega \mid \text{Im}(\omega) \in \mathbb{R}^{++}\}.\end{aligned}\quad (4.1)$$

These define the upper half-plane including and excluding the real axis, respectively. Similarly, Ω^- , $\Omega^{(-)}$ are the lower half-planes including and excluding the real axis, respectively.

The notation and properties used here for Fourier transforms of the various quantities of interest are outlined in many publications, including [20, 2].

Remark 4.1. Throughout this work, a subscript “+” attached to any quantity defined on Ω will imply that it is analytic on an open set including Ω^- , with all its singularities in $\Omega^{(+)}$. We shall abbreviate this description to simply a statement that it is analytic on Ω^- . Similarly, a subscript “-” will indicate that it is analytic on an open set including Ω^+ , with all its singularities in $\Omega^{(-)}$; again, this is abbreviated to a statement that it is analytic on Ω^+ .

Let us define the quantities

$$\begin{aligned}\tilde{G}_+(\omega) &= \int_0^\infty \tilde{G}(s)e^{-i\omega s} ds = \tilde{G}_c(\omega) - i\tilde{G}_s(\omega), \\ G'_+(\omega) &= \int_0^\infty G'(s)e^{-i\omega s} ds = G'_c(\omega) - iG'_s(\omega).\end{aligned}\quad (4.2)$$

The function $\tilde{G}_+(\omega)$ is analytic on Ω^- . This implies that any singularities of $\tilde{G}_+(\omega)$ are at least slightly off the real axis into $\Omega^{(+)}$, which in turn means that \tilde{G} decays exponentially at large positive times, though perhaps weakly. We shall be considering $\tilde{G}_+(\omega)$ both for values of ω on \mathbb{R} and off the real axis, into $\Omega^{(-)}$.

The quantity $\tilde{G}_+(\omega)$ is analytic in Ω^+ , its singularity structure being a mirror image, in the real axis, of that of $\tilde{G}_+(\omega)$. Thus, in particular, $\tilde{G}_c(\omega)$ has singularities in both $\Omega^{(+)}$ and $\Omega^{(-)}$ which are mirror images of one another. Similarly, its zeros will be mirror images of one another.

The standard properties that, for large ω ,

$$\begin{aligned}\tilde{G}_+(\omega) &\sim \frac{\tilde{G}'(0)}{i\omega} \quad \text{or} \quad \tilde{G}_s(\omega) \sim \frac{\tilde{G}(0)}{\omega}, \\ G'_+(\omega) &\sim \frac{G'(0)}{i\omega} \quad \text{or} \quad G'_s(\omega) \sim \frac{G'(0)}{\omega},\end{aligned}\quad (4.3)$$

will be required below.

The inverse relationships of (4.2) are given by

$$\tilde{G}(s) = \frac{1}{2\pi} \int_{-\infty}^\infty \tilde{G}_+(\omega)e^{i\omega s} d\omega, \quad G'(s) = \frac{1}{2\pi} \int_{-\infty}^\infty G'_+(\omega)e^{i\omega s} d\omega, \quad s > 0. \quad (4.4)$$

However, we have

$$G_0 - G_\infty = \tilde{G}(0) = \frac{1}{\pi} \int_{-\infty}^\infty \tilde{G}_+(\omega) d\omega = \frac{1}{\pi} \int_{-\infty}^\infty \tilde{G}_c(\omega) d\omega. \quad (4.5)$$

Relation (4.5)₂ follows by considering a contour integral over $\Omega^{(-)}$ and using (4.3), while (4.5)₃ results from the fact that $\tilde{G}_s(\omega)$ is an odd function. Applying a partial

integration in (4.2)₃ yields that

$$G_0 + G'_+(\omega) = G_\infty + i\omega\tilde{G}_+(\omega) = \mathcal{M}_+(\omega), \quad \omega \in \Omega^-, \quad (4.6)$$

where $\mathcal{M}_+(\omega)$ is the complex modulus of the material [24]. Its real and imaginary parts for $\omega \in \mathbb{R}$ are given by

$$\begin{aligned} \mathcal{M}_+(\omega) &= \mathcal{R}(\omega) + i\mathcal{I}(\omega), \\ \mathcal{R}(\omega) &= G_0 + G'_c(\omega) = G_\infty + \omega\tilde{G}_s(\omega), \\ \mathcal{I}(\omega) &= -G'_s(\omega) = \omega\tilde{G}_c(\omega). \end{aligned} \quad (4.7)$$

Important properties of $\tilde{G}_c(\omega)$ and $G'_s(\omega)$ include the equivalent conditions [11, 2]

$$\tilde{G}_c(\omega) \geq 0, \quad G'_s(\omega) \leq 0 \quad \forall \omega \in \mathbb{R}^{++}, \quad (4.8)$$

which are consequences of the second law. We note some properties of $\tilde{G}(s)$, which also apply to $G'(s)$. Because $\tilde{G}(s)$ is real, we have, from (4.2), that

$$\overline{\tilde{G}_+(\omega)} = \tilde{G}_+(-\bar{\omega}), \quad \overline{\tilde{G}_s(\omega)} = \tilde{G}_s(-\omega), \quad (4.9)$$

for all points $\omega \in \Omega$ where $\tilde{G}_+(\omega)$ is defined. Relation (4.9)₂ yields

$$\tilde{G}_c(\omega) = \tilde{G}_c(-\omega), \quad \tilde{G}_s(-\omega) = -\tilde{G}_s(\omega), \quad \tilde{G}_s(0) = 0, \quad \omega \in \mathbb{R}. \quad (4.10)$$

We also have

$$\tilde{G}_0 > 0, \quad G_\infty > 0, \quad (4.11)$$

the latter relation being true for a viscoelastic solid.

A quantity which will be of significant interest, particularly in the context of the minimum and related free energies, is

$$H(\omega) = -\omega G'_s(\omega) = \omega^2 \tilde{G}_c(\omega) = \omega \mathcal{I}(\omega) \geq 0, \quad \omega \in \mathbb{R}, \quad (4.12)$$

where the inequality is a consequence of (4.8) and (4.10). From (4.12)₂, it follows that the quantity $H(\omega)$ goes to zero quadratically at the origin. Using (4.3)₄ and (4.12), one can show that

$$H_\infty = \lim_{\omega \rightarrow \infty} H(\omega) = -G'(0) \geq 0. \quad (4.13)$$

We assume for present purposes that $G'(0)$ is non-zero so that H_∞ is a finite, positive number. Then $H(\omega) \in \mathbb{R}^{++} \forall \omega \in \mathbb{R}, \omega \neq 0$. The structure of its singularities are similar to those for $\tilde{G}_c(\omega)$, which are noted before (4.3).

The non-negative quantity $H(\omega)$ can always be expressed as the product of two factors ([17], [2], page 239)

$$H(\omega) = H_+(\omega)H_-(\omega), \quad (4.14)$$

where $H_+(\omega)$ has no zeros in $\Omega^{(-)}$ and is analytic in Ω^- . Similarly, $H_-(\omega)$ is analytic in Ω^+ with no zeros in $\Omega^{(+)}$. We put

$$H_\pm(\omega) = H_\mp(-\omega) = \overline{H_\mp(\omega)}, \quad H(\omega) = |H_\pm(\omega)|^2, \quad \omega \in \mathbb{R}. \quad (4.15)$$

The factorization (4.14) is the one relevant to the minimum free energy. For materials with only isolated singularities, there is a much broader class of factorizations, where the property that the zeros of $H_\pm(\omega)$ are in Ω^\pm respectively need not be true. These generate a range of free energies related to the minimum free energy, as discussed briefly in section 5.

The notation ω^\pm , which will be used below, was introduced in [17] and adopted in subsequent work. We have $\omega^\pm = \omega \pm i\epsilon$, $\omega \in \mathbb{R}$, where ϵ is a small positive

quantity. The limit $\epsilon \rightarrow 0$ can be taken after integrations have been carried out. It is useful for example in applying the Plemelj formulae.

The Fourier transform of $E^t(s)$, taken to be zero for $s \in \mathbb{R}^-$, has the form ([2], page 144)

$$E_+^t(\omega) = \int_0^\infty E^t(s)e^{-i\omega s} ds. \quad (4.16)$$

This quantity is analytic on Ω^- . The Fourier transform of E_{r+}^t , defined by (2.1)₂ and zero for $s \in \mathbb{R}^-$ has the form ([2], page 145)

$$E_{r+}^t(\omega) = E_+^t(\omega) - \frac{E(t)}{i\omega^-}. \quad (4.17)$$

Note the important connection

$$\frac{d}{dt}E_+^t(\omega) = \dot{E}_+^t(\omega) = -i\omega E_+^t(\omega) + E(t) = -i\omega E_{r+}^t(\omega), \quad (4.18)$$

between $\dot{E}_+^t(\omega)$ and $E_{r+}^t(\omega)$. Virtually all work on the minimum and related free energies up to and including [2] was based on $E_{r+}^t(\omega)$. Relations (4.18) provide the mechanism for changing to $\dot{E}_+^t(\omega)$. It follows also from (4.17) and (4.18) that

$$\frac{\partial}{\partial E(t)}\dot{E}_+^t(\omega) = 1. \quad (4.19)$$

For large ω (see (4.3)),

$$E_+^t(\omega) \sim \frac{E(t)}{i\omega}, \quad \dot{E}_+^t(\omega) \sim \frac{A(t)}{i\omega}, \quad (4.20)$$

where $A(t)$ is independent of ω .

The constitutive equation (2.3) in terms of frequency domain quantities has the form

$$\begin{aligned} T(t) &= G_\infty E(t) + \frac{1}{2\pi} \int_{-\infty}^\infty \overline{G_+(\omega)} \dot{E}_+^t(\omega) d\omega \\ &= G_\infty E(t) + \frac{1}{\pi} \int_{-\infty}^\infty \frac{H(\omega)}{\omega^2} \dot{E}_+^t(\omega) d\omega, \end{aligned} \quad (4.21)$$

where the second form follows from the argument given in [2], page 146.

The frequency domain representation for the work function, given by (3.9), has the form ([2], page 154):

$$W(t) = \phi(t) + \frac{1}{2\pi} \int_{-\infty}^\infty \frac{H(\omega)}{\omega^2} \left| \dot{E}_+^t(\omega) \right|^2 d\omega. \quad (4.22)$$

4.1. Frequency domain representations of dissipation rate and free energy kernels. We define

$$Z_{+-}(\omega_1, \omega_2) = \int_0^\infty \int_0^\infty Z(s, u) e^{-i\omega_1 s + i\omega_2 u} ds du, \quad (4.23)$$

where $Z(s, u)$ represents either of the kernels $\tilde{G}(s, u)$ or $K(s, u)$. Note that

$$\begin{aligned} Z_{+-}(\omega_1, \omega_2) &= Z_{+-}(-\omega_2, -\omega_1), \\ \overline{Z_{+-}(\omega_1, \omega_2)} &= Z_{+-}(-\overline{\omega_1}, -\overline{\omega_2}) = Z_{+-}(\overline{\omega_2}, \overline{\omega_1}), \quad \omega_1, \omega_2 \in \Omega, \end{aligned} \quad (4.24)$$

where the property $Z(s, u) = Z(u, s)$ has been used. These relations hold if ω_1, ω_2 are points of analyticity of $Z_{+-}(\omega_1, \omega_2)$. It follows from (4.24) that $Z_{+-}(\omega_1, \omega_2)$ is real if $\overline{\omega_2} = \omega_1$. In particular, $Z_{+-}(\omega_0, \omega_0)$ is real if ω_0 is real. The quantity $Z_{+-}(\omega_1, \omega_2)$ is analytic in the lower half of the ω_1 complex plane and in the upper

half of the ω_2 plane. Thus, $Z_{+-}(\omega_1, \omega_2)$ is given by analytic continuation from the real axis for $\omega_1 \in \Omega^{(-)}$ and $\omega_2 \in \Omega^{(+)}$.

It is shown in [20] for $\omega_1, \omega_2 \in \mathbb{R}$ that

$$i(\omega_1 - \omega_2)\tilde{G}_{+-}(\omega_1, \omega_2) = K_{+-}(\omega_1, \omega_2) + \tilde{G}_+(\omega_1) + \overline{\tilde{G}_+(\omega_2)}, \quad (4.25)$$

where $\tilde{G}_+(\omega)$ is defined by (4.2)₁. We will extrapolate this relationship by analytic continuation to $\omega_1 \in \Omega^{(-)}$ and $\omega_2 \in \Omega^{(+)}$.

Remark 4.2. Condition (3.8) ensures that Z_{+-} , defined by (4.23), exists. This has the consequence that $\psi(t)$ and $D(t)$, given by (3.1) and (3.5) respectively, are finite quantities for sinusoidal histories. It will emerge later that $W(t)$ diverges for such histories, so that $\mathcal{D}(t)$ must also become infinite in this case, by virtue of (2.10).

It follows from (4.12) and (4.25), by taking $\omega_1 = \omega_2 = \omega$ that [20]

$$K_{+-}(\omega, \omega) = -2\tilde{G}_c(\omega) = -2\frac{H(\omega)}{\omega^2} = -2\frac{\mathcal{I}(\omega)}{\omega}. \quad (4.26)$$

Let the quantity $K_{+-}(\omega_1, \omega_2)$, determined from each $K(s, u) \in \mathcal{K}$ by (4.23), form a set \mathcal{K}_F . Thus, the quantity $K_{+-}(\omega, \omega)$ is the same for all $K_{+-}(\omega_1, \omega_2) \in \mathcal{K}_F$.

5. THE MINIMUM AND RELATED FREE ENERGIES

It is shown in [12, 18, 2] that, for materials with only isolated singularities, the quantity $H(\omega)$ is a rational function and has many factorizations other than (4.14), denoted by

$$H(\omega) = H_+^f(\omega)H_-^f(\omega), \quad H_\pm^f(\omega) = H_\mp^f(-\omega) = \overline{H_\mp^f(\omega)}, \quad (5.1)$$

where f is an identification label distinguishing a particular factorization. These are obtained by exchanging the zeros of $H_+(\omega)$ and $H_-(\omega)$, leaving the singularities unchanged. Each factorization yields a different free energy and total dissipation given by

$$\begin{aligned} \psi_f(t) &= \phi(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} |p_-^{ft}(\omega)|^2 d\omega, \\ \mathcal{D}_f(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} |p_+^{ft}(\omega)|^2 d\omega, \\ p_\pm^{ft}(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{H_-^f(\omega') \dot{E}_+^t(\omega')}{\omega'(\omega' - \omega^\mp)} d\omega'. \end{aligned} \quad (5.2)$$

Note that each $\psi_f(t)$ is determined by the factors of $H(\omega)$. This latter quantity is determined from $G(s)$ by means of (4.12). Defining

$$K_f(t) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{H_-^f(\omega)}{\omega} \dot{E}_+^t(\omega) d\omega = \lim_{\omega \rightarrow \infty} [-i\omega p_-^{ft}(\omega)], \quad (5.3)$$

we can write the associated rate of dissipation in the form

$$D_f(t) = |K_f(t)|^2, \quad (5.4)$$

which can be expressed as a quadratic functional of the strain history. Relation (5.2)₁ can be expressed also as a quadratic functional (for example [20]). Note that $D_f(t)$ vanishes if $K_f(t) = 0$, which is a linear condition that can be satisfied for certain choices of strain history. Thus, the quadratic form for $D_f(t)$ is reduced from positive definite to positive semi-definite, indicating that each $\psi_f(t)$ is on the boundary of \mathcal{F} , as indicated earlier.

For these free energies and rates of dissipation, $K_{+-}(\omega_1, \omega_2)$ has the form

$$\omega_1 \omega_2 K_{+-}^f(\omega_1, \omega_2) = -2H_+^f(\omega_1)H_-^f(\omega_2). \quad (5.5)$$

These factorized quantities $K_{+-}^f(\omega_1, \omega_2)$ lie on the boundary of \mathcal{K}_F , by a similar argument as that applied to (5.4).

Remark 5.1. The factorization (4.14) yields the minimum free energy $\psi_m(t)$. This case is labeled as $f = 1$. Each exchange of zeros, starting from these factors, can be shown to yield a free energy which is greater than or equal to the previous quantity ([2], page 363). All these free energies are functionals of the minimal state. They are labeled by $f = 2, 3, \dots, N$ where N is the total number of distinct factorizations.

The quantity obtained by interchanging all the zeros is denoted by $\psi_f(t)$ for $f = N$. It can be identified as the maximum free energy among all those that are functionals of the minimal state. Reflecting this property, it is also denoted by $\psi_M(t)$. This quantity is less than the work function.

The most general rate of dissipation and free energy arising from these factorizations is given by

$$D(t) = \sum_{f=1}^N \lambda_f D_f(t), \quad \psi(t) = \sum_{f=1}^N \lambda_f \psi_f(t) \in \mathcal{F}, \quad \sum_{f=1}^N \lambda_f = 1, \quad \lambda_f \geq 0. \quad (5.6)$$

The question whether (5.6)₂ is the most general representation of a free energy in \mathcal{F} is discussed in subsection (8.1). From (4.19) and (5.2), we have

$$\frac{\partial}{\partial E(t)} p_-^{ft}(\omega) = -\frac{H_-^f(\omega)}{i\omega}, \quad (5.7)$$

which, with the help of (4.18) and ([2], page 249), yields

$$\frac{\partial}{\partial E(t)} \psi_f(t) = G_\infty E(t) + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{H(\omega)}{\omega^2} \dot{E}_+^t(\omega) d\omega = T(t), \quad (5.8)$$

where (4.21) has been used. This provides confirmation that the constitutive equation associated with all free energies of the form (5.6) is that given by (4.21) or (2.3).

The general form of $K_{+-}(\omega_1, \omega_2) \in \mathcal{K}_F$, which yields (5.6), is given as follows:

$$K_{+-}(\omega_1, \omega_2) = -\frac{2}{\omega_1 \omega_2} \sum_{f=1}^N \lambda_f H_+^f(\omega_1) H_-^f(\omega_2), \quad \sum_{f=1}^N \lambda_f = 1, \quad \lambda_f \geq 0, \quad (5.9)$$

where (5.5) has been used.

As already noted, the functionals $\psi_f(t)$, $f = 1, 2, \dots, N$ lie on the boundary of \mathcal{F} , in particular the minimum and maximum free energies which provide lower and upper bounds; similarly for $K_{+-}^f(\omega_1, \omega_2)$ with respect to \mathcal{K}_F . The factorizations (5.1) and therefore all these quantities are deduced from the parameters of the relaxation function. The size of the set \mathcal{F} (and \mathcal{K}_F or \mathcal{K}) is, in this sense, determined by the relaxation function.

6. FREE ENERGY AND DISSIPATION FUNCTIONALS FOR PARTICULAR HISTORIES

We seek to give detailed expressions for free energies and related quantities for general choices of the kernel $K(s, u) \in \mathcal{K}$ and histories with step function and SE behaviour. The latter will be considered both for semi-infinite and finite histories.

6.1. Step function histories. This is the simplest non-constant behaviour, given as follows. An alternative way of writing the history (2.1)₁ is $E(u)$, $u \leq t$ where t is the current time, assumed to be positive. We put

$$E(u) = \begin{cases} 0, & u \leq 0, \\ E_0, & 0 < u \leq t, \end{cases} \quad (6.1)$$

giving

$$\dot{E}(u) = \frac{dE(u)}{du} = E_0\delta(u), \quad (6.2)$$

in terms of the singular delta function. Thus, in the notation of (2.1)₁,

$$\dot{E}^t(s) = E_0\delta(t-s). \quad (6.3)$$

It follows from this relation and (3.5) that

$$D(t) = -\frac{E_0^2}{2}K(t, t). \quad (6.4)$$

Also, from (3.11), (2.8) and (3.1), we have

$$\begin{aligned} \psi(t) &= \phi(t) - \frac{E_0^2}{2} \int_0^\infty K(t+z, t+z) dz \\ &= \frac{1}{2}G_\infty E_0^2 - \frac{E_0^2}{2} \int_t^\infty K(y, y) dy, \quad t \geq 0. \end{aligned} \quad (6.5)$$

The integral term is non-negative, by virtue of (3.7)₂. Relation (3.13) yields that

$$\frac{1}{2}G_0 E_0^2 = \frac{1}{2}G_\infty E_0^2 - \frac{E_0^2}{2} \int_0^\infty K(y, y) dy. \quad (6.6)$$

Thus, on using (3.7)₂ again, we see that

$$\psi(t) \leq \frac{1}{2}G_0 E_0^2. \quad (6.7)$$

It follows from (3.9) that

$$W(t) = \frac{1}{2}G_0 E_0^2, \quad (6.8)$$

so that (3.10) is satisfied. Relation (2.10), together with (3.13), gives that

$$\mathcal{D}(t) = -\frac{E_0^2}{2} \int_0^t K(y, y) dy. \quad (6.9)$$

The finite range of the integral is easily understood, from a physical point of view. For the infinite period specified by (6.1)₁, there is no dissipation. At time $t = 0$, dissipation begins. Referring to (2.12), we see that

$$F_d(t) = -\frac{1}{G_0} \int_0^t K(y, y) dy, \quad F_s(t) = 1 - F_d(t). \quad (6.10)$$

Differentiating with respect to time, we obtain

$$\frac{d}{dt}F_d(t) = -\frac{1}{G_0}K(t, t), \quad \frac{d}{dt}F_s(t) = -\frac{d}{dt}F_d(t), \quad (6.11)$$

so that $F_d(t)$ is monotonically increasing and $F_s(t)$ is monotonically decreasing.

Referring to remark 2.2, a natural choice of selected time in this context is $t \rightarrow \infty$, which gives, by virtue of (3.13),

$$F_{dc} = \frac{G_0 - G_\infty}{G_0} = \chi = 1 - \beta, \quad F_{sc} = \frac{G_\infty}{G_0} = \beta, \quad (6.12)$$

in terms of the quantities introduced in (3.14). Thus, χ measures the energy dissipation and β the energy storage for any material in \mathcal{K} , due to a sudden step change in strain (see remark 3.1).

The quantity $F_d(t)$ is zero at $t = 0$ and increases monotonically to χ as $t \rightarrow \infty$, while $F_s(t) = 1$ at $t = 0$ and decreases monotonically to β at large t . Note that $K(y, y)$ must tend to zero as $y \rightarrow \infty$ to yield convergent integrals in (6.5) or (6.6).

Observe from (6.4) that, if $D(t)$ can be determined, this yields a measurement of $K(t, t)$. To obtain measurements of $K(s, u)$, $s, u \in \mathbb{R}^+$, one needs to consider histories with two steps ([2], page 132). Of course, this is not a very practical technique since step function histories are difficult to approximate closely.

6.2. SSE histories. Consider a history and current value $(E^t, E(t))$ defined by

$$E(t) = E_0 e^{i\omega_- t} + \overline{E_0} e^{-i\omega_+ t}, \quad E^t(s) = E(t-s), \quad s \in \mathbb{R}^+, \quad (6.13)$$

where E_0 is an amplitude and $\overline{E_0}$ its complex conjugate. Furthermore,

$$\omega_- = \omega_0 - i\eta, \quad \omega_+ = \overline{\omega_-}, \quad \omega_0, \eta \in \mathbb{R}^{++}. \quad (6.14)$$

The parameter η ensures finite results in certain quantities. For $\eta = 0$, we have purely sinusoidal behaviour, while for $\omega_0 = 0$, the history is exponentially growing. The derivative $\dot{E}^t(s)$, defined by (2.3)₃, has the form

$$\dot{E}^t(s) = i\omega_- E_0 e^{i\omega_-(t-s)} - i\omega_+ \overline{E_0} e^{-i\omega_+(t-s)}, \quad (6.15)$$

for SSE histories. Also, the quantity $E_+^t(\omega)$ (see (4.16)) is given by

$$E_+^t(\omega) = E_0 \frac{e^{i\omega_- t}}{i(\omega + \omega_-)} + \overline{E_0} \frac{e^{-i\omega_+ t}}{i(\omega - \omega_+)}, \quad (6.16)$$

while

$$\dot{E}_+^t(\omega) = E_0 \omega_- \frac{e^{i\omega_- t}}{\omega + \omega_-} - \overline{E_0} \omega_+ \frac{e^{-i\omega_+ t}}{\omega - \omega_+}. \quad (6.17)$$

Using (2.3) and (6.15), we find that the stress is given by

$$T(t) = \mathcal{M}_+(\omega_-) E_0 e^{i\omega_- t} + \mathcal{M}_+(-\omega_+) \overline{E_0} e^{-i\omega_+ t}, \quad (6.18)$$

where $\mathcal{M}_+(\omega)$ is defined by (4.6). Referring to (6.16) and (6.17), we see that

$$\begin{aligned} E_+^t(-i\alpha) &= E_0 \frac{e^{i\omega_- t}}{\alpha + i\omega_-} + \overline{E_0} \frac{e^{-i\omega_+ t}}{\alpha - i\omega_+}, \\ \dot{E}_+^t(-i\alpha) &= iE_0 \frac{\omega_- e^{i\omega_- t}}{\alpha + i\omega_-} - i\overline{E_0} \frac{\omega_+ e^{-i\omega_+ t}}{\alpha - i\omega_+}. \end{aligned} \quad (6.19)$$

The real quadratic form

$$\begin{aligned} V(t) &= ME_0^2 e^{2i\omega_- t} + \overline{M} \overline{E_0}^2 e^{-2i\omega_+ t} + N |E_0|^2 e^{i(\omega_- - \omega_+)t} \\ &= 2\operatorname{Re}[ME_0^2 e^{2i\omega_- t}] + N |E_0|^2 e^{i(\omega_- - \omega_+)t} \\ &= \left[2\operatorname{Re}\left(ME_0^2 e^{2i\omega_0 t} \right) + N |E_0|^2 \right] e^{2\eta t} \end{aligned} \quad (6.20)$$

will be denoted by

$$V(t) = \{M, N\}. \quad (6.21)$$

The quantity N is real. All free energies, total dissipations, rates of dissipation and work functions can be represented in the form $V(t)$, for histories given by (6.13). Note that

$$\int_{-\infty}^t V(s)ds = \left\{ \frac{M}{2i\omega_-}, \frac{N}{i(\omega_- - \omega_+)} \right\}, \quad (6.22)$$

$$\dot{V}(t) = \{2i\omega_- M, i(\omega_- - \omega_+)N\}.$$

We have, from (6.15) for $s = 0$ and (6.18),

$$\begin{aligned} T(t)\dot{E}(t) &= i\omega_- \mathcal{M}_+(\omega_-) E_0^2 e^{2i\omega_- t} - i\omega_+ \mathcal{M}_+(-\omega_+) \overline{E_0}^2 e^{-2i\omega_+ t} \\ &\quad + i[\omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)] |E_0|^2 e^{i(\omega_- - \omega_+)t} \\ &= \{i\omega_- \mathcal{M}_+(\omega_-), i[\omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)]\}. \end{aligned} \quad (6.23)$$

Using (2.11)₁, (6.23) and (6.22)₁, we see that

$$W(t) = \{M_W, N_W\}, \quad (6.24)$$

where

$$M_W = \frac{1}{2} \mathcal{M}_+(\omega_-), \quad N_W = \frac{\omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)}{\omega_- - \omega_+}. \quad (6.25)$$

The term N_W diverges in the purely sinusoidal limit. A general free energy (3.1)₁ for histories of the form (6.13) is given by

$$\psi(t) = \{M_\psi, N_\psi\}. \quad (6.26)$$

where

$$\begin{aligned} M_\psi &= \frac{1}{2} \left[G_\infty - \omega_-^2 \tilde{G}_{+-}(\omega_-, -\omega_-) \right] \\ &= \frac{1}{2} \left[\mathcal{M}_+(\omega_-) + \frac{i\omega_-}{2} K_{+-}(\omega_-, -\omega_-) \right], \end{aligned} \quad (6.27)$$

by virtue of (4.6), (4.9)₂, (4.23) and (4.25). Also, from (4.6), (4.24)₁ and subsequent observations,

$$\begin{aligned} N_\psi &= G_\infty + \frac{1}{2} \left\{ |\omega_-|^2 \tilde{G}_{+-}(\omega_-, \omega_+) + |\omega_+|^2 \tilde{G}_{+-}(-\omega_+, -\omega_-) \right\} \\ &= G_\infty + |\omega_-|^2 \tilde{G}_{+-}(\omega_-, \omega_+) \\ &= G_\infty + \frac{|\omega_-|^2}{i(\omega_- - \omega_+)} \left[K_{+-}(\omega_-, \omega_+) + \tilde{G}_+(\omega_-) + \overline{\tilde{G}_+(\omega_+)} \right] \\ &= \frac{-i|\omega_-|^2 K_{+-}(\omega_-, \omega_+) + \omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)}{\omega_- - \omega_+}, \end{aligned} \quad (6.28)$$

again using (4.25). From (3.5), (4.24) and (6.15), we find that

$$D(t) = \{M_D, N_D\}, \quad (6.29)$$

where

$$\begin{aligned} M_D &= \frac{\omega_-^2}{2} K_{+-}(\omega_-, -\omega_-), \\ N_D &= -\frac{|\omega_-|^2}{2} \{K_{+-}(\omega_-, \omega_+) + K_{+-}(-\omega_+, -\omega_-)\} \\ &= -|\omega_-|^2 K_{+-}(\omega_-, \omega_+). \end{aligned} \quad (6.30)$$

Let

$$\mathcal{D}(t) = \{M_{\mathcal{D}}, N_{\mathcal{D}}\}. \quad (6.31)$$

Then, from (6.22)₁,

$$M_{\mathcal{D}} = -\frac{i\omega_-}{4}K_{+-}(\omega_-, -\omega_-), \quad N_{\mathcal{D}} = i|\omega_-|^2 \frac{K_{+-}(\omega_-, \omega_+)}{\omega_- - \omega_+}. \quad (6.32)$$

We see from (6.25), (6.27), (6.28) and (6.32) that (2.10) is obeyed. Note that $N_{\mathcal{D}}$ diverges in the sinusoidal limit.

The ratios (2.12) are given by

$$F_d(t) = \frac{V_{\mathcal{D}}(t)}{V_W(t)}, \quad F_s(t) = 1 - F_d(t), \quad (6.33)$$

where $V_{\mathcal{D}}(t)$ has the form (6.20) with $M = M_{\mathcal{D}}$ and $N = N_{\mathcal{D}}$ given by (6.32). Also, $V_W(t)$ is similarly defined, with M_W and N_W given by (6.25).

The factor $e^{2\eta t}$, giving the exponential part of the history, cancels out of the ratios, yielding for $F_d(t)$,

$$F_d(t) = \frac{M_{\mathcal{D}}E_0^2 e^{2i\omega_0 t} + \overline{M_{\mathcal{D}}E_0^2} e^{-2i\omega_0 t} + N_{\mathcal{D}}|E_0|^2}{M_W E_0^2 e^{2i\omega_0 t} + \overline{M_W E_0^2} e^{-2i\omega_0 t} + N_W |E_0|^2}. \quad (6.34)$$

Now, we have

$$M_W E_0^2 e^{2i\omega_0 t} + \overline{M_W E_0^2} e^{-2i\omega_0 t} + N_W |E_0|^2 > 0, \quad (6.35)$$

which is a consequence of the fact that $W(t)$, given by (4.22), is positive, as is the cancelled factor $e^{2\eta t}$. Also, by averaging over any interval of duration π/ω_0 , the oscillatory terms vanish and we deduce that $N_W > 0$. The expression in (6.35) may be written as

$$N_W |E_0|^2 \left[1 + \frac{2|M_W| \cos(2\omega_0 t + \lambda)}{N_W} \right], \quad \lambda = \arg[M_W E_0^2], \quad (6.36)$$

where the term in brackets must be positive. It follows that, for all t ,

$$N_W > 2|M_W| \cos(2\omega_0 t + \lambda). \quad (6.37)$$

We can therefore write (6.34) as the numerator multiplying the factor

$$\frac{1}{N_W |E_0|^2} [1 + A], \quad (6.38)$$

where A is an infinite expansion of powers of terms involving $e^{\pm 2i\omega_0 t}$. This expansion is convergent by virtue of the inequality (6.37). If we take the average of $F_d(t)$ over any time interval of duration $\frac{\pi}{\omega_0}$, it reduces to

$$\begin{aligned} F_{dc} &= \frac{N_{\mathcal{D}}}{N_W} = \frac{i|\omega_-|^2 K_{+-}(\omega_-, \omega_+)}{\omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)}, \\ F_{sc} &= 1 - F_{dc} = \frac{N_{\psi}}{N_W} \\ &= \frac{-i|\omega_-|^2 K_{+-}(\omega_-, \omega_+) + \omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)}{\omega_- \mathcal{M}_+(-\omega_+) - \omega_+ \mathcal{M}_+(\omega_-)}, \end{aligned} \quad (6.39)$$

The quantities $N_{\mathcal{D}}$, N_{ψ} and the ratios F_{dc} , F_{sc} are parameters characterizing typical dissipated and stored energy for SSE histories, as discussed in remark 2.2.

6.3. Purely sinusoidal histories. For this case, the quantities $W(t)$ and $\mathcal{D}(t)$ diverge, as pointed out in remark 4.2, and after (6.25), (6.32). However, we now present expressions for those quantities that are finite, namely free energies and rates of dissipation.

In this limit, where $\eta \rightarrow 0$, (6.20) and (6.21) become

$$\{M, N\} = ME_0^2 e^{2i\omega_0 t} + \overline{M} \overline{E_0}^2 e^{-2i\omega_0 t} + N |E_0|^2. \quad (6.40)$$

Relation (6.23) converges to a finite result of the form

$$T(t)\dot{E}(t) = \{i\omega_0 \mathcal{M}_+(\omega_0), 2H(\omega_0)\}, \quad (6.41)$$

where (4.7) and (4.12) have been invoked. Also, (6.27) and (6.28) yield

$$\begin{aligned} M_\psi &= \frac{1}{2} \left\{ \mathcal{M}_+(\omega_0) + \frac{i\omega_0}{2} K_{+-}(\omega_0, -\omega_0) \right\}, \\ N_\psi &= \mathcal{R}(\omega_0) - \omega_0 \frac{d}{d\omega_0} \mathcal{R}(\omega_0) + U(\omega_0), \\ U(\omega_0) &= \frac{i\omega_0^2}{2} \left[-\frac{\partial}{\partial \omega_1} K_{+-}(\omega_1, \omega_2) + \frac{\partial}{\partial \omega_2} K_{+-}(\omega_1, \omega_2) \right] \Big|_{\omega_1 = \omega_2 = \omega_0}, \end{aligned} \quad (6.42)$$

where $\mathcal{R}(\omega)$ is defined by (4.7). Finally, from (6.29) and (6.30), we deduce that

$$D(t) = \left\{ \frac{\omega_0^2}{2} K_{+-}(\omega_0, -\omega_0), 2H(\omega_0) \right\}, \quad (6.43)$$

where (4.26) has been used. Applying (6.22)₂ in the sinusoidal limit, one can show that (2.9) is obeyed.

6.4. Comparison with special cases. We now compare these results with previously given particular examples of sinusoidal histories. The minimum free energy is discussed in detail for such histories in [1, 2]. Precisely analogous formulae apply to all the $\psi_f(t)$. Thus, we have, in the notation (6.40), using the complex modulus given by (4.6), rather than $G'(\omega_0)$ or $\tilde{G}(\omega_0)$,

$$\psi_f(t) = \left\{ \frac{1}{2} \left[\mathcal{M}_+(\omega_0) + \frac{i}{\omega_0} \left[H_-^f(-\omega_0) \right]^2 \right], R(\omega_0) - \omega_0 \frac{d}{d\omega_0} R(\omega_0) + Q_f(\omega_0) \right\}, \quad (6.44)$$

where $Q_f(\omega)$ is given by

$$Q_f(\omega) = i \left[\frac{d}{d\omega} H_+^f(\omega) H_-^f(\omega) - H_+^f(\omega) \frac{d}{d\omega} H_-^f(\omega) \right] \geq 0, \quad \omega \in \mathbb{R}. \quad (6.45)$$

The rate of dissipation is given by (5.4) and (5.3). It can be shown that

$$K_f(t) = H_-^f(-\omega_0) E_0 e^{i\omega_0 t} + H_-^f(\omega_0) \overline{E_0} e^{-i\omega_0 t}, \quad (6.46)$$

yielding

$$D_f(t) = \{[H_-^f(-\omega_0)]^2, 2H(\omega_0)\} = \{[H_+^f(\omega_0)]^2, 2H(\omega_0)\}, \quad (6.47)$$

where (5.1)₂ has been used.

We see that relations (6.44) and (6.47) are the special cases of (6.42) and (6.43) for $K_{+-}(\omega_1, \omega_2)$ given by (5.5). In particular, the quantity $Q_f(\omega)$ in (6.45) is equal to $U(\omega)$ in (6.42) for this choice of kernel.

6.5. Exponential histories. This can be treated either by direct calculation, or as a special case of the general formulae of subsection 6.2, where $\omega_0 \rightarrow 0$. We consider a history and current value $(E^t, E(t))$ given by (6.13) with $\omega_0 = 0$, so that

$$E(t) = E_e e^{\eta t}, \quad E^t(s) = E(t-s), \quad E_e = E_0 + \overline{E_0}. \quad (6.48)$$

The stress function, given by (6.18), has the form

$$T(t) = \mathcal{M}_+(-i\eta)E(t), \quad \mathcal{M}_+(-i\eta) = G_\infty + \eta \tilde{G}_+(-i\eta), \quad (6.49)$$

where the forms of $\mathcal{M}_+(-i\eta)$ can be deduced from (4.6). This quantity is real. From (6.49) or as special cases of (6.23) and (6.25), we have

$$\begin{aligned} T(t)\dot{E}(t) &= \eta \mathcal{M}_+(-i\eta)E^2(t) = \frac{1}{2} \mathcal{M}_+(-i\eta) \frac{d}{dt} E^2(t), \\ W(t) &= \frac{1}{2} \mathcal{M}_+(-i\eta)E^2(t). \end{aligned} \quad (6.50)$$

Also, (6.26), (6.27) and (6.28) reduce to

$$\psi(t) = \frac{1}{2} [\mathcal{M}_+(-i\eta) + \frac{\eta}{2} K_{+-}(-i\eta, i\eta)] E^2(t). \quad (6.51)$$

The rate of dissipation and total dissipation are special cases of (6.29) and (6.32), given by

$$D(t) = -\frac{\eta^2}{2} K_{+-}(-i\eta, i\eta) E^2(t), \quad \mathcal{D}(t) = -\frac{\eta}{4} K_{+-}(-i\eta, i\eta) E^2(t). \quad (6.52)$$

The results for the various quadratic quantities above can be summarized in a simple formula. Putting $\omega_0 = 0$ in (6.20), we have

$$V(t) = V_0 e^{2\eta t}, \quad V_0 = ME_0^2 + \overline{M} \overline{E_0}^2 + N |E_0|^2. \quad (6.53)$$

It can be shown using (3.1), (3.5) and (3.9), relating respectively to $\psi(t)$, $D(t)$ and $W(t)$, that

$$M = \overline{M} = \frac{N}{2}, \quad (6.54)$$

for exponential histories. This relation must therefore hold true for $\mathcal{D}(t)$, by virtue of (2.10). Equation (6.54) can also be shown using various explicit formulae from (6.25) to (6.32). It gives that $V_0 = ME_e^2$ or

$$V(t) = ME^2(t). \quad (6.55)$$

Each result in (6.50) - (6.52) has the form (6.55) where, for example, if $M = M(\omega_-, \omega_+)$ in the general sinusoidal/exponential case, this is replaced by $M = M(-i\eta, i\eta)$. The property (6.55) was first noted in [3].

The quantities F_s and F_d , defined by (2.12), are time-independent and given by

$$F_s = \frac{\mathcal{M}_+(-i\eta) + \frac{\eta}{2} K_{+-}(-i\eta, i\eta)}{\mathcal{M}_+(-i\eta)}, \quad F_d = -\frac{\eta}{2} \frac{K_{+-}(-i\eta, i\eta)}{\mathcal{M}_+(-i\eta)}. \quad (6.56)$$

Note that

$$F_s = F_{sc}, \quad F_d = F_{dc}, \quad (6.57)$$

where F_{sc} and F_{dc} are the quantities introduced in (6.39), with ω_\pm replaced by $\pm i\eta$, as in the comment after (6.55).

6.6. **Free energy and related functionals for SE histories which vanish for $t < 0$.** For such histories, (2.3) can be expressed as

$$T(t) = T_e(t) + \int_{-\infty}^t \tilde{G}(t-s)\dot{E}(s)ds = T_e(t) + \int_0^t \tilde{G}(t-s)\dot{E}(s)ds \quad (6.58)$$

with the aid of a simple change of variable. Also, (3.1)₁ and (3.5) become

$$\begin{aligned} \psi(t) &= \phi(t) + \frac{1}{2} \int_0^t \int_0^t \dot{E}(s)\tilde{G}(t-s, t-u)\dot{E}(u)dsdu, \\ D(t) &= -\frac{1}{2} \int_0^t \int_0^t \dot{E}(s)K(t-s, t-u)\dot{E}(u)dsdu. \end{aligned} \quad (6.59)$$

The work function is given by

$$W(t) = \int_0^t T(u)\dot{E}(u)du = \phi(t) + \frac{1}{2} \int_0^t \int_0^t \dot{E}(s)\tilde{G}(|s-u|)\dot{E}(u)duds, \quad (6.60)$$

by virtue of (2.11)₁ and (3.9).

7. DISCRETE SPECTRUM MATERIALS

The form of the relaxation function considered in this section is that for discrete spectrum materials, which will be used as our central illustrative example in later discussions. Let

$$\tilde{G}(s) = \sum_{i=1}^n G_i e^{-\alpha_i s}, \quad G'(s) = \sum_{i=1}^n g_i e^{-\alpha_i s}, \quad g_i = -\alpha_i G_i, \quad (7.1)$$

where n is a positive integer. The inverse decay times $\alpha_i \in \mathbb{R}^+$, $i = 1, 2, \dots, n$, and the coefficients G_i are also generally assumed to be positive, this being the simplest way to ensure the condition (4.8), which is clear from (7.3)₂ below. Note that

$$\tilde{G}(0) = G_0 - G_\infty = \sum_{i=1}^n G_i. \quad (7.2)$$

The parameters G_i , $i = 1, 2, \dots, n$, G_∞ and $\alpha_i \in \mathbb{R}^+$, $i = 1, 2, \dots, n$, are assumed to be known, given quantities. We arrange that $\alpha_1 < \alpha_2 < \alpha_3 \dots$. It follows from (4.2) that

$$\tilde{G}_+(\omega) = \sum_{i=1}^n \frac{G_i}{\alpha_i + i\omega}, \quad \tilde{G}_c(\omega) = \sum_{i=1}^n \frac{\alpha_i G_i}{\alpha_i^2 + \omega^2}, \quad \tilde{G}_s(\omega) = \omega \sum_{i=1}^n \frac{G_i}{\alpha_i^2 + \omega^2}. \quad (7.3)$$

Relation (4.12)₂ gives

$$H(\omega) = \omega^2 \sum_{i=1}^n \frac{\alpha_i G_i}{\alpha_i^2 + \omega^2} \geq 0. \quad (7.4)$$

This quantity can be expressed in the form [17]

$$H(\omega) = H_\infty \prod_{i=1}^n \left\{ \frac{\gamma_i^2 + \omega^2}{\alpha_i^2 + \omega^2} \right\}, \quad (7.5)$$

where the γ_i^2 are the zeros of $f(z) = H(\omega)$, $z = -\omega^2$ and obey the relations

$$\gamma_1 = 0, \quad \alpha_1^2 < \gamma_2^2 < \alpha_2^2 < \gamma_3^2 \dots \quad (7.6)$$

Recalling (4.13), we see from (7.1)₂ that

$$H_\infty = \sum_{i=1}^n \alpha_i G_i. \quad (7.7)$$

Let us define a vector \mathbf{e} in \mathbb{R}^n with components

$$e_i(t) = E(t) - \alpha_i E_+^t(-i\alpha_i) = \frac{d}{dt} E_+^t(-i\alpha_i) = \dot{E}_+^t(-i\alpha_i) = -\alpha_i E_{r+}^t(-i\alpha_i), \quad (7.8)$$

$$i = 1, 2, \dots, n,$$

where (4.18) has been used². The quantities $E_+^t(-i\alpha_i)$ are real. They are the Laplace transforms of $E^t(s)$, evaluated at α_i , $i = 1, 2, \dots, n$.

The complex modulus, defined by (4.6)₂, is given by

$$\mathcal{M}_+(\omega) = G_\infty + i\omega \sum_{i=1}^n \frac{G_i}{\alpha_i + i\omega}. \quad (7.9)$$

The stress function for discrete spectrum materials has the form

$$T(t) = G_\infty E(t) + \sum_{i=1}^n G_i e_i(t), \quad (7.10)$$

where (2.3)₁, (7.1)₁ and (7.8) have been used. Any quantity that depends on the history E^t only through the $e_i(t)$, defined by (7.8), is a functional of the minimal state ([20], for example). The work function, given by (2.11)₁, has the form

$$W(t) = \phi(t) + \sum_{i=1}^n G_i \int_{-\infty}^t e_i(u) \dot{E}(u) du, \quad (7.11)$$

which is not a functional of the minimal state.

8. FREE ENERGIES AND RELATED FUNCTIONALS FOR DISCRETE SPECTRUM MATERIALS

We now present a general form of a free energy functional for discrete spectrum materials ([2], page 362). Consider the quantity

$$\psi(t) = \phi(t) + \frac{1}{2} \mathbf{e}(t) \cdot \mathbf{C} \mathbf{e}(t) = \phi(t) + \frac{1}{2} \sum_{i,j=1}^n C_{ij} e_i(t) e_j(t), \quad (8.1)$$

where $\phi(t)$ is the equilibrium free energy, given by (2.8), and \mathbf{C} is a positive semidefinite (usually positive definite) symmetric matrix with components C_{ij} , $i, j = 1, 2, \dots, n$. The function $\psi(t)$ obeys (2.6) if \mathbf{C} obeys the conditions

$$\sum_{j=1}^n C_{ij} = G_i, \quad i = 1, 2, \dots, n. \quad (8.2)$$

This can be seen by means of (4.19), (7.8), (7.10) and (8.1). Referring to (7.7), we see that

$$\sum_{i,j=1}^n \alpha_i C_{ij} = \frac{1}{2} \sum_{i,j=1}^n (\alpha_i + \alpha_j) C_{ij} = H_\infty. \quad (8.3)$$

²Note that analytic continuation into Ω^- is straightforward since $E_+^t(\omega)$ is analytic in this half-plane.

The form (8.1) is the most general form of a free energy that is a functional of the minimal state, for discrete spectrum materials. One can show that

$$\begin{aligned}\dot{\psi}(t) + D(t) &= T(t)\dot{E}(t), \\ D(t) &= \frac{1}{2}\mathbf{e} \cdot \mathbf{\Gamma}\mathbf{e} = \frac{1}{2} \sum_{i,j=1}^n \Gamma_{ij} e_i(t)e_j(t), \\ \Gamma_{ij} &= (\alpha_i + \alpha_j)C_{ij},\end{aligned}\tag{8.4}$$

where Γ_{ij} are the components of the matrix $\mathbf{\Gamma}$. Condition (2.9)₂ requires that $\mathbf{\Gamma}$ must be at least positive semidefinite. It follows from (8.3) that

$$\sum_{i,j=1}^n \Gamma_{ij} = 2H_\infty.\tag{8.5}$$

Condition (8.2) is a restriction on \mathbf{C} and therefore $\mathbf{\Gamma}$, through (8.4)₄. Thus, $\mathbf{\Gamma}$ has $n(n-1)/2$ independent parameters, which are however subject to inequalities due to the positivity requirement on $\mathbf{\Gamma}$. By varying all these parameters within allowed ranges, we mark out the extent of the set \mathcal{K} , or under I2, the range of choices of $K(s, u)$ describing the different materials with constitutive relation (7.10) constructed from relaxation function (7.1). The kernels \tilde{G} and K , given by

$$\begin{aligned}\tilde{G}(s, u) &= \sum_{i,j=1}^n C_{ij} e^{-\alpha_i s - \alpha_j u} \in \mathcal{G}, \\ K(s, u) &= - \sum_{i,j=1}^n \Gamma_{ij} e^{-\alpha_i s - \alpha_j u} \in \mathcal{K},\end{aligned}\tag{8.6}$$

have the property that, when substituted into (3.1) and (3.5), they yield (8.1) and (8.4)₂ respectively. It follows from (4.23) and (8.6) that

$$\begin{aligned}\tilde{G}_{+-}(\omega_1, \omega_2) &= \sum_{i,j=1}^n \frac{C_{ij}}{(\alpha_i + i\omega_1)(\alpha_j - i\omega_2)}, \\ K_{+-}(\omega_1, \omega_2) &= - \sum_{i,j=1}^n \frac{\Gamma_{ij}}{(\alpha_i + i\omega_1)(\alpha_j - i\omega_2)},\end{aligned}\tag{8.7}$$

which can be shown to obey (4.25), by virtue of (8.2), (8.4)₄ and the use of partial fractions. Observe that

$$K_{+-}(\omega, \omega) = - \sum_{i,j=1}^n C_{ij} \left\{ \frac{1}{\alpha_i + i\omega} + \frac{1}{\alpha_j - i\omega} \right\} = - \frac{2H(\omega)}{\omega^2},\tag{8.8}$$

which may be shown with the aid of (7.3), (7.4) and (8.2). This agrees with (4.26).

The formulae presented in this section are for arbitrary histories, based on (7.8). It is of interest to check that the results are in agreement with the formulae of section 6 for specified histories but which apply to materials more general than the discrete spectrum category. It follows from (4.16), (6.3) and (7.8) that, for step function histories,

$$e_i(t) = E_0 e^{-\alpha_i t},\tag{8.9}$$

and we see that, for example, (8.1) agrees with (6.5), by virtue of (8.6)₂ and (8.4)₄. Also, for SSE histories, it can be shown that (8.4)_{2,3} is a special case of (6.30), with the aid of (6.19)₂, (7.8) and (8.7)₂. The other formulae for step function and SSE

histories in section 6 can also be shown to agree with the corresponding results in the present section.

For the discrete spectrum model, the set \mathcal{F} consists of all free energies of the form (8.1). The fundamental quantities are of course the $K(s, u) \in \mathcal{K}$, which are uniquely determined by the non-negative symmetric matrix $\mathbf{\Gamma}$, and the quantities $\alpha_i, i = 1, 2, \dots, n$.

8.1. Free energies ψ_f . Let us now consider important special cases of this formalism. Explicit forms of the factors $H_{\pm}^f(\omega)$, the free energies $\psi_f(t)$ and the dissipation rates $D_f(t)$ (see (5.2) - (5.4)) are given for discrete spectrum materials in for example [12, 18, 2]. The quantities $H_{\pm}^f(\omega)$ can be written in the form

$$\begin{aligned} H_-^f(\omega) &= ih_{\infty}\omega \sum_{i=1}^n \frac{R_i^f}{\alpha_i(\alpha_i - i\omega)}, \quad H_+^f(\omega) = \overline{H_-^f}(\omega), \\ R_i^f &= (\rho_i^f - \alpha_i) \prod_{\substack{j=1 \\ j \neq i}}^n \left\{ \frac{\rho_j^f - \alpha_i}{\alpha_j - \alpha_i} \right\}, \\ h_{\infty} &= H_{\infty}^{1/2}, \quad \gamma_1 = 0, \quad \rho_1 = 0, \\ \rho_i^f &= \epsilon_i^f \gamma_i, \quad \epsilon_i^f = \pm 1, \quad i = 2, \dots, n. \end{aligned} \tag{8.10}$$

Different choices of the vector with components ϵ_i^f yield different factorizations and free energies. There are $N = 2^{n-1}$ possible choices of the vector with components $\epsilon_i^f, i = 2, 3, \dots, n$. A way of generating them was suggested in [23], and is repeated here.

Remark 8.1. For each integer f , express $f - 1 \in [0, M - 1]$ as a binary number of length $n - 1$, and regard each digit of this number as a component of the matrix. Change each 0 in the matrix to -1 , which completes the construction.

This method is used to produce numerical results in the present work.

Taking the large ω limit of (8.10)₁, we see that

$$\sum_{i=1}^n \frac{R_i^f}{\alpha_i} = -1. \tag{8.11}$$

The function $p_-^{ft}(\omega)$, given by (5.2)₃, has the form

$$p_-^{ft}(\omega) = -ih_{\infty} \sum_{i=1}^n \frac{R_i^f e_i(t)}{\alpha_i(\omega + i\alpha_i)}. \tag{8.12}$$

Using (8.12) in (5.3)₂, we obtain

$$K_f(t) = -h_{\infty} \sum_{i=1}^n \frac{R_i^f e_i(t)}{\alpha_i}. \tag{8.13}$$

From (5.4) and (8.13), we see that

$$D_f(t) = H_{\infty} \left[\sum_{i=1}^n \frac{R_i^f}{\alpha_i} e_i(t) \right]^2 = H_{\infty} \sum_{i,j=1}^n \frac{R_i^f R_j^f}{\alpha_i \alpha_j} e_i(t) e_j(t). \tag{8.14}$$

Comparing with (8.4)₃, we obtain that

$$\Gamma_{ij} = 2H_\infty \frac{R_i^f R_j^f}{\alpha_i \alpha_j}, \quad (8.15)$$

for the family of free energies related to the factorizations (8.10). This identification also emerges from (5.5), (8.7)₂ and (8.10). Note that relation (8.5) holds for each factorization, by virtue of (8.11). It follows from (8.12) and (5.2)₁ that

$$\psi_f(t) = \phi(t) + H_\infty \sum_{i,j=1}^n \frac{R_i^f R_j^f}{(\alpha_i + \alpha_j) \alpha_i \alpha_j} e_i(t) e_j(t), \quad (8.16)$$

which, with the aid of (8.1) and (8.15), yields (8.4)₄. One can show directly that (8.2) is obeyed from an argument given in [2], page 267, which is valid for all subscripts f .

The central free energy, discussed below, is a linear combination of the forms (8.16), as in (5.6), for particular values of the λ_f .

A general form of $K_{+-}(\omega_1, \omega_2)$ for discrete spectrum materials can be given by (5.9), using (8.10). The question arises whether this is the most general representation, equivalent to (8.7)₂. This latter form has $n(n-1)/2$ independent parameters in $\mathbf{\Gamma}$, as determined after (8.5). Both the λ_f and the components of $\mathbf{\Gamma}$ are subject to positivity related inequalities. The number of independent λ_f is $2^{n-1} - 1$. Thus, for $n \geq 4$, there are more λ_f than independent elements of $\mathbf{\Gamma}$. Dependence on these parameters is linear in both cases. Thus, for $n \geq 4$, equivalence between the two representations can probably be demonstrated if the inequality constraints on the two sets of parameters are consistent.

Remark 8.2. Recalling (5.8) or (8.2), we see that the constitutive equation associated with each $\psi_f(t)$ and any linear combination of them, as in (5.6), is that given by (2.3), with relaxation function specified by (7.1).

8.2. The Day free energy. For the case $n = 1$, the relations (8.1) and (8.4) reduce to the formulae for the Day free energy and rate of dissipation [6, 2]. A relaxation function given by (7.1), but with only one decaying exponential, has the form

$$G_D(t) = G_\infty + G_d e^{-\alpha t}, \quad G_d = G_0 - G_\infty. \quad (8.17)$$

This behaviour has, in some contexts, been referred to as the standard linear model [24]. By virtue of (8.2) and (8.4)₄, we must have

$$C_{11} = G_d, \quad \Gamma_{11} = 2\alpha G_d. \quad (8.18)$$

The Day free energy functional is given by

$$\psi_D(t) = \phi(t) + \frac{G_d}{2} e_1^2(t), \quad (8.19)$$

in terms of $e_1(t)$ defined by (7.8). The corresponding rate of dissipation is

$$D_D(t) = \alpha G_d e_1^2(t). \quad (8.20)$$

From (6.25) and (7.9), we can determine M_W and N_W for this case. In particular,

$$N_W = G_\infty + G_d \frac{(\omega_0^2 + \eta^2)(\alpha + \eta)}{\eta[(\alpha + \eta)^2 + \omega_0^2]}. \quad (8.21)$$

The kernels (8.6) reduce to

$$\tilde{G}(s, u) = G_d e^{-\alpha(s+u)}, \quad K(s, u) = -2\alpha G_d e^{-\alpha(s+u)}, \quad (8.22)$$

and (8.7) becomes

$$\begin{aligned}\tilde{G}_{+-}(\omega_1, \omega_2) &= \frac{G_d}{(\alpha + i\omega_1)(\alpha - i\omega_2)}, \\ K_{+-}(\omega_1, \omega_2) &= -\frac{2\alpha G_d}{(\alpha + i\omega_1)(\alpha - i\omega_2)},\end{aligned}\tag{8.23}$$

which yield explicit functions for $M_{\mathcal{D}}$ and $N_{\mathcal{D}}$, given by (6.32). Thus, we obtain that

$$M_{\mathcal{D}} = \frac{iG_d}{2} \frac{(w_0 - i\eta)\alpha}{(\alpha + \eta + i\omega_0)^2}, \quad N_{\mathcal{D}} = G_d \frac{\alpha(\omega_0^2 + \eta^2)}{\eta[(\alpha + \eta)^2 + \omega_0^2]}.\tag{8.24}$$

Relations (8.14) and (8.16) are particular cases of the general formulae (8.4) and (8.1), and must have the same limit for $n = 1$. This can be seen by noting that

$$H_{\infty} = -G'(0) = \alpha G_d,\tag{8.25}$$

and from (8.11),

$$R_1^1 = -\alpha,\tag{8.26}$$

for $n = 1$.

The fundamental point made in [22] is that a material with memory is completely characterized by choosing $K(s, u)$ rather than the relaxation function. However, for the $n = 1$ case, specifying the relaxation function parameters fixes uniquely the kernel $K(s, u)$ and therefore determines the material completely. Thus, the set \mathcal{K} for $n = 1$ is a singleton given by (8.22)₂, and there is only one material with the constitutive relation generated by the relaxation function (8.17), with parameters as specified.

This is essentially the observation in the Introduction that there is only one free energy which is a functional of the minimal state ([2], page 150 for example) for $n = 1$, namely (8.19).

Remark 8.3. If a material behaviour can be adequately simulated by one decay constant α , together with coefficients G_{∞} and G_d , then $\psi_{\mathcal{D}}(t)$, given by (8.19), is the physical free energy for that material.

9. FUNCTIONALS TO BE PLOTTED FOR COMPARISON PURPOSES

The free energy functional proposed in [18] (see also [2], page 367) is given by (5.6)₂ with $\lambda_f = 1/N$, $f = 1, 2, \dots, N$ for discrete spectrum materials. It was proposed as a candidate for the physical free energy. Adopting viewpoint I2, we see that it is the physical free energy of the material described by kernel $K(s, u) \in \mathcal{K}$ with Fourier transform $K_{+-}(\omega_1, \omega_2)$ given by (5.9), with equal λ_f . This may indeed be a reasonable approximation to many choices of material behaviour. Similarly, the rate of dissipation has the form (5.6)₁, for the same λ_f . Closed formulae for these quantities were established, which can be put in the form

$$\begin{aligned}\psi_c(t) &= \phi(t) + H_{\infty} \sum_{i,j=1}^n \frac{P_n(\alpha_i, \alpha_j)}{\alpha_i + \alpha_j} e_i(t) e_j(t), \\ D_c(t) &= H_{\infty} \sum_{i,j=1}^n P_n(\alpha_i, \alpha_j) e_i(t) e_j(t),\end{aligned}\tag{9.1}$$

where

$$P_n(\alpha_i, \alpha_j) = \frac{\prod_{k=2}^n \{\alpha_i \alpha_j + \gamma_k^2\}}{\prod_{\substack{k=1 \\ k \neq i}}^n (\alpha_i - \alpha_k) \prod_{\substack{k=1 \\ k \neq j}}^n (\alpha_j - \alpha_k)}. \quad (9.2)$$

We shall refer to $\psi_c(t)$ as the central free energy.

In subsection 11.4, we will present plots of total dissipations associated with the central free energy, and also the minimum and maximum free energies, as specified in remark 5.1. The quantities R_i^1 for the minimum free energy and associated dissipation, are given by (8.10) with $\epsilon_i^1 = 1$, $i = 2, \dots, N$, while for the maximum free energy and dissipation, the quantities R_i^N have $\epsilon_i^N = -1$, $i = 2, \dots, N$. The ratios defined in (2.12), or related quantities (see remark 2.2), are also presented. Using (8.10) and (9.2), the matrix Γ in (8.4) for these three cases can be expressed as

$$\begin{aligned} \Gamma_{ij} &= 2H_\infty \frac{F_{ij}(r)}{\prod_{\substack{k=1 \\ k \neq i}}^n (\alpha_i - \alpha_k) \prod_{\substack{k=1 \\ k \neq j}}^n (\alpha_j - \alpha_k)}, \\ F_{ij}(1) &= \prod_{l=1}^n (\gamma_l - \alpha_i) \prod_{l=1}^n (\gamma_l - \alpha_j) \\ &= \prod_{l=1}^n [\alpha_i \alpha_j + \gamma_l^2 - \gamma_l(\alpha_i + \alpha_j)], \\ F_{ij}(2) &= \prod_{l=1}^n (\alpha_i \alpha_j + \gamma_l^2), \\ F_{ij}(3) &= \prod_{l=1}^n (\gamma_l + \alpha_i) \prod_{l=1}^n (\gamma_l + \alpha_j) \\ &= \prod_{l=1}^n [\alpha_i \alpha_j + \gamma_l^2 + \gamma_l(\alpha_i + \alpha_j)], \end{aligned} \quad (9.3)$$

where the minimum, central and maximum free energies are labeled by $r = 1, 2, 3$, respectively. We can determine C_{ij} from (8.4)₄.

The quantities $K(s, u)$ and $K_{+-}(\omega_1, \omega_2)$ are given by (8.6)₂ and (8.7)₂ in terms of Γ_{ij} . All the functionals of interest are presented in section 6 for step function and SE histories, in terms of $K(s, u)$ and $K_{+-}(\omega_1, \omega_2)$. The total dissipation for SSE histories in the Day case is given explicitly by (8.23).

10. CHOICE OF PARAMETERS FOR THE RELAXATION FUNCTION

The inverse decay times are given by the formula

$$\begin{aligned} \alpha_r &= \alpha_n \kappa_r, & \kappa_r &= \frac{\sin^2 \frac{r\pi}{2(n+1)}}{\sin^2 \frac{n\pi}{2(n+1)}}, \\ r &= 1, 2, \dots, n, & \kappa_n &= 1, \quad \kappa_r \leq 1, \end{aligned} \quad (10.1)$$

based on a simple polymeric model ([15, 3] and references therein).

The quantities R_i/α_i , $i = 1, 2, \dots, n$, given by (8.10) for $f = 1$, can clearly be expressed in terms of the dimensionless parameters κ_r , $r = 1, 2, \dots, n$, and γ_j/α_n , $j = 1, 2, \dots, n$. Now, (7.5), expressed in terms of the variable ω^2/α_n^2 , has

zeros at $-(\gamma_j/\alpha_n)^2$, which are dimensionless numbers denoted by μ_j^2 . Thus, we have

$$\gamma_r = \alpha_n \mu_r, \quad r = 1, 2, \dots, n, \quad (10.2)$$

where the quantities κ_r and μ_r obey (7.6) with κ_r replacing α_r and μ_r replacing γ_r . However, the simplest way of proceeding is to keep the notation α_r and γ_r rather than κ_r and μ_r , and put α_n equal to unity. In fact, we absorb α_n into the time (or frequency) variable, taken to be the dimensionless quantity $\alpha_n t$ (or ω/α_n); it is then understood that when α_n appears in formulae, it is equal to unity. Of course, in a practical situation, it must be ascribed its physical value, but we need not concern ourselves with what that value is, in the present work.

Also based on this polymeric model [15], we choose all the G_i in (7.1) to be equal to G_1 , so that, from (7.2),

$$\frac{G_1}{G_0} = \frac{\chi}{n}, \quad (10.3)$$

in the notation of (3.14). It follows from (7.7) that

$$H_\infty = \frac{\chi}{n} G_0 \sum_{i=1}^n \alpha_i. \quad (10.4)$$

We take

$$G_0 = 1. \quad (10.5)$$

In order to choose an appropriate value for n , we initially consider values between 4 and 8, since 2, 3 are perhaps too simple and 8 is where the material is a close approximation to the continuous spectrum case [23]. The relaxation functions, for $n = 4, 5, \dots, 8$, with the α_i defined by (10.1) and G_1 , given by (10.3), are very close in value. This is indicated by a plot of the relaxation functions for $n = 4, 8$ on Figure 1; the $n = 5, 6, 7$ cases fall between these two. Note that the $n = 8$ function has not converged to its infinite limit β , even at $\alpha_n t = 40$. This is because the smallest inverse decay time α_1 for this case is equal to 0.0311.

We will adopt (10.1) and the equality of all the G_i , yielding (10.3). Full knowledge of the matrix $\mathbf{\Gamma}$ for material I, or whatever other kernel in \mathcal{K} is of interest, remains to be established, presumably by measurement.

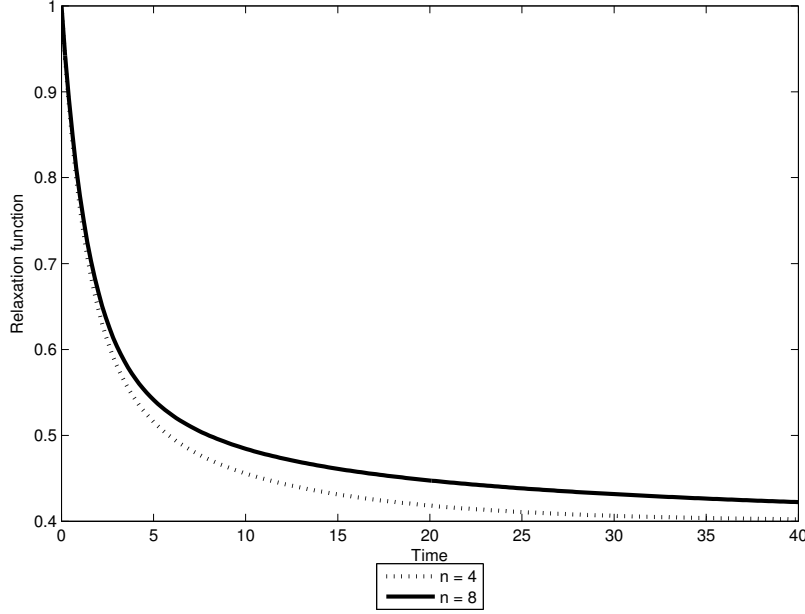
10.1. Closest Day relaxation function. We now seek the Day relaxation function which is closest to the actual relaxation function for the materials in \mathcal{K} .

The α_i , $i = 1, 2, \dots, n$, in (7.1) are given by (10.1), while the G_i , $i = 1, 2, \dots, n$, are determined by (10.3), together with the assumption that the G_i are all equal. This equality will be explicitly invoked later. We choose G_0 , G_∞ and α such that the resulting $n = 1$ relaxation function approximates (7.1) as closely as possible.

We choose G_0 and G_∞ to be the same for the materials with relaxation function given by (7.1) and (8.17), respectively. Then, G_d is given by (8.17)₂.

Choosing the optimal value of α is somewhat more difficult. Consider

$$\begin{aligned} f(\alpha) &= \frac{1}{G_d^2} \int_0^\infty [G_D(s) - G(s)]^2 ds \\ &= \frac{1}{G_d^2} \int_0^\infty \left[G_d e^{-\alpha s} - \sum_{i=1}^n G_i e^{-\alpha_i s} \right]^2 ds, \end{aligned} \quad (10.6)$$

FIGURE 1. Relaxation functions for $n = 4, 8$ where $\beta = 0.4$.

which is a $L^2(\mathbb{R}^+)$ norm of the difference between the relaxation functions for the Day case and that in (7.1). Then, we put

$$f_m = \min_{\alpha > 0} f(\alpha), \quad (10.7)$$

and this minimum is achieved at α_d , so that

$$f(\alpha_d) = f_m \leq f(\alpha) \quad \forall \alpha \in \mathbb{R}^+. \quad (10.8)$$

The quantity α_d is the inverse time decay constant that will be used in the Day free energy and dissipation. We have, from (10.6) that

$$f_m = \int_0^\infty d^2(s) ds, \quad d(s) = e^{-\alpha_d s} - \frac{1}{G_d} \sum_{i=1}^n G_i e^{-\alpha_i s}. \quad (10.9)$$

Note that $d(0) = 0$ and $\lim_{s \rightarrow \infty} d(s) = 0$. It is assumed that the fit sought by the limiting process (10.7) is reasonably good, so that $f_m \ll 1$. For the specific example considered below, $f_m = 0.1$. It follows that $d(s)$ must be small except perhaps on regions of \mathbb{R}^+ with small measure.

Let $W_D(t)$ denote the Day work function. It follows from (3.9) that

$$\frac{1}{G_d} [W_D(t) - W(t)] = \frac{1}{2} \int_0^\infty \int_0^\infty d(|s-u|) \dot{E}^t(s) \dot{E}^t(u) ds du. \quad (10.10)$$

The conclusion that $d(s)$ is typically small suggests that $\frac{1}{G_d} [W_D(t) - W(t)]$ should also be small. In the examples presented later, it is indeed always the case that $W_D(t)$ and $W(t)$ are very close in value.

$f(\alpha_d), n = 4, 5, \dots, 8$	0.0603	0.0968	0.1347	0.1722	0.2088
$\alpha_d, n = 4, 5, \dots, 8$	0.3536	0.3225	0.3030	0.2896	0.2798
$f''(\alpha_d), n = 4, 5, \dots, 8$	8.6	10.7	12.4	13.8	14.9

TABLE 1. The function defined by (10.12), the solution of (10.14), denoted by α_d and the second derivatives of $f(\alpha)$ at α_d .

The quantity $f(\alpha)$, given by (10.6), can be explicitly calculated. Let us replace α by α_0 . Then

$$f(\alpha_0) = \sum_{i,j=0}^n \frac{c_i c_j}{\alpha_i + \alpha_j}, \quad \alpha_0 \in (0, 1], \quad (10.11)$$

$$c_i = \begin{cases} 1, & i = 0, \\ -\frac{G_i}{G_d}, & i = 1, 2, \dots, n. \end{cases}$$

This can be written in the form

$$f(\alpha_0) = \frac{1}{2\alpha_0} + 2 \sum_{i=1}^n \frac{c_i}{\alpha_0 + \alpha_j} + \sum_{i,j=1}^n \frac{c_i c_j}{\alpha_i + \alpha_j}, \quad (10.12)$$

so that

$$f'(\alpha_0) = -\frac{1}{2\alpha_0^2} - 2 \sum_{i=1}^n \frac{c_i}{(\alpha_0 + \alpha_j)^2}. \quad (10.13)$$

Thus, the α_0 satisfying (10.8) is the solution of the equation

$$1 + 4 \sum_{i=1}^n \frac{c_i \alpha_0^2}{(\alpha_0 + \alpha_j)^2} = 0, \quad (10.14)$$

which is a minimum if $f''(\alpha_0) > 0$. This α_0 is equal to α_d .

Note that the values of α_d on Table 1 do not vary greatly with n . The quantities $f''(\alpha_d)$ are all positive so that the extrema of $f(\alpha)$ at $\alpha = \alpha_d$ are all minima.

It seems therefore to matter little what value of n is adopted. We choose $n = 5$ for the remainder of this work. The numerical values of α_r , $r = 1, 2, 3, 4, 5$, given by (10.1), are 0.0718, 0.2679, 0.5359, 0.8038 and 1.0.

Referring to remark 8.1 and the developments of subsection 8.1, we find that the vectors with components ϵ_i^f , $i = 2, 3, 4, 5$ are as shown on Table 2.

The appropriate Day relaxation function is determined by (10.6) - (10.8) where $f(\alpha)$ has the form (10.12). Since the G_i are all equal, (10.11)₂ becomes

$$c_i = \begin{cases} 1, & i = 0, \\ -\frac{1}{n}, & i = 1, 2, \dots, n, \end{cases} \quad (10.15)$$

with the aid of (7.2) and (8.17)₂. We look for a solution to (10.14) where $\alpha_0 \in (0, 1]$. This is denoted by α_d , which from Table 1 is equal to 0.3225, with optimum choice $f(\alpha_d) = f_m = 0.0968$.

The quantities $G(s)$ and $G_D(s)$, where the latter is given by (8.17)₁ with $\alpha = \alpha_d$, are plotted on Figure 2. We see that the curves are reasonably close. The relaxation

$f =$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1
	1	1	1	1	-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1
	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1
	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1

TABLE 2. Vectors with components ϵ_i^f , $i = 2, 3, 4, 5$, where $f = 1, 2, \dots, 16$, as generated by the algorithm described in remark 8.1. Note that $f = 1$ and 16 relate to the minimum and maximum free energies, respectively.

function $G(s)$ converges very slowly to zero because the least inverse decay time, $\alpha_1 = 0.0718$ is small; see paragraph after (10.5).

Figure 2 clearly suggests that $d(s)$, defined in (10.9), is small for most s , which is empirical confirmation of the discussion around (10.10).

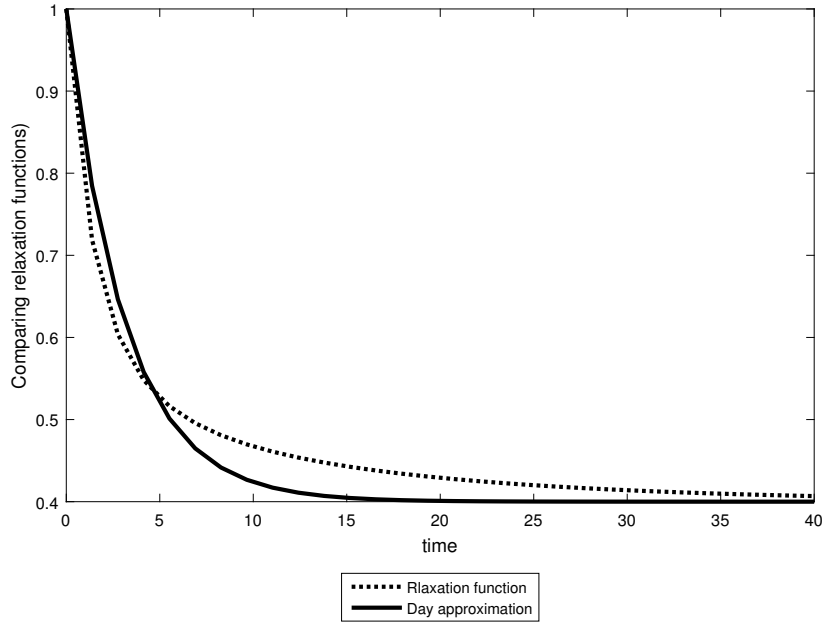


FIGURE 2. The relaxation function for $n = 5$, $\beta = 0.4$ and the Day relaxation function approximating it.

Observe that if all the α_i in (8.6) are replaced by α_d , then these relations reduce to (8.22), on using (8.5) and (8.25).

It is of interest to compare the Day free energy and total dissipation with various free energies and total dissipations derivable from different choices of $K(s, u) \in \mathcal{K}$ for relaxation function (7.1). This will be done for total dissipation in various plots presented in subsection 11.4.

10.2. Closest kernel to the Day form. All free energies and total dissipations related to each $K(s, u) \in \mathcal{K}$ reduce to the unique Day versions for $n = 1$. It might be expected therefore that the latter are close to the average of those for general n . What emerges from the numerical work is however that the Day free energy is closer to the minimum free energy than the maximum free energy for $n = 5$, with corresponding results for the total dissipations.

This can be demonstrated directly by seeking the kernel $K(s, u) \in \mathcal{K}$ which is closest to the Day kernel given by (8.22)₂ for $\alpha = \alpha_d$, that is

$$K_D(s, u) = -2\alpha_d G_d e^{-\alpha_d(s+u)}, \quad (10.16)$$

Referring to (8.6)₂ and (8.22)₂, we define

$$\begin{aligned} m(\boldsymbol{\lambda}) &= \frac{1}{G_d^2} \int_0^\infty \int_0^\infty [K_D(s, u) - K(s, u)]^2 ds du \\ &= \frac{1}{G_d^2} \int_0^\infty \int_0^\infty \left[2\alpha_d G_d e^{-\alpha_d(s+u)} - \sum_{i,j=1}^n \Gamma_{ij} e^{-\alpha_i s - \alpha_j u} \right]^2 ds du \\ &= 1 - \frac{4\alpha_d}{G_d} \sum_{i,j=1}^n \frac{\Gamma_{ij}}{(\alpha_d + \alpha_i)(\alpha_d + \alpha_j)} + \frac{1}{G_d^2} \sum_{i,j,k,l=1}^n \frac{\Gamma_{ij}\Gamma_{kl}}{(\alpha_i + \alpha_k)(\alpha_j + \alpha_l)}. \end{aligned} \quad (10.17)$$

Varying the general matrix Γ_{ij} has the drawback that it is difficult to ensure that the optimum matrix determined by such variational procedures is non-negative. However, the linear combination of $D_f(t)$ given by (5.6) and (8.14) has non-negativity requirements built in, and also the constraints (8.2). Noting (8.15), we see that this choice amounts to using the following expression for Γ_{ij} :

$$\Gamma_{ij} = \frac{2H_\infty}{\alpha_i \alpha_j} \sum_{f=1}^N \lambda_f R_i^f R_j^f, \quad \lambda_f > 0, \quad f = 1, 2, \dots, N, \quad \sum_{f=1}^N \lambda_f = 1. \quad (10.18)$$

Substituting for Γ_{ij} in (10.17), we obtain

$$m(\boldsymbol{\lambda}) = 1 - \mathbf{A} \cdot \boldsymbol{\lambda} + \boldsymbol{\lambda} \cdot \mathbf{B} \boldsymbol{\lambda}, \quad (10.19)$$

where the vector $\boldsymbol{\lambda} \in \mathbb{R}^N$ has components λ_f , $f = 1, 2, \dots, N$, $\mathbf{A} \in \mathbb{R}^N$ while \mathbf{B} is in the space of symmetric linear operators on \mathbb{R}^N . These are given explicitly by

$$\begin{aligned} A_f &= \frac{8H_\infty \alpha_d}{G_d} \sum_{i,j=1}^n \frac{R_i^f R_j^f}{\alpha_i \alpha_j (\alpha_d + \alpha_i)(\alpha_d + \alpha_j)}, \\ B_{fg} &= \frac{2H_\infty^2}{G_d^2} \sum_{i,j,k,l=1}^n \frac{R_i^f R_j^f R_k^g R_l^g}{\alpha_i \alpha_j \alpha_k \alpha_l} \left[\frac{1}{(\alpha_i + \alpha_k)(\alpha_j + \alpha_l)} \right. \\ &\quad \left. + \frac{1}{(\alpha_i + \alpha_l)(\alpha_j + \alpha_k)} \right], \end{aligned} \quad (10.20)$$

$f, g = 1, 2, \dots, N.$

The matrix \mathbf{B} is non-negative by construction.

The idea is to minimize $m(\boldsymbol{\lambda})$, given by (10.19), by varying the λ_f , under the constraints given in (10.18). This is a classic quadratic programming problem. The number of parameters λ_f is typically large, equal to 16 for example in the particular case dealt with here. Maple 2016 was used to obtain a solution.

We also consider an approximation to (5.6) [23] which involves retaining only the minimum and maximum free energies, and related dissipations, in the sum of terms. The vector $\mathbf{A} \in \mathbb{R}^2$ and matrix $\mathbf{B} \in \mathbb{R}^2 \times \mathbb{R}^2$. There are only two λ_i , namely λ_1 and λ_N obeying $\lambda_1 + \lambda_N = 1$ and both must be non-negative, so that $\lambda_1 = \lambda \in [0, 1]$ and $\lambda_N = 1 - \lambda \geq 0$. Relation (10.18) becomes

$$\Gamma_{ij} = \frac{2H_\infty}{\alpha_i \alpha_j} [\lambda R_i^1 R_j^1 + (1 - \lambda) R_i^N R_j^N]. \quad (10.21)$$

The quantities R_i^1 and R_i^N for the minimum and maximum free energies and associated dissipations are described before (9.3). Relation (10.19) is replaced by

$$m(\lambda) = F_0 + F_1 \lambda + F_2 \lambda^2, \quad (10.22)$$

where

$$\begin{aligned} F_0 &= 1 - A_N + B_{NN}, \\ F_1 &= A_N - A_1 + 2(B_{1N} - B_{NN}), \\ F_2 &= B_{11} + B_{NN} - 2B_{1N}. \end{aligned} \quad (10.23)$$

The value of λ yielding an optimum value of $m(\lambda)$ is given by

$$\lambda_0 = -\frac{F_1}{2F_2}. \quad (10.24)$$

This model is discussed further in subsection 10.3. It emerges that, for the parameters chosen, $\lambda_0 \in (0, 1)$, as required without this constraint being explicitly applied.

10.3. Results of the optimization process. Let us now consider the result of the optimization problem described after (10.20). It emerges that the matrix \mathbf{B} is positive semidefinite since five of its eigenvalues are zero or extremely small (less than 0.006 in magnitude). This implies that there may be many choices of the 16 dimensional vector $\boldsymbol{\lambda}$ which give the same optimal behaviour. The results are as follows. The parameters λ_3 to λ_{16} are zero or negligible. The parameters λ_1 and λ_2 are equal to 0.9464 and 0.1067 respectively. Thus, the member of \mathcal{F} closest to the Day free energy has the form

$$\psi_{m2}(t) = 0.9464\psi_m(t) + 0.1067\psi_2(t). \quad (10.25)$$

The last constraint of (10.19) should give that $\lambda_1 + \lambda_2 = 1$, which is not fully enforced by the numerical procedure. This is a difficulty in that it means that $\psi_{m2}(t)$ may not obey the requirements for a free energy. Let us therefore accept that only two of the λ_f are non-zero and implement the procedure leading to (10.22) - (10.24), with the subscript N , replaced by 2, relating to $\psi_2(t)$ in (10.25). Instead of (10.25), we have

$$\psi_{m2}(t) = \lambda_2 \psi_m(t) + (1 - \lambda_2) \psi_2(t), \quad (10.26)$$

where λ_2 must be chosen to minimize $m(\lambda_2)$, defined by

$$m(\lambda_2) = N_0 + N_1 \lambda_2 + N_2 \lambda_2^2, \quad (10.27)$$

with

$$\begin{aligned} N_0 &= 1 - A_2 + B_{22}, \\ N_1 &= A_2 - A_1 + 2(B_{12} - B_{22}), \\ N_2 &= B_{11} + B_{22} - 2B_{12}. \end{aligned} \quad (10.28)$$

The value of λ_2 yielding an optimum value of $m(\lambda_2)$ is given by

$$\lambda_2 = -\frac{N_1}{2N_2} = 0.9169. \quad (10.29)$$

It follows that $1 - \lambda_2 = 0.0831$. The quantity $N_2 = 1.7761 > 0$ so that the optimum point is a minimum. The optimal value of $m(\lambda_2)$ is 0.071.

There is also the second alternative, generated by the solution to (10.22). The quantity λ_0 , given by (10.24), is equal to 0.98 which is therefore the desired optimum point. We have $F_2 = 2.0 > 0$, which again ensures a minimum. Thus, within this approximate treatment, the free energy in \mathcal{F} closest to the Day free energy is given by

$$\psi_{mM}(t) = 0.98\psi_m(t) + 0.02\psi_M(t). \quad (10.30)$$

The total dissipations corresponding to these two choices are compared with the Day total dissipation on Figure 9 and the results discussed in subsection 11.4.

However, it is clear from (10.30) that the Day free energy is very close to $\psi_m(t)$ and not close to $\psi_M(t)$. Also, from (10.26) and (10.29), the proximity of $\psi_D(t)$ to $\psi_m(t)$ is clear.

11. FUNCTIONAL FORMS TO BE EVALUATED AND PLOTTED

The various functional expressions for step function and SE histories are summarized in this section.

11.1. Step function histories. Convenient expressions can be given for step function histories in the case of discrete spectrum materials. We take $E_0 = 1$ in (6.1). The general results (6.5), (6.9) and (6.10) together with relations (8.4)₄, (8.6)₂ and (10.5) yield that

$$\begin{aligned} 2\mathcal{D}(t) = F_d(t) &= \sum_{i,j=1}^n \frac{\Gamma_{ij}}{\alpha_i + \alpha_j} \left[1 - e^{-(\alpha_i + \alpha_j)t} \right] \\ &= \sum_{i,j=1}^n C_{ij} \left[1 - e^{-(\alpha_i + \alpha_j)t} \right], \\ 2\psi(t) = F_s(t) &= 1 - F_d(t). \end{aligned} \quad (11.1)$$

Given the close numerical connection between the total dissipation and $F_d(t)$, only the latter is plotted in subsection 11.4. The various choices of the symmetric matrix Γ are presented in (9.3).

For the case of the Day free energy, we have $n = 1$ and

$$\begin{aligned} F_d(t) &= \chi \left[1 - e^{-2\alpha dt} \right], \\ F_s(t) &= (1 - \chi) \left[1 + \frac{\chi}{1 - \chi} e^{-2\alpha dt} \right], \end{aligned} \quad (11.2)$$

where $\chi \in (0, 1)$ is defined by (3.14)₂.

The formulae (11.1) and (11.2) provide examples of (6.12), for discrete spectrum materials.

11.2. SSE histories. We choose a special case of (6.13) where $E_1 = iE_0 = \overline{E_1}$, so that the history and current value ($E^t, E(t)$) have the forms

$$\begin{aligned} E(t) &= -iE_1[e^{i\omega_-t} - e^{-i\omega_+t}] = 2E_1e^{\eta t} \sin(\omega_0t), \\ E^t(s) &= E(t-s), \quad s \in \mathbb{R}^+, \end{aligned} \quad (11.3)$$

where the ω_{\pm} are defined by (6.14) and $2E_1e^{\eta t}$ is the amplitude. It will be assumed that $E_1 = 1$.

For the total dissipation and F_{dc} , given respectively by (6.32) and (6.39)₁, we use (8.7)₂. The work function is given by (6.24), (6.25) and (7.9). These quantities are plotted in subsection 11.4, together with analogous functions related to the Day free energy.

Recalling (6.19) and (7.8), relation (8.4)₃ can be put in the form (6.30), on using (8.7)₂. Similarly, (8.1) can be shown to be equal to (6.26) by virtue of (8.7)₁, (6.27)₁ and (6.28)₁.

For the Day free energy, the formulae are compact enough to write explicitly. The form of $\mathcal{D}_D(t)$ follows from (6.31) and (8.24). From (8.21) and (8.24), we find that

$$F_{dc} = \frac{(\omega_0^2 + \eta^2)\alpha_d\chi}{\beta\eta[\omega_0^2 + (\alpha_d + \eta)^2] + (\omega_0^2 + \eta^2)\chi(\alpha_d + \eta)}, \quad F_{sc} = 1 - F_{dc}. \quad (11.4)$$

The ratios F_{dc} and F_{sc} are functions of the positive quantities β , ω_0 and η . For exponential histories, we put $\omega_0 = 0$ in (11.4) to obtain

$$F_{dc} = \frac{\eta\alpha_d\chi}{(\beta\alpha_d + \eta)(\alpha_d + \eta)}, \quad F_{sc} = 1 - F_{dc}. \quad (11.5)$$

In this case, one can easily show that $0 \leq F_{dc} \leq 1$ by noting firstly that the quadratic $q(\eta) = (\beta\alpha_d + \eta)(\alpha_d + \eta) - \alpha_d\chi\eta$ has no real zeros for $\beta \leq 1$, and secondly that $q(0) > 0$.

11.3. SE histories which vanish for $t < 0$. The quantity $e_i(t)$, defined by (7.8), becomes

$$\begin{aligned} e_i(t) &= \int_0^\infty e^{-\alpha_i u} \dot{E}^t(u) du = \int_{-\infty}^t e^{-\alpha_i(t-s)} \dot{E}(s) ds \\ &= e^{-\alpha_i t} \int_0^t e^{\alpha_i s} \dot{E}(s) ds, \quad t \geq 0. \end{aligned} \quad (11.6)$$

Relations (7.10), (7.11), (8.1) and (8.4) remain unchanged. The total dissipation is given by

$$\mathcal{D}(t) = \frac{1}{2} \sum_{i,j=1}^n \Gamma_{ij} \int_0^t e_i(u) e_j(u) du = W(t) - \psi(t), \quad (11.7)$$

where the integral is clearly finite.

The history (11.3), nonzero only for $t > 0$, will be used. The parameter η will be allowed have both positive, negative and zero values for such histories. If $\eta = -|\eta| < 0$, the exponential behaviour of the history is decaying rather than increasing. We have

$$\dot{E}(t) = E_1[\omega_- e^{i\omega_-t} + \omega_+ e^{-i\omega_+t}], \quad t > 0, \quad (11.8)$$

and

$$e_i(t) = 2E_1 \operatorname{Re} \left\{ \frac{\omega_-}{\alpha_i + i\omega_-} \left[e^{i\omega_-t} - e^{-\alpha_i t} \right] \right\}. \quad (11.9)$$

Also, from (7.11) and (11.8),

$$\begin{aligned}
 W(t) = & \frac{1}{2}G_\infty E^2(t) + 2E_1^2 \sum_{i=1}^n G_i \operatorname{Re} \left\{ \frac{\omega_-}{2i(\alpha_i + i\omega_-)} (e^{2i\omega_- t} - 1) \right. \\
 & + \frac{|\omega_-|^2}{2\eta(\alpha_i + i\omega_-)} (e^{2\eta t} - 1) \\
 & \left. + \frac{2\omega_-}{(\alpha_i + i\omega_-)} \operatorname{Re} \left[\frac{\omega_-}{(\alpha_i - i\omega_-)} (e^{(i\omega_- - \alpha_i)t} - 1) \right] \right\}.
 \end{aligned} \tag{11.10}$$

The total dissipation is conveniently evaluated by (11.7)₂ and (11.10). The fraction $F_d(t)$, defined by (2.12), can also be determined from these relations. They are plotted in subsection 11.4.

For $\eta < 0$, we see from (11.9) that each $e_i(t)$ tends to zero as $t \rightarrow \infty$, so that $\psi(t)$ and $D(t)$ also have this property. However, $W(t)$ and $\mathcal{D}(t) = W(t) - \psi(t)$ tend to some finite value, which, by neglecting all exponential decay terms in (11.10), can be deduced to be

$$W(\infty) = \mathcal{D}(\infty) = -E_1^2 \sum_{i=1}^n G_i \frac{\alpha_i \omega_0^2}{\eta[(\alpha_i - \eta)^2 + \omega_0^2]}. \tag{11.11}$$

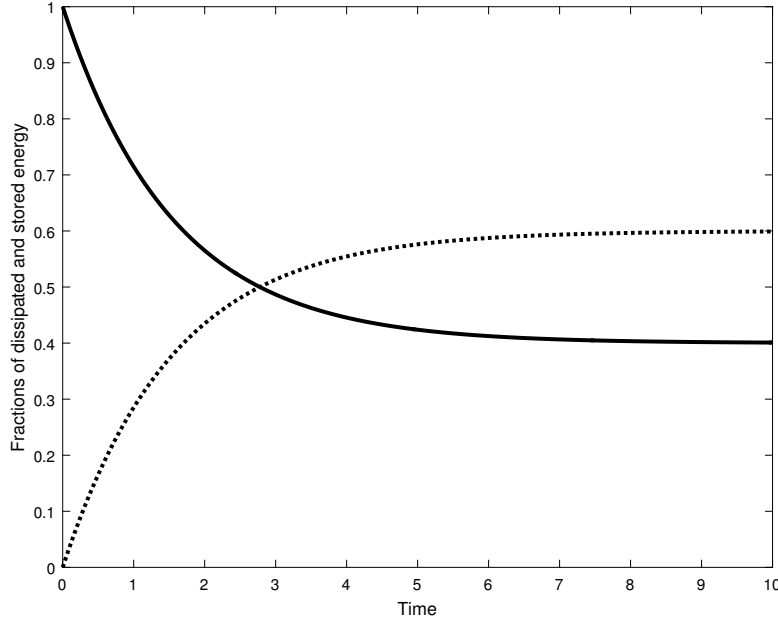


FIGURE 3. The fraction of dissipated (dotted line) and stored (continuous line) energy for the Day functional with a step function history, where $\beta = 0.4$.

11.4. Plotting total dissipation functionals and fractions. The quantities $F_d(t)$, $F_s(t)$ for the Day free energy, given by (11.2), are plotted on Figure 3. The asymptotic limits $F_d(t) \rightarrow \chi$ and $F_s(t) \rightarrow \beta$ are apparent. These curves must always meet at $F_d(t) = F_s(t) = 0.5$.

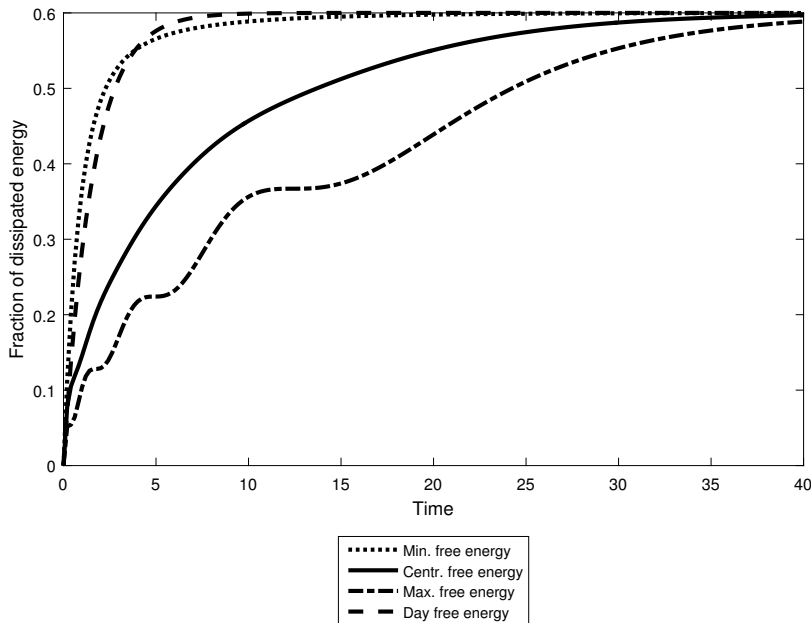


FIGURE 4. The fraction of dissipated energy for minimum, central, maximum and Day free energies with a step-function history, where $\beta = 0.4$.

In all remaining plots, we present only the total dissipations, work functions and the ratios $F_d(t)$, F_{dc} ; free energies and the quantities $F_s(t)$, F_{sc} are easily deduced from (2.10) and (2.12)₃. The total dissipation associated with the minimum, central and maximum free energies are denoted by $\mathcal{D}_m(t)$, $\mathcal{D}_c(t)$ and $\mathcal{D}_M(t)$. The total dissipation for the Day free energy is $\mathcal{D}_D(t)$, introduced before (11.4).

The three fractions $F_d(t)$ derived from (9.3) (or total dissipations; see comment after (11.1)) and the corresponding quantity for the Day free energy in the case of step function histories are plotted on Figure 4, where $\beta = 0.4$. These are the quantities given by (11.1)_{2,3} and (11.2)₁. Note that $\mathcal{D}_m(t)$ is the largest, while $\mathcal{D}_M(t)$ is the smallest. For all other free energies, the total dissipation is intermediate, in particular, $\mathcal{D}_c(t)$. These assertions are obvious consequences of (2.10).

The Day free energy used here and below is such that $\alpha_d = 0.3225$, as observed after (10.15). Also, (7.2), (8.17)₂, (10.3) and (10.5) determine $G_d = nG_1$ to be equal to χ . This free energy yields a dissipation fraction very close to that for the minimum free energy. Note that some curves on Figure 4 approach their asymptotic value χ quite slowly. This is due to the smallness of α_1 , as pointed out after (10.15) in the context of Figure 2.

For all the curves presented below, there is a proximity between $\mathcal{D}_D(t)$ and $\mathcal{D}_m(t)$; in some cases, this is true for $\mathcal{D}_c(t)$. Similar statements must apply to $\psi_D(t)$ and $\psi_m(t)$ (or, where applicable, $\psi_c(t)$), since, as argued below, $W(t)$ and $W_D(t)$ are close. This phenomenon is supported by (10.26), (10.29) and (10.30). The very simple formula for the Day free energy could in many circumstances provide a quick,

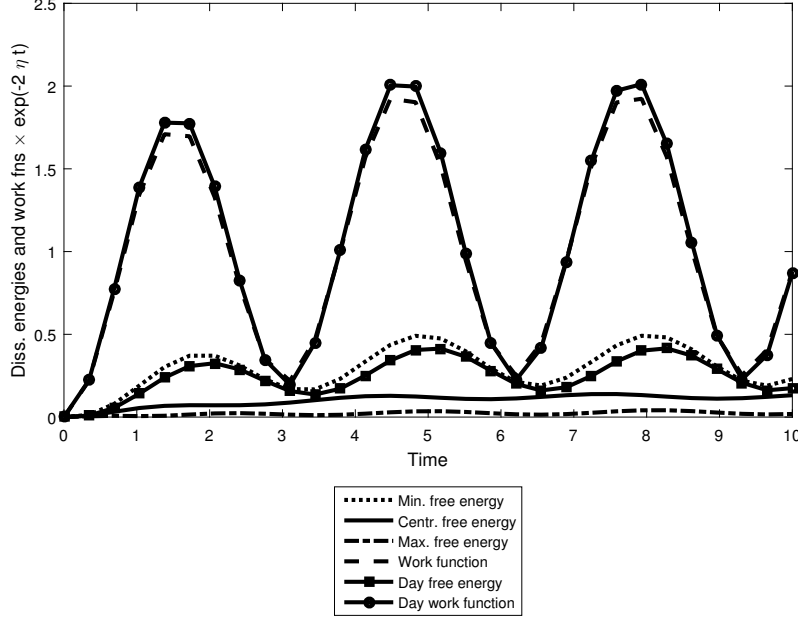


FIGURE 5. Dissipated energies $\times e^{-2\eta t}$ related to the listed free energies for SE histories vanishing for $t < 0$ where $\eta = 0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$; also the listed work functions.

fairly accurate approximation³ to the minimum free energy. This feature may be useful in a practical sense.

Figures 5 and 6 are plots of dissipated energy and of these quantities divided by the work functions, for SE histories vanishing if $t < 0$. Figures 10 and 11 are similar plots for SSE histories. We multiply all quantities plotted on Figures 5 and 10 by $e^{-2\eta t}$, which shows the relative positions of the various curves with greater clarity.

The quantities $\mathcal{D}_c(t)$ and $\mathcal{D}_M(t)$ exhibit reduced oscillations in Figures 5 and 10. These are presented with a larger scale on Figure 9, showing the same effect. The work function is strongly oscillatory, which produces the more marked oscillation in the fractions involving $\mathcal{D}_c(t)$ and $\mathcal{D}_M(t)$ on Figures 6 and 11.

On Figure 6 (and Figure 11), we notice that the fractions related to the minimum and Day total dissipations coincide near the oscillation peaks.

Figures 5, 10 and 6, 11 are very similar, but distinguished by a time translation; $t = 0$ on Figures 5, 6 correspond roughly to $t = 2$ on Figures 10, 11. This indicates that transient effects quickly vanish for the histories that are zero when $t < 0$.

On Figures 5, 7, 10, 12, 14 and 16, it is clear that the work function $W(t)$ is very close to the Day work function $W_D(t)$. We refer in this context to the paragraph after (10.10).

The same plots for the same parameters are presented on Figures 7 and 8 as on Figures 5 and 6, except that $\eta = -0.5$. The oscillatory nature of the histories is reflected in both plots. On Figure 7, the difference between $W(t)$ and $W_D(t)$ is slightly more substantial than on the other plots.

³The free energy $\psi_F(t)$ referred to in the Introduction, also has the property that, in at least some cases, it is a close approximation of $\psi_m(t)$ [3].

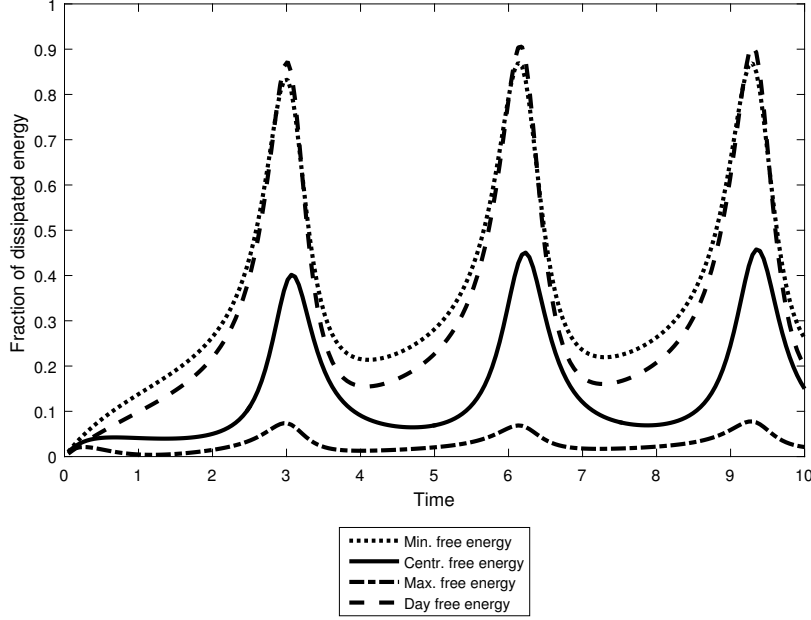


FIGURE 6. Fraction of dissipated energy related to the listed free energies for SE histories vanishing for $t < 0$ where $\eta = 0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$.

The phenomenon described in the context of (11.11) is clear from Figure 7. Indeed, if the formula (11.11) is evaluated for the stated parameters, it yields that $W(\infty) = \mathcal{D}(\infty) = 0.26$.

On Figure 9, the total dissipations associated with ψ_{m2} and ψ_{mM} (denoted by $\mathcal{D}_{m2}(t)$ and $\mathcal{D}_{mM}(t)$), defined in subsection 10.3, are compared, for SSE histories, with $\mathcal{D}_D(t)$ and $\mathcal{D}_m(t)$. It emerges from this plot that $\mathcal{D}_{mM}(t)$ is very close to $\mathcal{D}_m(t)$ and less close to $\mathcal{D}_D(t)$, while $\mathcal{D}_{m2}(t)$ is intermediate between the two and is a better fit to $\mathcal{D}_D(t)$, though not a close fit.

The plots from Figure 12 onwards are illustrations of the dependence of the average total dissipation and the quantity F_{dc} (defined by (6.39)₁, (7.9) and (8.7)₂) on the parameters η , ω_0 and β . The first two are parameters of the history, while the last one is a property of the material. Also, the equivalent quantity for the Day free energy, as given by (11.4), is plotted. All these are for SSE histories.

On Figure 12 and 13, we have plots of the average total dissipations and F_{dc} for SSE histories as a function of η , with ω_0 and β as specified, and the corresponding quantities for the Day free energy. Also, the work function and the Day work function are plotted on Figure 12. Figure 14 and 15 are plots of these quantities as a function of ω_0 , with η and β fixed, while Figure 16 and 17 present them as a function of β , with η and ω_0 specified. Note that there is a magnification of difference for each of these cases between the plots of total dissipation and those of fractions.

All curves decline with increasing η and β but become larger with ω_0 . These are in line with intuitive expectations. Regarding the variation with β , we recall

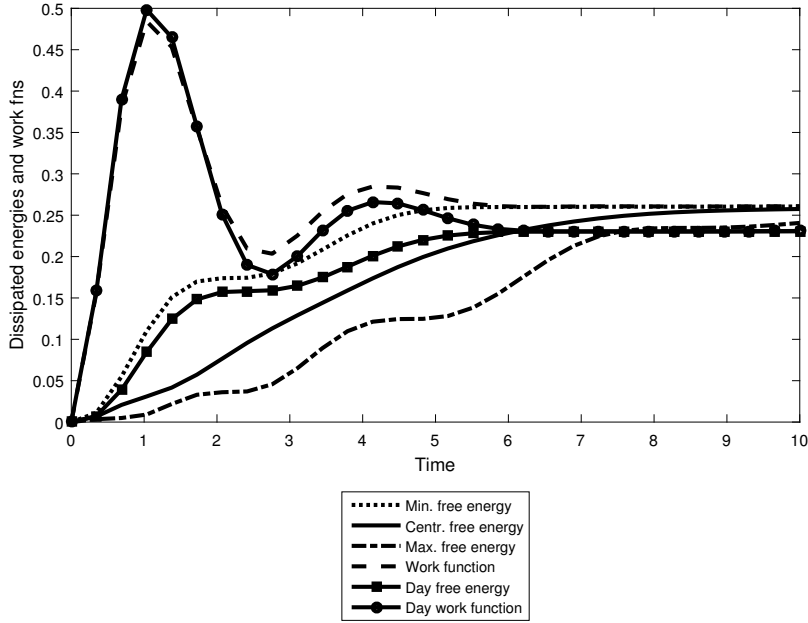


FIGURE 7. Dissipated energy related to the listed free energies for SE histories vanishing for $t < 0$ where $\eta = -0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$; also the listed work functions.

remark 3.1; also, it is consistent with (11.2)₁ for large times since χ decreases as β increases.

The Day average total dissipation (referred to as \mathcal{D}_{Da}) is close to the average total dissipation associated with the minimum free energy, \mathcal{D}_{ma} , as η varies, though, particularly for lower values of η , it is perceptibly separate and more evenly spaced between \mathcal{D}_{ma} and the dissipations associated with the central free energy (the latter referred to as \mathcal{D}_{ca}). As a function of ω_0 , this quantity is close to \mathcal{D}_{ma} at low values, but moves over to \mathcal{D}_{ca} as ω_0 increases. The quantity \mathcal{D}_{Da} is closer to \mathcal{D}_{ma} than \mathcal{D}_{ca} for all values of β , though the three converge as $\beta \rightarrow 1$.

A plausible choice to represent the Day energy loss fraction is the curve, indeed almost straight line, on Figure 17, describing the behaviour of F_{dc} given by (11.4). This formula depends only weakly on ω_0 , which can be seen by considering the plot of the Day total dissipation on Figure 14. Putting $\omega_0 = 0$ yields (11.5) and near $\beta = 0$ gives, for $\alpha = \alpha_d$, the form

$$F_{dc} = \frac{\alpha_d \chi}{\alpha_d + \eta}. \quad (11.12)$$

This simple relation in fact is a good fit for the Day fraction on Figure 17, because of the near linearity of the curve and the fact that F_{dc} vanishes at $\chi = 0$. Equation (11.12) holds for values of η other than 0.5, provided the curve remains nearly linear. For small η , it reduces to $F_{dc} = \chi$, as in the step function case. However, (11.12) provides only a very rough approximation to the Day curve on Figure 13.

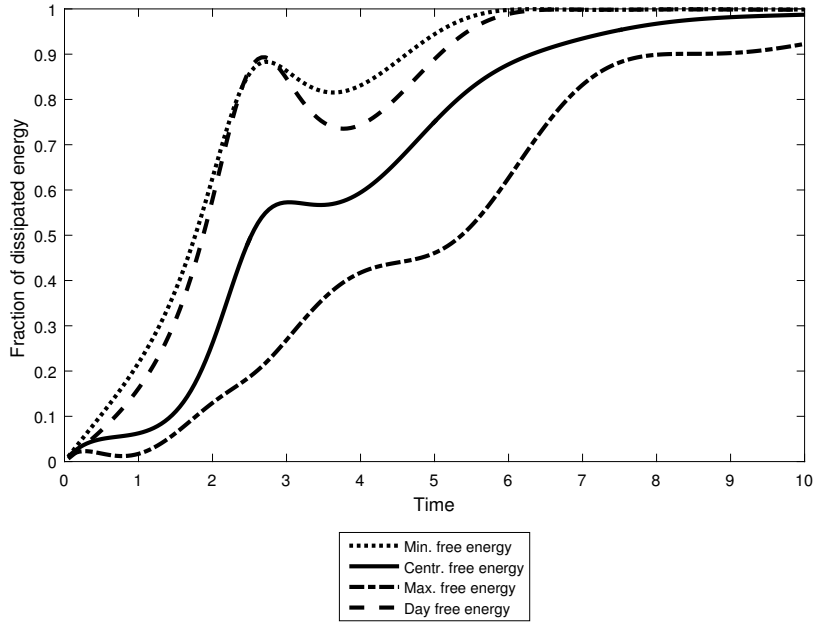


FIGURE 8. Fraction of dissipated energy related to the listed free energies for SE histories vanishing for $t < 0$ where $\eta = -0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$.

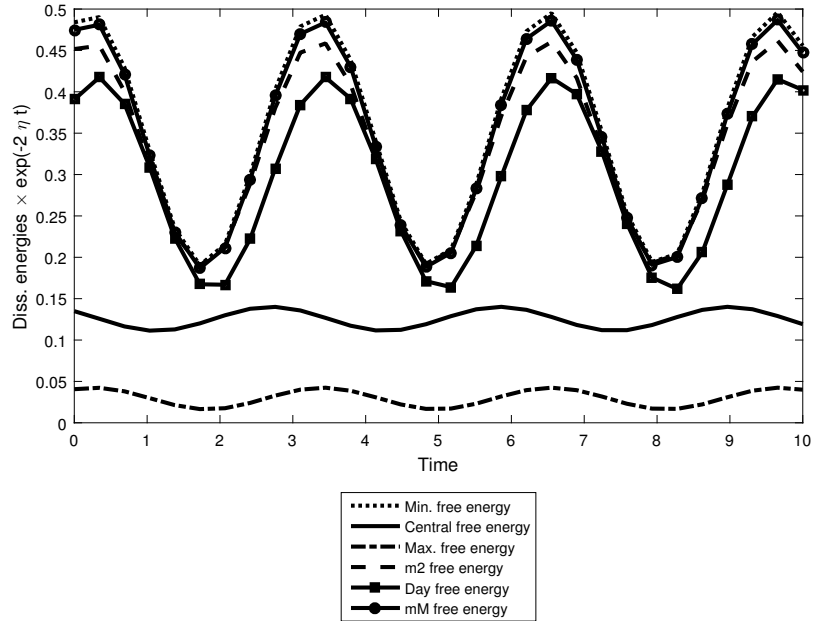


FIGURE 9. Comparison of dissipated energies $\times e^{-2\eta t}$ related to the listed free energies for SSE histories, where $\eta = 0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$.

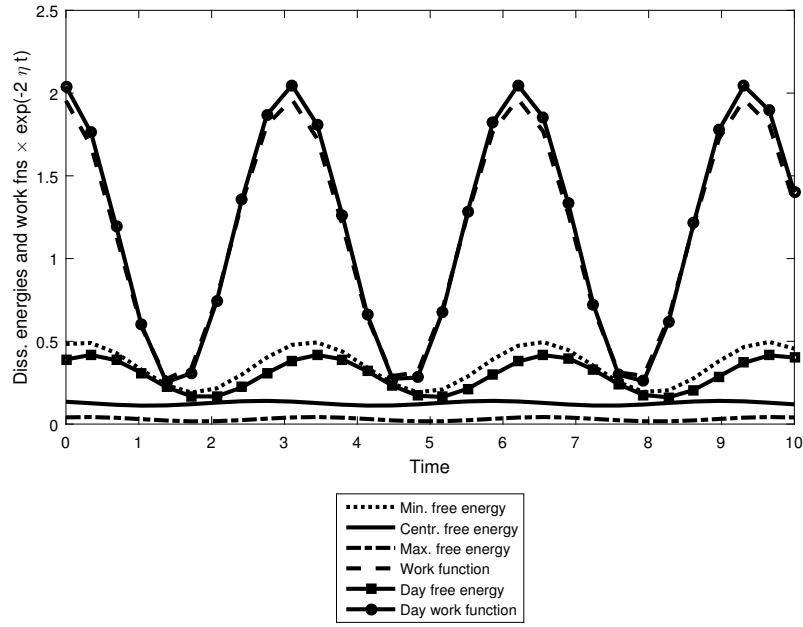


FIGURE 10. Dissipated energies $\times e^{-2\eta t}$ related to the listed free energies for SSE histories, where $\eta = 0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$;

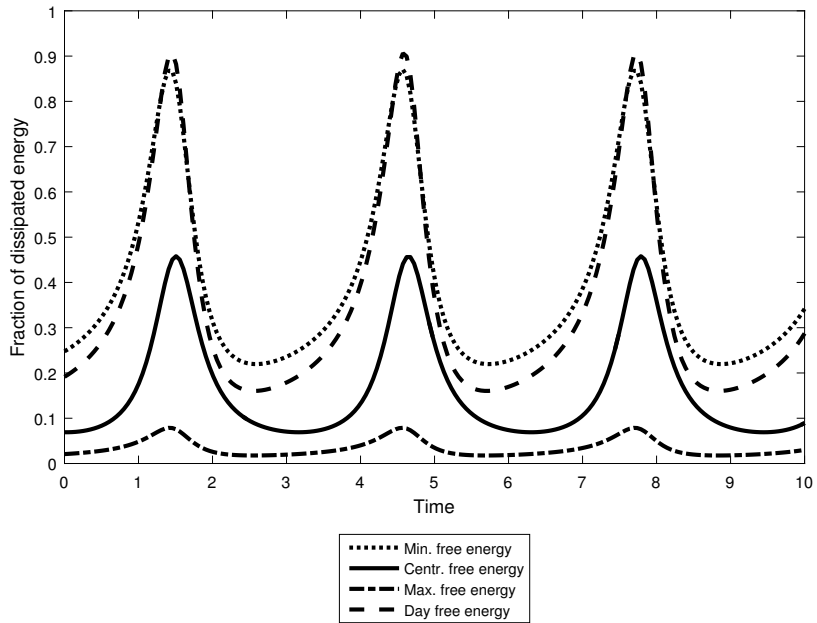


FIGURE 11. Fraction of dissipated energy related to the listed free energies for SSE histories, where $\eta = 0.5$, $\omega_0 = 1.0$ and $\beta = 0.4$.

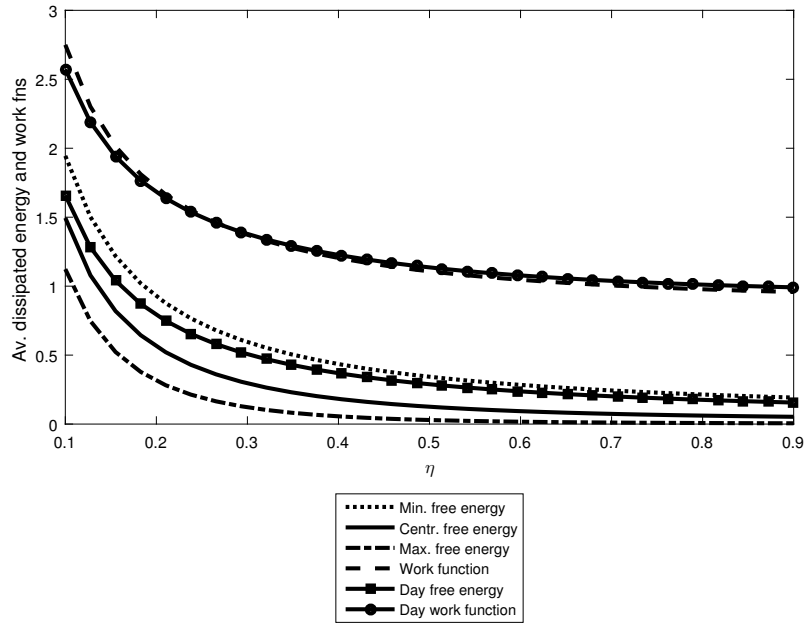


FIGURE 12. The average dissipated energy related to the listed free energies and work functions for SSE histories as functions of η with $\omega_0 = 1.0$ and $\beta = 0.4$.

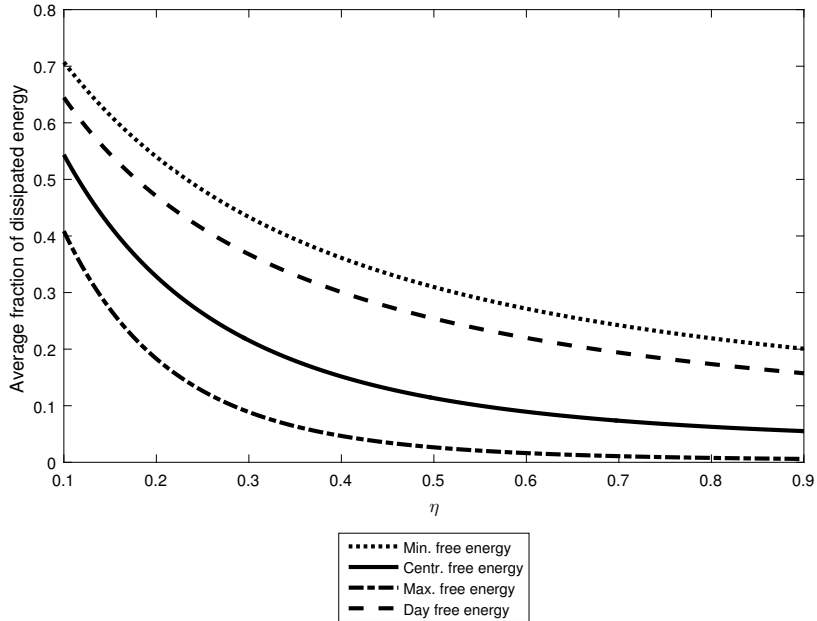


FIGURE 13. The average fraction of dissipated energy related to the listed free energies for SSE histories as functions of η , with $\omega_0 = 1.0$ and $\beta = 0.4$.

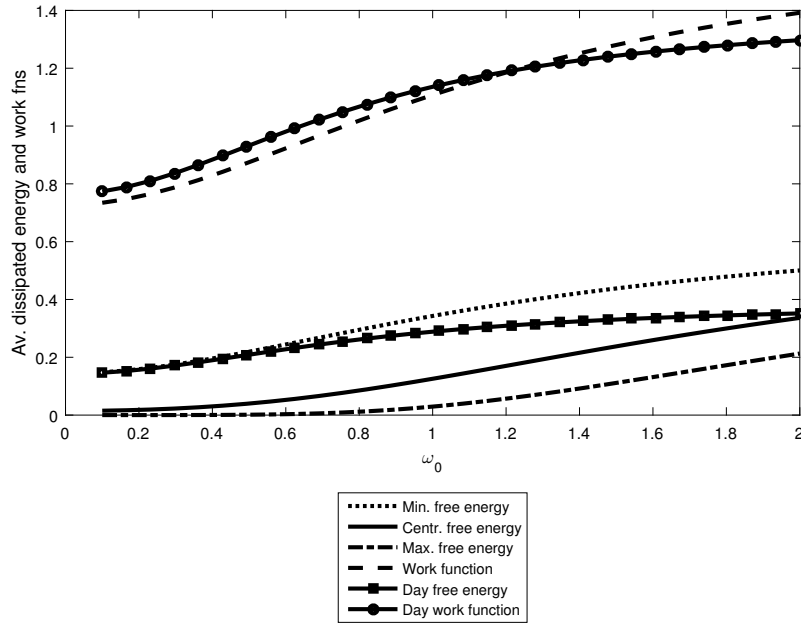


FIGURE 14. The average dissipated energy related to the listed free energies and work functions for SSE histories as functions of ω_0 with $\eta = 0.5$ and $\beta = 0.4$.

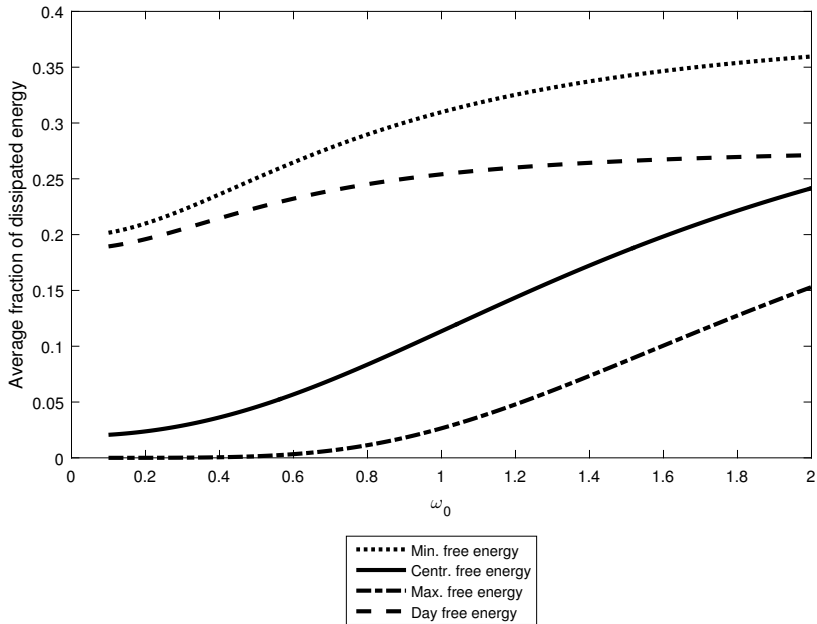


FIGURE 15. The average fraction of dissipated energy related to the listed free energies for SSE histories as functions of ω_0 , with $\eta = 0.5$ and $\beta = 0.4$.

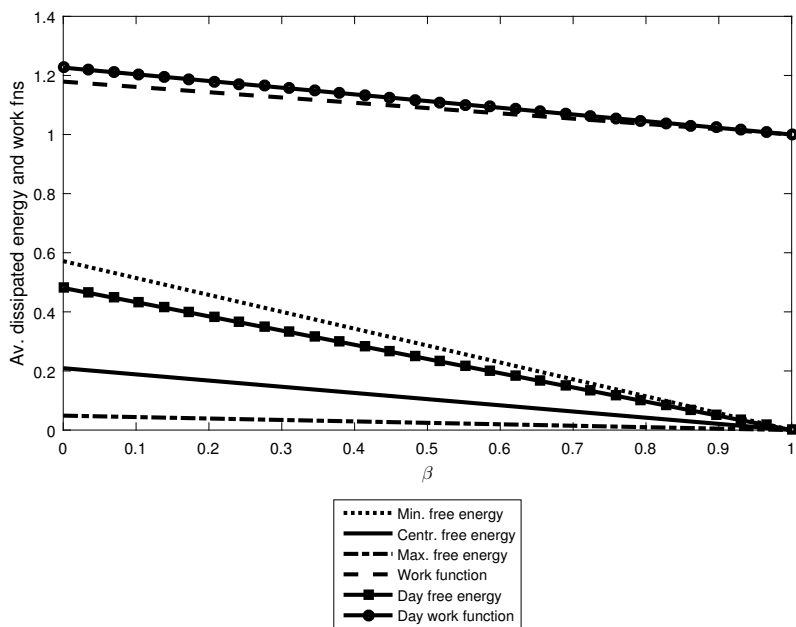


FIGURE 16. The average dissipated energy related to the listed free energies and work functions for SSE histories as functions of β with $\alpha = 0.5$ and $\omega_0 = 1$.

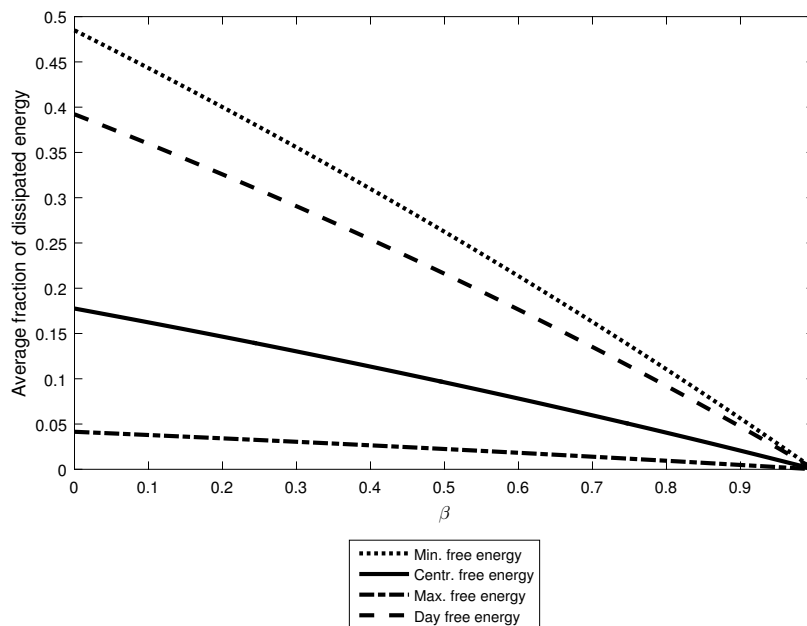


FIGURE 17. The average fraction of dissipated energies related to the listed free energies for SSE histories as functions of β with $\eta = 0.5$ and $\omega_0 = 1$.

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