

# THE MINIMUM FREE ENERGY FOR CONTINUOUS SPECTRUM MATERIALS

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ABSTRACT. A general closed expression is given for the isothermal minimum free energy of a linear viscoelastic material with continuous spectrum response. Two quite distinct approaches are adopted, which give the same final result. The first involves expressing a positive quantity, closely related to the loss modulus of the material, defined on the frequency domain, as a product of two factors with specified analyticity properties. The second is the continuous spectrum version of a method used by Breuer and Onat [1] for materials with relaxation function given by sums of exponentials. It is further shown that minimal energy states [6] are uniquely related to histories and the work function is the maximum free energy with the property that it is a function of state.

## 1. INTRODUCTION.

A general expression for the minimum free energy of a linear viscoelastic material under isothermal conditions was given in [2]. This was for a scalar constitutive relation. A generalization to the full tensor case has also been presented [4]. Detailed, explicit expressions for the minimum free energy and related quantities were given in [2, 4] for discrete spectrum materials, namely those for which the relaxation function is a sum of exponentials. The minimum free energy of compressible viscoelastic fluids was determined in [9] while materials with finite memory were considered in [7]. These results are used in the context of the viscoelastic Saint-Venant problem in [10].

A definition of a viscoelastic state, based on the ideas of Noll [11], has been given and explored in [20, 19] (see also [12]). Such a state has been termed a minimal state in [6].

Also, a formalism has been developed [6] for the scalar case, which allows expressions for a family of free energies related to a particular minimal state to be derived for discrete spectrum models, including minimum and maximum free energies. Generalization of this work to the full tensor, non-isothermal case was presented in [8]. A generalization of the formalism in [6] has been used recently to propose a closed formula for the physical free energy and rate of dissipation.

It is not clear how the formulae emerging from the methodology developed in [2, 4] apply to materials other than those exhibiting a discrete spectrum response, in particular for materials with a continuous spectrum response *i.e.* those for which the relaxation function is given by an integral of a density function multiplying a decaying exponential. The object of the present work is to address this issue. We

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will confine the treatment to the scalar case. There is no great loss of generality in doing so because, in the general tensor case, explicit solutions have been given only if the eigenspaces of the relaxation tensor derivative are time-independent, and on each such eigenspace, the explicit results are precisely those of the scalar case [4, 8]

All the above papers are based on the same methodology, which involves factorizing a quantity closely related to the loss modulus of the material, in order to solve the relevant Wiener-Hopf equation (or equivalent variational problem) for the optimal future continuation required to determine the minimum free energy. Another method was used in [1] for the discrete spectrum case. This involved making a very natural assumption on the form of the optimal future continuation and solving algebraic equations for the various parameters. The need for factorization did not arise. This method is also developed in the present work for continuous spectrum materials. The assumption involved in this case is also a very natural one, namely that the optimal future continuation has a singularity structure determined only by that of the Fourier transform of the relaxation function derivative.

The layout of the paper is as follows. In section 2, fundamental relationships are written down and the basic factorization property is introduced. The Wiener-Hopf equation relating to the maximum recoverable work is derived in section 3. The factorization procedure is discussed in depth for the continuous spectrum case in section 4; and some related formulae are considered in section 5. The minimum free energy is discussed in section 6. The alternative approach referred to in the previous paragraph is discussed in detail in section 7. The concept of a minimal state for continuous spectrum materials is explored in section 8. Some examples are presented in section 9.

## 2. BASIC RELATIONSHIPS

We consider a linear viscoelastic solid, subject to stress in such a way that there is only one non-zero component of stress  $T(t)$  and strain  $E(t)$  related by

$$\begin{aligned} T(t) &= G_0 E(t) + \int_0^\infty G'(s) E^t(s) ds, & E^t(s) &= E(t-s), & s \in \mathcal{R} \\ &= G_\infty E(t) + \int_0^\infty G'(s) E_r^t(s) ds, & E_r^t(s) &= E^t(s) - E(t) \end{aligned} \quad (2.1)$$

where  $E^t \in L^1(\mathcal{R}^+) \cap L^2(\mathcal{R}^+) \cap C^1(\mathcal{R}^+)$  and  $G' \in L^1(\mathcal{R}^+) \cap L^2(\mathcal{R}^+)$  using the notation here and below:  $\mathcal{R}$  is the set of reals,  $\mathcal{R}^+$  the positive reals, and  $\mathcal{R}^{++}$  the strictly positive reals; similarly  $\mathcal{R}^-$ ,  $\mathcal{R}^{--}$  are the negative and strictly negative reals. The relative history  $E_r^t$  will be used extensively later <sup>1</sup>. The relaxation function

$$G(s) = G_0 + \int_0^s G'(u) du \quad (2.2)$$

is well-defined along with  $G_\infty = \lim_{s \rightarrow \infty} G(s)$ . We take

$$G_\infty > 0 \quad (2.3)$$

so that the body is a solid.

A viscoelastic state is defined in general by the current value of strain and the history  $(E(t), E^t)$ . The concept of a minimal state ([6] based on ideas introduced in

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<sup>1</sup>Note that this notation differs from that in [2]

[11, 12, 19, 20, 4, 17]) can be expressed as follows: two viscoelastic states  $(E_1(t), E_1^t)$ ,  $(E_2(t), E_2^t)$  are equivalent or in the same minimal state if

$$E_1(t) = E_2(t); \quad \int_0^\infty G'(s + \tau) [E_1^t(s) - E_2^t(s)] ds = 0 \quad \forall \tau \geq 0. \quad (2.4)$$

Let  $\Omega$  be the complex  $\omega$  plane and

$$\begin{aligned} \Omega^+ &= \{\omega \in \Omega \mid \text{Im}(\omega) \in \mathcal{R}^+\} \\ \Omega^{(+)} &= \{\omega \in \Omega \mid \text{Im}(\omega) \in \mathcal{R}^{++}\} \end{aligned} \quad (2.5)$$

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

For any  $f \in L^2(\mathcal{R})$ , its Fourier transform  $f_F \in L^2(\mathcal{R})$  is given by

$$f_F(\omega) = \int_{-\infty}^\infty f(\xi) e^{-i\omega\xi} d\xi. \quad (2.6)$$

If  $f$  is a real-valued function in the time domain - which will be the case for all functions of interest here - then

$$\bar{f}_F(\omega) = f_F(-\omega) \quad (2.7)$$

where the bar denotes complex conjugate.

We have

$$\begin{aligned} f_F(\omega) &= f_+(\omega) + f_-(\omega) \\ f_+(\omega) &= \int_0^\infty f(\xi) e^{-i\omega\xi} d\xi \\ f_-(\omega) &= \int_{-\infty}^0 f(\xi) e^{-i\omega\xi} d\xi, \quad f_\pm \in L^2(\mathcal{R}) \end{aligned} \quad (2.8)$$

where  $f_+$  is analytic in  $\Omega^{(-)}$ . For the cases of interest in the present work, we also assume that it is analytic on an open set including  $\Omega^-$ , so that we include  $\mathcal{R}$  in the region of analyticity. Similarly,  $f_-$  is analytic on an open set which includes  $\Omega^+$ . We will abbreviate these statements in what follows as:  $f_\pm$  is analytic in  $\Omega^\mp$ . We have

$$\lim_{\omega \rightarrow \infty} i\omega f_+(\omega) = f(0^+), \quad \lim_{\omega \rightarrow \infty} i\omega f_-(\omega) = -f(0^-). \quad (2.9)$$

Functions on  $\mathcal{R}$  which vanish identically on  $\mathcal{R}^{--}$  are defined as functions on  $\mathcal{R}^+$ . For such quantities,  $f_F = f_c - if_s$  where  $f_c, f_s$  are the Fourier cosine and sine transforms

$$\begin{aligned} f_c(\omega) &= \int_0^\infty f(\xi) \cos \omega\xi d\xi = f_c(-\omega) \\ f_s(\omega) &= \int_0^\infty f(\xi) \sin \omega\xi d\xi = -f_s(-\omega). \end{aligned} \quad (2.10)$$

Thus

$$F(\omega) = G'_F(\omega) = \int_0^\infty G'(s) e^{-i\omega s} ds = G'_c(\omega) - iG'_s(\omega) \quad (2.11)$$

The notation  $F$  is introduced to simplify later formulae. We shall require the property of  $F$  that

$$\lim_{\omega \rightarrow \infty} i\omega F(\omega) = G'(0). \quad (2.12)$$

which is a special case of (2.9)<sub>1</sub>. Properties of  $G'_s(\omega)$  include [18]

$$\begin{aligned} G'_s(\omega) &\leq 0 \quad \forall \omega \in \mathcal{R}^{++} \\ G'_s(-\omega) &= -G'_s(\omega), \quad \forall \omega \in \mathcal{R} \end{aligned} \quad (2.13)$$

the first relation being a consequence of the second law of thermodynamics and the second being a particular case of (2.10). It follows that  $G'_s(0) = 0$ . We also have [18]

$$G_\infty - G_0 = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{G'_s(\omega)}{\omega} d\omega < 0 \quad (2.14)$$

so that  $G'_s(\omega)/\omega \in L^1(\mathcal{R})$ . It follows from (2.3) and (2.14) that  $G_0$  is positive definite.

The function  $F$  is analytic on  $\Omega^{(-)}$ . This is a consequence of the fact that  $G'$  vanishes on  $\mathcal{R}^{--}$  which is essentially the requirement of Causality [21]. As noted above, it is assumed that  $F$  is analytic in  $\Omega^-$ . Relation (2.11)<sub>1</sub> can be used to define  $F(\omega)$  where the integral converges, namely  $\Omega^-$  and possibly a strip of  $\Omega^{(+)}$ . Elsewhere, it is defined by analytic continuation from the region in which the integral exists. In fact, such continuation will generally be possible to all of  $\Omega^{(+)}$ , excluding singular points.

Letting the bar denoted complex conjugate, we write  $\overline{F(\omega)}$  for the quantity  $\overline{F(\overline{\omega})}$  and  $\overline{F}(\omega)$  for the complex conjugate if  $\omega \in \mathcal{R}$ , or more generally  $\overline{F(\overline{\omega})}$ . For  $\omega \in \mathcal{R}$ , we have  $F(-\omega) = \overline{F}(\omega)$ . The quantity  $\overline{F}$  is analytic in  $\Omega^+$ , a mirror image, in the real axis, of the singularity structure of  $F(\omega)$ . Thus,  $G'_s(\omega)$  has singularities in both  $\Omega^{(+)}$  and  $\Omega^{(-)}$  which are mirror images of one another. Similarly, its zeros will be mirror images of one another. We will be interested in the singularity structure of

$$\begin{aligned} H(\omega) &= \frac{\omega}{2i} (F(\omega) - \overline{F}(\omega)) \\ &= -\omega G'_s(\omega) = H(-\omega) \geq 0 \quad \forall \omega \in \mathcal{R} \end{aligned} \quad (2.15)$$

$$H(\omega) = H_1(\omega^2)$$

This last relation is a consequence of the analyticity of  $H(\omega)$  on the real axis. It follows that  $H(\omega)$  goes to zero at least quadratically at the origin. It is assumed that the behaviour is in fact quadratic, *i.e.*  $H(\omega)/\omega^2$  tends to a finite, non-zero quantity as  $\omega$  tends to zero. Note that  $H(\omega)$  is positive semi-definite. The singularities of  $H$  are the same as those of  $F$  in  $\Omega^{(+)}$  and of  $\overline{F}$  in  $\Omega^{(-)}$ . It will be required in later developments that  $H(\omega)$  can be written in the form

$$H(\omega) = H_+(\omega)H_-(\omega) \quad (2.16)$$

where  $H_+(\omega)$  has no singularities or zeros in  $\Omega^{(-)}$  and is thus analytic in  $\Omega^-$ . Similarly,  $H_-(\omega)$  is analytic in  $\Omega^+$  with no zeros in  $\Omega^{(+)}$ . Therefore the singularities of  $F$  must all occur in  $H_+$  and those of  $\overline{F}$  in  $H_-$ . There may be other singularities

in  $H_{\pm}$  which cancel on multiplication. That such a factorization is always possible is shown for general tensor constitutive relations in [4].

Using (2.12) and (2.15), one can show that

$$H_{\infty} = \lim_{|\omega| \rightarrow \infty} H(\omega) = -G'(0) \geq 0 \quad (2.17)$$

The sign of  $G'(0)$  has been deduced by various authors from thermodynamic constraints in the general three-dimensional case [23, 15, 18]. We assume for present purposes that  $G'(0)$  is non-zero so that  $H_{\infty}$  is a finite, positive number. Then  $H(\omega) \in \mathcal{R}^{++} \forall \omega \in \mathcal{R}, \omega \neq 0$ .

The factorization (2.16) is unique up to a constant phase factor. We put [2]

$$\begin{aligned} H_{\pm}(\omega) &= H_{\mp}(-\omega) = \overline{H_{\mp}(\omega)} \\ H(\omega) &= |H_{\pm}(\omega)|^2, \end{aligned} \quad (2.18)$$

one consequence of which is that the factorization is now unique up to a change of sign.

A general method is outlined in [2] for determining the factors of  $H$ . A modification of this method is presented here, which is more convenient for the present application. As observed in [2], the function  $T(\omega)H(\omega)$ , where <sup>2</sup>

$$T(\omega) = \frac{\omega^2 + \omega_0^2}{H_{\infty}\omega^2}, \quad (2.19)$$

is positive-definite on  $\mathcal{R}$ , non-singular at the origin and approaches unity for large  $\omega$ . The frequency  $\omega_0 \in \mathcal{R}^{++}$  may be chosen arbitrarily. Therefore, the function  $\log(T(\omega)H(\omega))$  is well-defined on  $\mathcal{R}$  and approaches zero for large  $\omega$ . Let [2]

$$\begin{aligned} H_+(\omega) &= \frac{\omega h_{\infty}}{\omega - i\omega_0} e^{-M^+(\omega)} \\ h_{\infty} &= H_{\infty}^{1/2} \end{aligned} \quad (2.20)$$

where  $M^+$  is given by <sup>3</sup>

$$\begin{aligned} M^+(\omega) &= \lim_{\beta \rightarrow 0^-} M(\omega + i\beta) \\ M(z) &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log[T(\omega')H(\omega')]}{\omega' - z} d\omega', \quad z \in \Omega \setminus \mathcal{R}. \end{aligned} \quad (2.21)$$

Using (2.15), we can write

$$\begin{aligned} \log(T(\omega)H(\omega)) &= \log \left[ -i \frac{\omega - i\omega_0}{H_{\infty}} F(\omega) \right] + \log U(\omega) \\ U(\omega) &= \frac{1}{2} \left[ 1 - \frac{\overline{F(\omega)}}{F(\omega)} \right] \left[ \frac{\omega + i\omega_0}{\omega} \right]. \end{aligned} \quad (2.22)$$

The standard branch of the logarithm function is chosen, namely that which vanishes for argument unity. The function  $U$  is complex but non-zero on the real line and approaches unity for large  $\omega$ , by virtue of (2.12). Similarly for the argument of

<sup>2</sup>The introduction of the parameter  $\omega_0$  represents a slight modification (improvement) of the formula in [2]

<sup>3</sup>The quantity  $M^+(\omega)$  was denoted by  $M^-(\omega)$  in [2] and *vice versa*. The present usage is more consistent with the rest of the paper.

the first term on the right of (2.22)<sub>1</sub>. This term has all its singularities in  $\Omega^{(+)}$  so that if we close on  $\Omega^{(-)}$  for  $Imz < 0$  then, by Cauchy's theorem, its contribution to  $M(z)$  is simply the negative of itself. Thus, we have

$$\begin{aligned} H_+(\omega) &= \frac{-i\omega}{h_\infty} F(\omega) e^{-N^+(\omega)}, \quad \omega \in \mathcal{R} \\ N^+(\omega) &= \lim_{\beta \rightarrow 0^-} N(\omega + i\beta) \\ N(z) &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log U(\omega')}{\omega' - z} d\omega', \quad z \in \Omega \setminus \mathcal{R}. \end{aligned} \tag{2.23}$$

Using the relation (2.18)<sub>1</sub> we deduce that

$$\begin{aligned} H_-(\omega) &= \frac{i\omega}{h_\infty} \bar{F}(\omega) e^{-N^-(\omega)}, \quad \omega \in \mathcal{R} \\ N^-(\omega) &= \lim_{\beta \rightarrow 0^-} \bar{N}(\omega - i\beta) \\ \bar{N}(z) &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log \bar{U}(\omega')}{\omega' - z} d\omega', \quad z \in \Omega \setminus \mathcal{R}. \end{aligned} \tag{2.24}$$

The extraction of the factor  $F$  in (2.23) and  $\bar{F}$  in (2.24) has the advantage that the correct behaviour of  $H_\pm$  at small and large  $\omega$  is assured. This is of course true of (2.20) but the apparent singularity at  $\omega = i\omega_0$  must be eliminated, and the procedures for doing this after the transformations described in section 4 have been carried out is not straightforward. Using (2.23), (2.24) the parameter  $\omega_0$  drops out of the formulae in a simple manner, as we shall see later. Furthermore, the singularities of  $F$  in  $\Omega^{(+)}$  must occur also in  $H_+$  (though in fact  $H_+$  may have other singularities), while a similar statement applies to  $H_-$  and  $\bar{F}$ . If the transformation carried out on  $N^+$  in section 4 were instead carried out on  $M^+$  (and this is the natural first approach), it is in fact rather difficult to ensure that the singularity structures of  $H_\pm$  in  $\Omega^\pm$  are correct. This is particularly true of logarithmic singularities which can, as we shall see, occur at the end points of the branch cuts.

Consider now the strain history  $E^t$ . Define

$$E_+^t(\omega) = \int_0^\infty E^t(s) e^{-i\omega s} ds, \quad E_+^t \in L^2(\mathcal{R}^+) \tag{2.25}$$

It is analytic in  $\Omega^{(-)}$ , a property which will be assumed to extend to  $\Omega^-$ . This region can be extended to include  $\Omega^{(+)}$ , excluding singular points, by analytic continuation. From (2.9)<sub>1</sub>, it follows that

$$\lim_{\omega \rightarrow \infty} i\omega E_+^t(\omega) = E^t(0^+) = E(t). \tag{2.26}$$

We also require the Fourier transform of the relative history.

$$\begin{aligned} E_{r+}^t(\omega) &= E_+^t(\omega) - E(t) \int_0^\infty e^{-i\omega s} ds \\ &= E_+^t(\omega) - \frac{E(t)}{i\omega^-}; \quad \omega^- = \lim_{\alpha \rightarrow 0^+} (\omega - i\alpha) \end{aligned} \tag{2.27}$$

where the limit being taken after any integration involving the quantity  $(\omega^-)^{-1}$  has been carried out. Under a similar assumption to that for  $E_+^t$ , we have that  $E_{r+}^t$  is analytic on  $\Omega^-$ . Note that, by virtue of (2.9)<sub>1</sub>,  $E_{r+}^t$  goes to zero at large  $\omega$  as  $\omega^{-2}$ .

Let us also define

$$E_-^t(\omega) = \int_{-\infty}^0 E^t(s)e^{-i\omega s} ds, \quad E_-^t \in L^2(\mathcal{R}^-) \quad (2.28)$$

It is analytic in  $\Omega^{(+)}$ , a property which will be assumed to extend to  $\Omega^+$ . It is defined on  $\Omega^{(-)}$ , excluding singular points, by analytic continuation. From (2.9), it follows that

$$\lim_{\omega \rightarrow \infty} i\omega E_-^t(\omega) = -E^t(0^-) = -E(t^+). \quad (2.29)$$

We also require the Fourier transform of the relative history.

$$\begin{aligned} E_{r-}^t(\omega) &= E_-^t(\omega) - E(t) \int_{-\infty}^0 e^{-i\omega s} ds \\ &= E_-^t(\omega) + \frac{E(t^+)}{i\omega^+}; \quad \omega^+ = \lim_{\alpha \rightarrow 0^+} (\omega + i\alpha) \end{aligned} \quad (2.30)$$

where the limit being taken after any integration involving the quantity  $(\omega^-)^{-1}$  has been carried out. Under a similar assumption to that for  $E_-^t$ , we have that  $E_{r-}^t$  is analytic in  $\Omega^+$  and  $E_{r+}^t$  goes to zero at large  $\omega$  as  $\omega^{-2}$ .

### 3. THE MAXIMUM RECOVERABLE WORK AND THE WIENER-HOPF EQUATION

The total work done on the material up to time  $t$  is given by [4]

$$W(t) = \int_{-\infty}^t T(s)\dot{E}(s)ds = \phi(t) + \frac{1}{2} \int_0^\infty \int_0^\infty E_r^t(s)G_{12}(|s-u|)E_r^t(u)dsdu \quad (3.1)$$

where  $\phi$  has the form

$$\phi(t) = \frac{1}{2}G_\infty E^2(t). \quad (3.2)$$

This quantity is the equilibrium free energy. Also

$$G_{12}(|s-u|) = \frac{\partial^2}{\partial s \partial u} G(|s-u|). \quad (3.3)$$

The maximum recoverable work from a given state of a material with memory is equal to the minimum free energy of that state, as can be shown under very general conditions (*e.g.* [5] and references therein). Thus, we seek to maximize the

$$W_r(t) = - \int_t^\infty T(s)\dot{E}(s)ds \quad (3.4)$$

or to minimize

$$W(\infty) = \int_{-\infty}^\infty T(s)\dot{E}(s)ds \quad (3.5)$$

where  $E$  is varied only on  $[t, \infty)$ . When taking the variation, we can assume that  $E(\infty)$  vanishes [4]. It follows from (3.1), on changing the integration range to  $(-\infty, t]$ , that

$$W(\infty) = \frac{1}{2} \int_{-\infty}^\infty \int_{-\infty}^\infty E(s)G_{12}(|s-u|)E(u)dsdu. \quad (3.6)$$

It is easily deduced that the optimization condition is

$$\int_{-\infty}^\infty G_{12}(|s-u|)E(u)du = \int_{-\infty}^\infty G_{12}(|s-u|)E_r^t(u)du = 0, \quad s \in \mathcal{R}^-. \quad (3.7)$$

We can remove the derivative with respect to  $s$  since  $G_2$  tends to zero as  $s$  tends to infinity. Also, the derivative with respect to  $u$  can be replaced by a derivative with respect to  $s$ . Thus, we obtain the relation

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial s} G(|s-u|) E_r^t(u) du = 0, \quad s \in \mathcal{R}^-. \quad (3.8)$$

or

$$\int_{-\infty}^0 \frac{\partial}{\partial s} G(|s-u|) E_o^t(u) du = \int_0^{\infty} G'(u-s) E_r^t(u) du = 0, \quad s \in \mathcal{R}^- \quad (3.9)$$

where  $E_o^t : \mathcal{R}^- \mapsto \mathcal{R}$  is the future continuation which yields the maximum recoverable work.

#### 4. FACTORIZATION OF $H$ FOR CONTINUOUS SPECTRUM MATERIALS

We adopt the following continuous spectrum form for the relaxation function

$$G'(t) = \int_a^b k(\alpha) e^{-\alpha t} d\alpha, \quad t \in \mathcal{R}^+, \quad b > a \geq 0. \quad (4.1)$$

It is assumed that  $k \in L^1([a, b])$ . The upper limit  $b$  may be infinite. If  $a = 0$  then  $k(0)$  is constrained to be zero also. We take the Fourier transform of (4.1) to obtain

$$F(\omega) = \int_a^b \frac{k(\alpha)}{\alpha + i\omega} d\alpha, \quad \omega \in \mathcal{R}. \quad (4.2)$$

This formula can be extended by analytic continuation to  $\Omega$ , excluding singular points. We restrict the density function  $k$  to be Hölder continuous on  $(a, b)$ . It may be singular at the end points with a power less than unity. It is assumed that

$$k(\alpha) \leq 0, \quad \alpha \in [a, b]. \quad (4.3)$$

This assumption is not essential but is the simplest which ensures compatibility with thermodynamic constraint (2.13)<sub>1</sub>. Note that it renders  $G$  completely monotonic in the sense discussed in [19]. Also, it is easily shown that  $F$  has no zeros on the finite part of  $\Omega \setminus [ia, ib]$ . Taking the complex conjugate of (4.2), we have

$$\overline{F}(\omega) = \int_a^b \frac{k(\alpha)}{\alpha - i\omega} d\alpha, \quad \omega \in \mathcal{R}. \quad (4.4)$$

which can similarly be continued into the complex plane.

The quantity  $F$  has a branch cut on  $[ia, ib]$  and  $\overline{F}$  on  $[-ia, -ib]$ . As  $\omega$  tends to  $i\alpha$ , where  $\alpha \in \mathcal{R} \setminus [-a, -b]$

$$\overline{F}(i\alpha) = F(-i\alpha) = \int_a^b \frac{k(\beta)}{\beta + \alpha} d\beta = K(\alpha) \quad (4.5)$$

while if  $\alpha \in (a, b)$ , we have, by virtue of the Plemelj formulae [22],

$$\begin{aligned} F_R(i\alpha) &= R(\alpha) + iI(\alpha) \\ F_L(i\alpha) &= R(\alpha) - iI(\alpha) \end{aligned} \quad (4.6)$$

with

$$R(\alpha) = P \int_a^b \frac{k(\beta)}{\beta - \alpha} d\beta, \quad I(\alpha) = -\pi k(\alpha) \geq 0 \quad (4.7)$$



where  $F_R(i\alpha), F_L(i\alpha)$  are the limiting values of  $F(\omega)$ , approaching from the right and the left respectively as one moves from  $ia$  to  $ib$ . Similarly

$$\begin{aligned}\overline{F}_R(-i\alpha) &= R(\alpha) + iI(\alpha) \\ \overline{F}_L(-i\alpha) &= R(\alpha) - iI(\alpha)\end{aligned}\tag{4.8}$$

for  $\alpha \in (a, b)$ , where  $\overline{F}_R(-i\alpha), \overline{F}_L(-i\alpha)$  are the limiting values of  $\overline{F}(\omega)$  from the right and left respectively as one moves from  $-ia$  to  $-ib$ . The symbol  $P$  in (4.7) indicates a principal value.

From (2.15), we have

$$H(\omega) = -\omega^2 \int_a^b \frac{k(\alpha)}{\alpha^2 + \omega^2} d\alpha.\tag{4.9}$$

Let us consider the behaviour of  $F(\omega)$  at the end points  $ia$  and  $ib$  for various limiting behaviours of  $k(\alpha)$  as  $\alpha$  approaches  $a$  or  $b$  [22]. If  $k(a) = 0$  then  $F(\omega)$  has a definite, finite non-zero limit as  $\omega \rightarrow ia$ . A similar statement applies to the limit  $\omega \rightarrow ib$  if  $k(b) = 0$ .

If

$$k(a) = k_a < 0\tag{4.10}$$

and  $k$  is Hölder continuous near and at  $a$ , then  $F(\omega)$  has a logarithmic singularity at  $\omega = ia$ . As  $\omega$  approaches this end point along any path off  $[ia, ib]$  then

$$F(\omega) = k_a \log \frac{1}{a + i\omega} + F_1(\omega)\tag{4.11}$$

where  $F_1(a)$  is well-defined. Similarly, if

$$k(b) = k_b < 0\tag{4.12}$$

and  $k$  is Hölder continuous near and at  $b$ , then, as  $\omega$  approaches  $ib$ , not along  $[ia, ib]$  we have

$$F(\omega) = -k_b \log \frac{1}{b + i\omega} + F_2(\omega)\tag{4.13}$$

where  $F_2(b)$  is well-defined. For points on  $(ia, ib)$ , relations (4.11) and (4.13) are replaced by

$$\begin{aligned}R(\alpha) &\xrightarrow{\alpha \rightarrow ia^+} k_a \log \frac{1}{\alpha - a} \\ &\xrightarrow{\alpha \rightarrow ib^-} -k_b \log \frac{1}{b - \alpha}\end{aligned}\tag{4.14}$$

where  $R(\alpha)$  is given by (4.7). If  $k(\alpha)$  has dominant behaviour as  $\alpha \rightarrow a^+$  along  $(a, b)$  of the form

$$k(\alpha) \xrightarrow{\alpha \rightarrow a^+} \frac{k_1}{(\alpha - a)^\gamma}, \quad 0 < \gamma < 1, \quad k_1 < 0\tag{4.15}$$

then for  $\omega \notin (ia, ib)$

$$F(\omega) \xrightarrow{\omega \rightarrow ia} \frac{Ak_1}{(a + i\omega)^\gamma}.\tag{4.16}$$

The detailed form of  $A$  is given in [22]. A similar observation applies to the case where  $k$  has such behaviour at  $b$ . For points on  $(ia, ib)$ , relation (4.16) is replaced by

$$R(\alpha) \xrightarrow{\alpha \rightarrow a^+} \frac{A_1 k_1}{(\alpha - a)^\gamma}\tag{4.17}$$

where again the form of  $A_1$  may be found in [22]. A similar observation applies at  $b$ .

We return our attention to (2.23). The function  $U(i\alpha)$ ,  $\alpha > 0$  is real for  $\alpha \notin [a, b]$ . It is discontinuous across  $[a, b]$ . We define, for  $\alpha \in [a, b]$ ,

$$\begin{aligned} U_R(i\alpha) &= \lim_{\omega \rightarrow \omega_R} U(\omega), \quad \omega_R = \alpha e^{\frac{i\pi}{2}} \\ U_L(i\alpha) &= \lim_{\omega \rightarrow \omega_L} U(\omega), \quad \omega_L = \alpha e^{-\frac{3i\pi}{2}}. \end{aligned} \quad (4.18)$$

As noted earlier, the function  $U(\omega)$  is non-zero on  $\Omega^{(+)}$  and approaches unity as  $\omega \rightarrow \infty$ . Thus,  $\log U(\omega)$  has a branch cut on  $[ia, ib]$  and no other singularity in  $\Omega^{(+)}$ . The factor  $\log \left[ \frac{\omega + i\omega_0}{\omega} \right]$  is assigned a branch cut on  $[0, -i\omega_0]$ . Moving the line of integration in (2.23)<sub>3</sub> to the infinite half-circle in  $\Omega^{(+)}$  while going around the branch cut, we obtain

$$\begin{aligned} N(z) &= \frac{1}{2\pi i} \int_a^b \frac{\Delta(\alpha)}{\alpha + iz} d\alpha \\ \Delta(\alpha) &= \log U_R(i\alpha) - \log U_L(i\alpha) \end{aligned} \quad (4.19)$$

where the branch of the logarithm function is as specified earlier. Its imaginary part lies in  $[-\pi, \pi]$ . Note that the factor  $\left[ \frac{\omega + i\omega}{\omega} \right]$  in  $U(\omega)$  cancels out of  $\Delta(\alpha)$ . It can henceforth be omitted. Thus, we put

$$\begin{aligned} Y(\omega) &= \frac{1}{2} \left( 1 - \frac{\bar{F}(\omega)}{F(\omega)} \right), \\ \Delta(\alpha) &= \log Y_R(i\alpha) - \log Y_L(i\alpha) \end{aligned} \quad (4.20)$$

where, from (4.5) and (4.6),

$$\begin{aligned} Y_R(i\alpha) &= \frac{1}{2} \left[ 1 - \frac{K(\alpha)}{R(\alpha) + iI(\alpha)} \right], \\ Y_L(i\alpha) &= \frac{1}{2} \left[ 1 - \frac{K(\alpha)}{R(\alpha) - iI(\alpha)} \right] = \overline{Y_R(i\alpha)}. \end{aligned} \quad (4.21)$$

We can write

$$\Delta(\alpha) = 2iA(\alpha), \quad A(\alpha) = \arg Y_R(\alpha), \quad -\pi \leq A(\alpha) \leq \pi \quad (4.22)$$

and

$$\begin{aligned} H_+(\omega) &= -\frac{i\omega}{h_\infty} F(\omega) e^{-N^+(\omega)} \\ N^+(\omega) &= \frac{1}{\pi} \int_a^b \frac{A(\alpha)}{\alpha + i\omega} d\alpha. \end{aligned} \quad (4.23)$$

while

$$\begin{aligned} H_-(\omega) &= \frac{i\omega}{h_\infty} \bar{F}(\omega) e^{-N^-(\omega)} \\ N^-(\omega) &= \frac{1}{\pi} \int_a^b \frac{A(\alpha)}{\alpha - i\omega} d\alpha. \end{aligned} \quad (4.24)$$

In the notation of (4.7), we have

$$V(\alpha) = 2[R(\alpha)^2 + I(\alpha)^2] \operatorname{Re} Y_R(i\alpha) = R(\alpha)^2 + I(\alpha)^2 - K(\alpha)R(\alpha) \quad (4.25)$$

where  $K(\alpha)$ , given by (4.5), is real and negative for  $\alpha > -a$ . Also,

$$W(\alpha) = 2[R(\alpha)^2 + I(\alpha)^2]ImY_R(i\alpha) = K(\alpha)I(\alpha) \leq 0. \quad (4.26)$$

from which it follows that  $-\pi \leq A(\alpha) \leq 0$ . Then

$$\begin{aligned} A(\alpha) &= -B(\alpha), \quad V(\alpha) \geq 0, \\ &= -\pi + B(\alpha), \quad V(\alpha) < 0; \\ B(\alpha) &= \arctan \left| \frac{W(\alpha)}{V(\alpha)} \right|, \quad 0 \leq B(\alpha) \leq \frac{\pi}{2}. \end{aligned} \quad (4.27)$$

Note the following result.

**Proposition 4.1.** *The quantity*

$$V(\alpha) = R(\alpha)^2 + I(\alpha)^2 - K(\alpha)R(\alpha), \quad \alpha \in (a, b) \quad (4.28)$$

*is non-negative in the vicinity of the end-points  $a$  and  $b$ . It is also non-negative when  $R(\alpha) \in \mathcal{R}^+$ .*

*Proof.* The latter statement follows immediately from the fact that  $K(\alpha) \leq 0$  for  $\alpha \in (a, b)$ . The statement is trivially true when  $R(\alpha)$  vanishes. Non-negativity near a given end point is manifestly true if  $R$  is unbounded at that end point, which is true even if  $k$  is finite but non-zero at the end points (see (4.14)). Thus, we must consider only the case where the density function  $k$  vanishes at the end point. Consider first the lower end point  $a$ . We have

$$R(a) = P \int_a^b \frac{k(\beta)}{\beta - a} d\beta \leq 0. \quad (4.29)$$

Then

$$V(a) \geq R(a)^2 - K(a)R(a) \geq 0 \quad (4.30)$$

if

$$-R(a) \geq -K(a). \quad (4.31)$$

Observing that

$$K(a) = \int_a^b \frac{k(\beta)}{\beta + a} d\beta. \quad (4.32)$$

we see that (4.31) is true. Also,

$$R(b) = \int_a^b \frac{k(\beta)}{\beta - b} d\beta \geq 0. \quad (4.33)$$

so that  $V(b) \geq 0$  □

If  $V \geq 0$  on  $(a, b)$  then

$$\begin{aligned} H_+(\omega) &= -\frac{i\omega}{h_\infty} F(\omega) \exp \left\{ \frac{1}{\pi} \int_a^b \frac{B(\alpha) d\alpha}{\alpha + i\omega} \right\} \\ H_-(\omega) &= \frac{i\omega}{h_\infty} \bar{F}(\omega) \exp \left\{ \frac{1}{\pi} \int_a^b \frac{B(\alpha) d\alpha}{\alpha - i\omega} \right\} \end{aligned} \quad (4.34)$$

where  $B$  is defined by (4.27)<sub>3</sub>

## 5. SOME CONSEQUENCES OF THE FACTORIZATION FORMULAE

It is of interest to consider the limits of  $H_{\pm}$ , given by (4.23) and (4.24), as  $\omega$  approaches the branch cuts on  $[ia, ib]$  and  $[-ia, -ib]$ . Consider (4.24) as  $\omega \rightarrow -i\alpha$ ,  $\alpha \in (a, b)$ , from the left, *i.e.* from the fourth quadrant. Noting (4.8), we obtain

$$\begin{aligned} H_{-L}(-i\alpha) &= \frac{\alpha}{h_{\infty}}(R(\alpha) - iI(\alpha))P(\alpha)e^{-iA(\alpha)} \\ P(\alpha) &= \exp \left\{ -\frac{1}{\pi}P \int_a^b \frac{A(\beta)}{\beta - \alpha} d\beta \right\} \end{aligned} \quad (5.1)$$

where the Plemelj formulae have been used. Also, from (4.5) and (4.23)

$$\begin{aligned} H_{+L}(-i\alpha) &= -\frac{\alpha}{h_{\infty}}K(\alpha)Q(\alpha) = H_{+R}(-i\alpha) \\ Q(\alpha) &= \exp \left\{ -\frac{1}{\pi} \int_a^b \frac{A(\beta)}{\beta + \alpha} d\beta \right\}. \end{aligned} \quad (5.2)$$

Multiplying  $H_{\pm L}$  together, we obtain the limit of  $H(\omega)$  as  $\omega \rightarrow -i\alpha$ ,  $\alpha \in (a, b)$ , namely

$$H_L(-i\alpha) = -\frac{\alpha^2}{H_{\infty}}(R(\alpha) - iI(\alpha))K(\alpha)P(\alpha)Q(\alpha)e^{-iA(\alpha)}. \quad (5.3)$$

Also, from (2.15), we have

$$H_L(-i\alpha) = \frac{\alpha}{2}(R(\alpha) - K(\alpha) - iI(\alpha)). \quad (5.4)$$

Equating the arguments of these two expressions for  $H_L(-i\alpha)$  gives

$$\arg(R(\alpha) - K(\alpha) - iI(\alpha)) = -A(\alpha) + \arg(R(\alpha) - iI(\alpha)). \quad (5.5)$$

or, taking complex conjugates,

$$A(\alpha) = \arg \left[ 1 - \frac{K\alpha}{R(\alpha) + iI(\alpha)} \right] \quad (5.6)$$

which is of course simply (4.22)<sub>2</sub>. Equating the magnitudes of the two expressions given by (5.3) and (5.4), we obtain

$$-2\alpha K(\alpha)P(\alpha)Q(\alpha) = H_{\infty} \sqrt{\frac{(R(\alpha) - K(\alpha))^2 + I^2(\alpha)}{R^2(\alpha) + I^2(\alpha)}}. \quad (5.7)$$

With the aid of (5.5), we can write (5.1) in the form

$$\begin{aligned} H_{-L}(-i\alpha) &= \frac{\alpha}{h_{\infty}}(R(\alpha) - K(\alpha) - iI(\alpha)) \sqrt{\frac{R^2(\alpha) + I^2(\alpha)}{(R(\alpha) - K(\alpha))^2 + I^2(\alpha)}} P(\alpha) \\ &= -\frac{h_{\infty}}{2} \frac{(R(\alpha) - K(\alpha) - iI(\alpha))}{K(\alpha)Q(\alpha)}. \end{aligned} \quad (5.8)$$

The second form follows from (5.7).

Finally, we observe that (2.15)<sub>1</sub>, (2.16), (4.23) and (4.24) give

$$W(\omega) = \frac{H_{\infty}}{2i\omega} \left( \frac{1}{\overline{F(\omega)}} - \frac{1}{F(\omega)} \right) = \exp \left\{ -\frac{1}{\pi} \int_a^b \frac{A(\alpha)d\alpha}{\alpha + i\omega} - \frac{1}{\pi} \int_a^b \frac{A(\alpha)d\alpha}{\alpha - i\omega} \right\} \quad (5.9)$$

Let us show this directly, noting that the left-hand side does not vanish at the origin and is unity at infinity. Consider the contour  $C$ , taken clockwise at infinity except that it excludes the positive imaginary axis above  $ia$ , and the negative imaginary axis below  $-ia$ . The quantity  $W$  is finite and non-zero within  $C$ . Then we see that

$$W(\omega) = \exp \left\{ -\frac{1}{2\pi i} \int_C \frac{\log(W(u)du}{u - \omega} \right\} \quad (5.10)$$

where  $\omega$  is in the interior of  $C$ . Invoking an argument similar to that leading to (4.19) and (4.20), the result follows on noting that

$$\log W_R(i\alpha) - \log W_L(i\alpha) = \log Y_R(i\alpha) - \log Y_L(i\alpha) \quad (5.11)$$

for  $\alpha \in (a, b)$ , since real, positive factors in the arguments of the logarithms cancel.

## 6. THE MINIMUM FREE ENERGY

Firstly, we derive the expression for the continuation that yields the maximum recoverable work - which is equal to the minimum free energy - when  $F$  is given by (4.2), from the Wiener-Hopf equation (3.8) or (3.9). The unique factorization of  $H$  is given by (4.23), (4.24) and (4.27). We shall use the formalism for relative histories, defined by (2.1)<sub>2</sub>, as in [9, 7, 8, 10] rather than in [2, 4]. Taking the Fourier transform of (3.8) yields

$$\frac{2i}{\omega} H(\omega)(E_{r+}^t(\omega) + E_m^t(\omega)) = R_+^t(\omega) \quad (6.1)$$

where  $E_m^t$  is the Fourier transform of the optimum relative continuation  $E_o^t$  in (3.9) and  $R_+^t$  is an unknown function, analytic in  $\Omega^-$ . Equation (6.1) is an immediate consequence of the relation

$$\int_{-\infty}^{\infty} \frac{d}{ds} G(|s|) e^{-i\omega s} ds = -2iG'_s(\omega) \quad (6.2)$$

and (2.15). Using the factorization property of  $H$ , we can write (6.1) as

$$H_-(\omega)E_{r+}^t(\omega) + H_-(\omega)E_m^t(\omega) = \frac{\omega R_+^t(\omega)}{2iH_+(\omega)}. \quad (6.3)$$

Let us define

$$\begin{aligned} p^t(z) &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \frac{H_-(\omega')E_{r+}^t(\omega')}{\omega' - z} \\ p_{\pm}^t(\omega) &= \lim_{\alpha \rightarrow 0^+} p^t(\omega \mp i\alpha). \end{aligned} \quad (6.4)$$

By the Plemelj formulae [22]

$$H_-(\omega)E_{r+}^t(\omega) = p_-^t(\omega) - p_+^t(\omega). \quad (6.5)$$

Then (6.3) can be written in the form

$$p_-^t(\omega) + H_-(\omega)E_m^t(\omega) = p_+^t(\omega) + \frac{\omega R_+^t(\omega)}{2iH_+(\omega)}. \quad (6.6)$$

Recalling that  $E_m^t$  is analytic in  $\Omega^+$  (see after (2.28)), we see that the lefthand side of this relation is analytic in  $\Omega^+$  and the righthand side is analytic in  $\Omega^-$ . Also, the lefthand side goes to zero as  $\omega^{-1}$  as we see by applying (2.29) to  $E_m^t$ . Thus,

both sides are analytic in  $\Omega$  and vanish at infinity; and are therefore individually zero. Therefore

$$E_m^t(\omega) = -\frac{p_-^t(\omega)}{H_-(\omega)} \quad (6.7)$$

and the minimum free energy is given by ([2, 4, 7], for example)

$$\begin{aligned} \psi_m(t) &= \phi(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} H(\omega) |E_m^t(\omega)|^2 d\omega \\ &= \phi(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} |p_-^t(\omega)|^2 d\omega \end{aligned} \quad (6.8)$$

where  $\phi$  is given by (3.2). The quantity  $\psi_m(t)$  was shown in [2, 4] to be a free energy by the Graffi definition [24, 25] and in [4] by the Coleman-Owen definition [13, 14] for the general tensor case.

Note that  $p_-^t$  can be written in the form

$$\begin{aligned} p_-^t(\omega) &= \frac{1}{2\pi} \int_a^b \frac{\Delta_h(\alpha) E_{r+}^t(-i\alpha)}{\alpha - i\omega} d\alpha \\ \Delta_h(\alpha) &= -i(H_{-L}(-i\alpha) - H_{-R}(-i\alpha)) \end{aligned} \quad (6.9)$$

by closing the contour on  $\Omega^{(-)}$  around the branch cut and changing variables. The quantity  $H_{-L}$  is given by (5.8), while  $H_{-R}$  is its complex conjugate. Thus, we have

$$\begin{aligned} \Delta_h(\alpha) &= -\frac{2\alpha}{h_\infty} I(\alpha) P(\alpha) \sqrt{\frac{R^2(\alpha) + I^2(\alpha)}{(R(\alpha) - K(\alpha))^2 + I^2(\alpha)}} \\ &= h_\infty \frac{I(\alpha)}{K(\alpha)Q(\alpha)} \leq 0, \quad \alpha \in [a, b]. \end{aligned} \quad (6.10)$$

The second form has the advantage that the need to evaluate a principal value integral is avoided. Using (6.8) and (6.9), we can write the minimum free energy in the form (*cf.* (3.1))

$$\psi_m(t) = \phi(t) + \frac{1}{2} \int_0^\infty \int_0^\infty E_r^t(s) G_{12}(s, u) E_r^t(u) ds du \quad (6.11)$$

where

$$G_{12}(s, u) = \frac{1}{2\pi^2} \int_a^b \int_a^b \frac{\Delta_h(\alpha) e^{-\alpha s} \Delta_h(\beta) e^{-\beta u}}{\alpha + \beta} d\alpha d\beta \quad (6.12)$$

and we understand the subscripts to mean differentiation with respect to the first and second variable. It follows that

$$G(s, u) = G(\infty, \infty) + \frac{1}{2\pi^2} \int_a^b \int_a^b \frac{\Delta_h(\alpha) e^{-\alpha s} \Delta_h(\beta) e^{-\beta u}}{(\alpha + \beta)\alpha\beta} d\alpha d\beta \quad (6.13)$$

if we require that [2]

$$G(\infty, \infty) = G(s, \infty) = G(\infty, s), \quad s \in \mathcal{R}^+ \quad (6.14)$$

yielding  $G_1(s, \infty) = G_2(\infty, s) = 0$ . It is also required that [2]

$$G(s, 0) = G(0, s) = G(s), \quad s \in \mathcal{R}^+ \quad (6.15)$$

where  $G(s)$  is defined by (2.2). We deduce from (6.14) and (6.15) that

$$G(\infty, \infty) = G(\infty) = G_\infty \quad (6.16)$$

in the notation of (2.1). To show that (6.15) holds, observe that for  $z \in \Omega^-$ ,

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{H_-(\omega')}{(\omega' - z)\omega'} d\omega' = -\frac{H_-(z)}{z} = \frac{i}{2\pi} \int_a^b \frac{\Delta_h(\beta)}{(\beta - iz)\beta} d\beta \quad (6.17)$$

where the first relation follows by closing the contour in  $\Omega^{(-)}$  and the second results in the same manner as (6.9). It follows from (5.2) and  $H_-(i\alpha) = H_+(-i\alpha)$  that

$$\frac{1}{2\pi} \int_a^b \frac{\Delta_h(\beta)}{(\beta + \alpha)\beta} d\beta = \frac{1}{h_\infty} K(\alpha) Q(\alpha). \quad (6.18)$$

Noting that

$$G(s) = G_\infty - \int_a^b \frac{k(\alpha)}{\alpha} e^{-\alpha s} d\alpha \quad (6.19)$$

we deduce from (6.10)<sub>2</sub> that (6.15) holds. Observe that both  $G$  and  $G_{12}$  are positive quantities.

The rate of dissipation associated with the minimum free energy is given by [2]

$$\begin{aligned} D_m(t) &= \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} H_-(\omega) E_{r+}^t(\omega) d\omega \right\}^2 \\ &= \left\{ \frac{1}{2\pi} \int_a^b \Delta_h(\alpha) E_{r+}^t(-i\alpha) d\alpha \right\}^2 \\ &= \left\{ \frac{1}{2\pi} \int_0^\infty \int_a^b \Delta_h(\alpha) E_r^t(u) e^{-\alpha y} d\alpha du \right\}^2 \geq 0. \end{aligned} \quad (6.20)$$

## 7. AN ALTERNATIVE APPROACH

Another approach to finding the minimum free energy of a continuous spectrum material is outlined in this section. Its most remarkable feature is that it does not require explicit factorisation of the function  $H$ . It was motivated initially by the method of Breuer and Onat [1] who propose an ansatz for the optimal continuation in the discrete spectrum case and solve the problem by this means. A similar ansatz can be written down without difficulty for the continuous spectrum case. However, it turns out that no such explicit assumption is required.

We start from the form (6.1) of the Wiener-Hopf equation, absorbing the factor  $2i$  in  $R_+$  and seeking not  $E_m^t(\omega)$  but

$$\Xi_m^t(\omega) = i\omega \bar{F}(\omega) E_m^t(\omega) \quad (7.1)$$

which is also analytic in  $\Omega^+$ . The reason for this change of unknown is so that we end up with formulae that are directly comparable with earlier results, in particular (6.7), based on the factorization of  $H$  with factors  $F$  and  $\bar{F}$  extracted. as in (2.23), (2.24) and later formulae.

Thus, recalling (2.15), we consider the relation

$$H(\omega) \left[ E_{r+}^t(\omega) + \frac{\Xi_m^t(\omega)}{i\omega \bar{F}(\omega)} \right] = H(\omega) E_{r+}^t(\omega) + \bar{Y}(\omega) \Xi_m^t(\omega) = R_+(\omega) \quad (7.2)$$

where  $Y$  is defined by (4.20). We consider the discontinuity of both sides across the cut  $(-ia, -ib)$ . The quantities  $E_{r+}^t$  and  $R_+$  are analytic in  $\Omega^-$  and therefore

have no discontinuity across the cut. Using (5.4) and its complex conjugate which gives  $H_{-R}(-i\alpha)$ , we obtain

$$\begin{aligned} \bar{Y}_L(-i\alpha)\Xi_L^t(-i\alpha) - \bar{Y}_R(-i\alpha)\Xi_R^t(-i\alpha) &= i\alpha I(\alpha)E_{r+}^t(-i\alpha), \quad \alpha \in (a, b) \\ &= 0, \quad \alpha \notin (a, b) \end{aligned} \quad (7.3)$$

where  $\Xi_L^t, \Xi_R^t$  are the limits of  $\Xi_m^t$  on  $[-ia, -ib]$  from the left and right respectively. If it were assumed that  $\Xi_m^t$  can be written as a Cauchy integral over  $[-ia, -ib]$ , which amounts to the continuous version of the Breuer - Onat ansatz, then (7.3) could be put in the form of a singular integral equation. As remarked earlier, this is unnecessary. The only and very natural assumption needed is that the only singularity of  $E_m^t$  is a branch cut on  $[-ia, -ib]$ . Note that

$$\Xi_m^t(\omega) \approx \frac{1}{\omega} \quad (7.4)$$

for large frequencies, which follows from (2.9) and (7.1). Relation (7.3) is a Hilbert problem, which we can write in the form

$$\begin{aligned} \Xi^{t+}(\alpha) &= C_1(\alpha)\Xi^{t-}(\alpha) + C_2(\alpha) \\ \Xi^{t+}(\alpha) &= \Xi_L^t(-i\alpha), \quad \Xi^{t-}(\alpha) = \Xi_R^t(-i\alpha) \\ C_1(\alpha) &= \frac{\bar{Y}_R(-i\alpha)}{\bar{Y}_L(-i\alpha)}, \quad C_2(\alpha) = \frac{i\alpha I(\alpha)E_{r+}^t(-i\alpha)}{\bar{Y}_L(-i\alpha)}. \end{aligned} \quad (7.5)$$

Note that, from the complex conjugate of (4.21),

$$C_1(a) = C_1(b) = 1. \quad (7.6)$$

This is clear for singular end points as given by (4.14) and (4.17). For the non-singular case,  $I(a)$  and  $I(b)$  vanish.

Equation (7.5) will now be solved for  $\Xi^t(z) = \Xi_m^t(-iz)$  which has a branch cut on  $[a, b]$  and where  $\Xi^{t\pm}(\alpha)$  are the limits of this function from the left and the right of the cut. The solution is subject to (7.4) and to the condition that it is bounded except possibly at  $a$  or  $b$  where it may diverge logarithmically or as a power less than unity. This latter property reflects the assumptions made relating to the density function  $k$ . The general solution is ([22], pg 237)

$$\begin{aligned} \Xi^t(z) &= \frac{X(z)}{2\pi i} \int_a^b \frac{C_2(\beta)}{X^+(\beta)(\beta - z)} d\beta + X(z)P(z) \\ X(z) &= \Pi(z)e^{N(iz)} \\ N(iz) &= \frac{1}{2\pi i} \int_a^b \frac{\log C_1(\lambda)}{\lambda - z} d\lambda \\ \Pi(z) &= (z - a)^{\lambda_1} (z - b)^{\lambda_2} \end{aligned} \quad (7.7)$$

where  $\lambda_1, \lambda_2$  are integers and  $P(z)$  is an arbitrary polynomial of degree not less than  $\kappa - 1$  with

$$\kappa = -\lambda_1 - \lambda_2.$$

Observe that  $N(iz)$  is the quantity defined by (4.19) and (4.20) since

$$\bar{Y}_R(-i\alpha) = Y_R(i\alpha), \quad \bar{Y}_L(-i\alpha) = Y_L(i\alpha) \quad (7.8)$$



by virtue of (4.6) and (4.8). The quantity  $X^+(\beta)$  is the limit of  $X(z)$  as  $z \rightarrow \beta \in (a, b)$  from the positive half-plane. Near  $z = a, b$  the quantity  $N$  is finite because of (7.6) so that

$$\begin{aligned} X(z) &\underset{z \rightarrow a}{\approx} K_1(z-a)^{\lambda_1} \\ &\underset{z \rightarrow b}{\approx} K_2(z-b)^{\lambda_2} \end{aligned} \quad (7.9)$$

where  $K_1, K_2$  are constants. To ensure no divergence in  $\Xi$  of order unity or stronger, we must have  $\lambda_1, \lambda_2 \geq 0$  and  $\kappa \leq 0$ . For  $\kappa < 0$ , solutions vanishing at infinity are possible only if restrictions are placed on  $C_2$  which depends only on given physical parameters [22]. Thus, we must have  $\kappa = 0$  and  $\lambda_1 = \lambda_2 = 0$ . The polynomial  $P$  is zero. Therefore

$$X(z) = e^{N(iz)}$$

and

$$\Xi^t(i\omega) = \Xi_m^t(\omega) = \frac{X(i\omega)}{2\pi i} \int_a^b \frac{C_2(\beta)}{X^+(\beta)(\beta - i\omega)} d\beta. \quad (7.10)$$

Observe that, from (4.24),

$$X(i\omega) = \frac{i\omega \bar{F}(\omega)}{h_\infty H_-(\omega)} \quad (7.11)$$

and

$$X^+(\beta) = \frac{\beta \bar{F}_L(-i\beta)}{h_\infty H_{-L}(-i\beta)} = \frac{1}{P(\beta)} e^{iA(\beta)}, \quad \beta \in (a, b) \quad (7.12)$$

where (4.8) and (5.1) have been used. Now, from (4.21) and (7.8).

$$\bar{Y}_L(-i\beta) = \frac{1}{2} \left[ 1 - \frac{K(\beta)}{R(\beta) - iI(\beta)} \right] = \frac{1}{2} \sqrt{\frac{(R(\beta) - K(\beta))^2 + I^2(\beta)}{R^2(\beta) + I^2(\beta)}} e^{-iA(\beta)}. \quad (7.13)$$

by virtue of (5.5). Thus

$$\frac{C_2(\beta)}{X^+(\beta)} = 2i\beta P(\beta) I(\beta) \sqrt{\frac{R^2(\beta) + I^2(\beta)}{(R(\beta) - K(\beta))^2 + I^2(\beta)}} = -ih_\infty \Delta_h(\beta) E_{r+}^t(-i\beta) \quad (7.14)$$

in the notation of (6.10). Then, we finally obtain from (7.1), (7.10) and (7.14)

$$E_m^t(\omega) = -\frac{1}{2\pi H_-(\omega)} \int_a^b \frac{\Delta_h(\beta) E_{r+}^t(-i\beta)}{\beta - i\omega} d\beta$$

which agrees with (6.7) and (6.9).

Note that the quantity  $X$ , given by (7.11), is closely related to the factor  $H_-$ . This is how the factors of  $H$  enter the formulae. The quantity  $X$  is the solution of the homogeneous part of the Hilbert problem (7.5). We note that the factorization problem of  $H$  can be expressed as a homogeneous Hilbert problem on the real axis:

$$H_-(w) = H(w) [H_+(w)]^{-1}.$$

It is straightforward to show that this is equivalent to the homogeneous problem associated with (7.5)<sub>1</sub> by taking the limit of this relation on both sides of the branch cut on  $[-ia, -ib]$  in  $H_-$  and  $H$ , and using (7.11)

## 8. MINIMAL STATES

Finally, let us explore the concept of minimal states, defined by (2.4), in the context of continuous spectrum materials.

**Proposition 8.1.** *For the relaxation function derivative given by (4.1), where  $k$  is negative on  $(a, b)$ , except possibly at a finite number of isolated points, and for histories with  $E_+^t$  analytic on  $\mathcal{R}$  (see the remark after (2.25)) the minimal states are singletons. In other words,  $(E(t), E^t)$  is the minimal state.*

*Proof.* We define  $(E_d(t), E_d^t)$  as

$$\begin{aligned} E_d(t) &= E_1(t) - E_2(t) \\ E_d^t(s) &= E_1^t(s) - E_2^t(s), \quad s \in \mathcal{R}^+. \end{aligned} \quad (8.1)$$

Then (2.4) becomes

$$\begin{aligned} E_d(t) &= 0 \\ \int_0^\infty G'(s + \tau) E_d^t(s) ds &= \int_a^b k(\alpha) e^{-\alpha\tau} E_{d+}^t(-i\alpha) d\alpha = 0, \quad \forall \tau \geq 0. \end{aligned} \quad (8.2)$$

The function

$$Z(\tau) = \int_a^b k(\alpha) e^{-\alpha\tau} E_{d+}^t(-i\alpha) d\alpha \quad (8.3)$$

can be extended to the complex  $\tau$  plane. It is analytic (and therefore zero) for  $\text{Re } \tau > 0$ . Taking the inverse Laplace transform, we deduce that  $k(\alpha) E_{d+}^t(-i\alpha)$  vanishes for  $\alpha \in \mathcal{R}^+$ . Thus, since  $k(\alpha)$  does not vanish for  $\alpha \in (a, b)$ , except at most at a finite number of isolated points, we have

$$E_{d+}^t(-i\alpha) = 0, \quad (8.4)$$

over  $(a, b)$  or some open sub-interval of this region, which in turn implies that  $E_{d+}^t(\omega)$  vanishes in the region of analyticity connected to  $(-ia, -ib)$ . This certainly includes  $\Omega^-$  and in particular the real axis. We conclude that

$$E_d(t) = 0, \quad E_d^t(s) = 0, \quad s \in \mathcal{R}^{++} \quad (8.5)$$

□

This result is in sharp contrast with the situation prevailing for discrete spectrum materials [6, 3].

It follows from proposition 8.1 that the work function is a function of state and is the maximum free energy, for relaxation functions obeying a strong dissipativity condition [20].

A generalization of proposition 8.1 is given in [3].

## 9. PARTICULAR CASES AND APPROXIMATIONS

Explicit expressions for  $F(\omega)$ ,  $R(\alpha)$ ,  $K(\alpha)$  and  $G'(0) = -h_\infty^2$  corresponding to a number of choices of  $k(\alpha)$  are presented on Table 1. These are the quantities required to determine  $H_\pm$  in (4.23) and (4.24) or indeed the free energy functional (6.11). A multiplying positive constant may of course be included in  $k$  in all cases.

In addition, we note the following formulae which allow simple generalizations of those tabulated. If  $k(\alpha)$  yields  $F(\omega)$  then  $\alpha k(\alpha)$  yields  $F_1(\omega)$  where

$$\begin{aligned} F_1(\omega) &= G'(0) - i\omega F(\omega) \\ G'(0) &= \int_a^b k(\alpha) d\alpha. \end{aligned} \quad (9.1)$$

Also

$$\begin{aligned} R_1(\alpha) &= G'(0) + \alpha R(\alpha) \\ K_1(\alpha) &= G'(0) - \alpha K(\alpha) \\ G'_1(0) &= \int_a^b \alpha k(\alpha) d\alpha. \end{aligned} \quad (9.2)$$

where the subscript '1' indicates the various quantities corresponding to  $\alpha k(\alpha)$ . Furthermore, all quantities are linear in  $k$  so that formulae for linear combinations of density functions may be constructed without difficulty.

A choice of  $k$  which is of some physical interest is [26]

$$k(\alpha) = -A\alpha^\lambda, \quad 0 < \lambda \leq 1, \quad 0 < \alpha < \infty, \quad A > 0, \quad (9.3)$$

particularly for  $\lambda = 0.5$ . However,  $G'(0)$  is infinite for this relaxation spectrum, a problem that is easily remedied in principle by taking the range of integrations to be finite. In this case, it would probably be simpler in this case to evaluate all the quantities of interest by numerical methods. Note however that the seventh and the fifth rows of Table 1 provide a good approximation to (9.3) if  $a$  is put equal to zero and  $b$  is taken to be large. In any case, the relevance of (9.3) is weakened by the fact that the power  $\lambda$  may depend on the value of  $\alpha$ .

Note that the behaviour of  $H_\pm$ , given by (4.23) and (4.24), for large  $\omega$ , is approximated by

$$\begin{aligned} H_+(\omega) &\approx -\frac{i\omega}{h_\infty} F(\omega) \\ H_-(\omega) &\approx \frac{i\omega}{h_\infty} \bar{F}(\omega). \end{aligned} \quad (9.4)$$

At small  $\omega$ , they are approximately given by a real constant times the quantities on the right of (9.4).

This suggests that (9.4), perhaps with multiplying constants, may provide a reasonable approximation for the factors at all frequencies. However, the functional (6.8) has the properties of a free energy (see [2]) only approximately, if (9.4) is used.

Table 1: The quantities  $F, K, R$  and  $G'(0)$  required to determine the factors of  $H$  and the minimum free energy for various choices of the density function  $k$ . The function  $I(\alpha) = -\pi k(\alpha)$ . The quantity  $c = (a + b)/2$ . The function Ei is the exponential-integral function. The fourth and fifth rows are of course special cases ( $\theta = 1/2$ ) of the sixth and seventh rows. The branch of  $[(a - z)(b - z)]^{1/2}$  is chosen to be the one that approaches  $-z$  as  $|z|$  becomes large. Similarly for  $(a - z)^\theta (b - z)^{1-\theta}$ . The quantity  $\theta \in (0, 1)$ .

	$k(\alpha), \alpha \in (a, b)$	$F(\omega)$	$K(\alpha), \alpha > -a$	$R(\alpha), \alpha \in (a, b)$	$G'(0)$
(1)	-1	$\log \frac{\omega - ia}{\omega - ib}$	$\log \frac{\alpha + a}{\alpha + b}$	$\log \frac{\alpha - a}{b - \alpha}$	$-(b - a)$
(2)	$-(\alpha - a)(b - \alpha)$	$-(b - a)(c + i\omega)$ $+(a + i\omega)(b + i\omega) \log \frac{b + i\omega}{a + i\omega}$	$-(b - a)(c + \alpha)$ $+(a + \alpha)(b + \alpha) \log \frac{b + \alpha}{a + \alpha}$	$-(b - a)(c - \alpha)$ $+(\alpha - a)(b - \alpha) \log \frac{\alpha - a}{b - \alpha}$	$-\frac{(b - a)^3}{6}$
(3)	$-e^{-\alpha t_0}, \alpha \geq a > 0$	$e^{i\omega t_0} \text{Ei}(-(a + i\omega)t_0)$	$e^{\alpha t_0} \text{Ei}(-(a + \alpha)t_0)$	$e^{-\alpha t_0} \text{Ei}((\alpha - a)t_0)$	$-\frac{e^{-at_0}}{t_0}$
(4)	$-\frac{1}{\sqrt{(\alpha - a)(b - \alpha)}}$	$-\frac{\pi}{[(a + i\omega)(b + i\omega)]^{1/2}}$	$-\frac{\pi}{\sqrt{(a + \alpha)(b + \alpha)}}$	0	$-\pi$
(5)	$-\sqrt{(\alpha - a)(b - \alpha)}$	$-\pi \{c + i\omega$ $-\left. [(a + i\omega)(b + i\omega)]^{1/2} \right\}$	$-\pi \{c + \alpha$ $-\left. \sqrt{(a + \alpha)(b + \alpha)} \right\}$	$-\pi(c - \alpha)$	$-\frac{\pi(b - a)^2}{8}$
(6)	$-\frac{1}{(\alpha - a)^{1-\theta}(b - \alpha)^\theta}$	$-\frac{\pi}{\sin \pi \theta} \frac{1}{(a + i\omega)^{1-\theta}(b + i\omega)^\theta}$	$-\frac{\pi}{\sin \pi \theta} \frac{1}{(a + \alpha)^{1-\theta}(b + \alpha)^\theta}$	$\frac{\pi \cot \pi \theta}{(\alpha - a)^{1-\theta}(b - \alpha)^\theta}$	$-\frac{\pi}{\sin \pi \theta}$
(7)	$-(\alpha - a)^{1-\theta}(b - \alpha)^\theta$	$-\frac{\pi}{\sin \pi \theta} \{a(1 - \theta) + b\theta + i\omega$ $-\left. (a + i\omega)^{1-\theta}(b + i\omega)^\theta \right\}$	$-\frac{\pi}{\sin \pi \theta} \{a(1 - \theta) + b\theta + \alpha$ $-\left. (a + \alpha)^{1-\theta}(b + \alpha)^\theta \right\}$	$-\frac{\pi}{\sin \pi \theta} \{a(1 - \theta) + b\theta - \alpha$ $+\left. \cos \pi \theta (\alpha - a)^{1-\theta}(b - \alpha)^\theta \right\}$	$-\frac{\pi(b - a)^2 \theta(1 - \theta)}{2 \sin \pi \theta}$

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