

Relation between the inverse Laplace transforms of $I(t^\beta)$ and $I(t)$: Application to the Mittag-Leffler and asymptotic inverse power law relaxation functions

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The relation between $H(k)$, inverse Laplace transform of a relaxation function $I(t)$, and $H_\beta(k)$, inverse Laplace transform of $I(t^\beta)$, is obtained. It is shown that for $\beta < 1$ the function $H_\beta(k)$ can be expressed in terms of $H(k)$ and of the Lévy one-sided distribution $L_\beta(k)$. The obtained results are applied to the Mittag-Leffler and asymptotic inverse power law relaxation functions. A simple integral representation for the Lévy one-sided density function $L_{1/4}(k)$ is also obtained.

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1. Introduction

In several relaxation processes, including luminescence spectroscopy, the time-dependent relaxation function $I(t)$ is the Laplace transform of $H(k)$, distribution of rate constants [1]. The function $I(t^\beta)$, usually with $0 < \beta < 1$, also arises in many cases, and it is therefore of interest to relate $H_\beta(k)$, inverse Laplace transform of $I(t^\beta)$, with $H(k)$. In this work, the relation between $H(k)$ and $H_\beta(k)$ is obtained. It is also shown that for $\beta \leq 1$ the function $H_\beta(k)$ can be expressed in terms of $H(k)$ and of the Lévy one-sided probability density function $L_\beta(k)$. The obtained results are applied to the Mittag-Leffler and asymptotic inverse power law relaxation functions.

2. General inverse Laplace transform

A simple form of the inverse Laplace transform of a relaxation function can be obtained by the method outlined in [1]. Briefly, the three following equations

can be used for the direct inversion of a function $I(t)$ to obtain its inverse $H(k)$,

$$H(k) = \frac{e^{ck}}{\pi} \int_0^\infty [Re[I(c + i\omega)] \cos(k\omega) - Im[I(c + i\omega)] \sin(k\omega)] d\omega, \quad (1)$$

$$H(k) = \frac{2e^{ck}}{\pi} \int_0^\infty Re[I(c + i\omega)] \cos(k\omega) d\omega \quad k > 0, \quad (2)$$

$$H(k) = -\frac{2e^{ck}}{\pi} \int_0^\infty Im[I(c + i\omega)] \sin(k\omega) d\omega \quad k > 0, \quad (3)$$

where c is a real number larger than c_0 , c_0 being such that $I(z)$ has some form of singularity on the line $Re(z) = c_0$ but is analytic in the complex plane to the right of that line, i.e., for $Re(z) > c_0$.

The relaxation function $I(t)$ is given by

$$I(t) = \int_0^\infty e^{-kt} H(k) dk, \quad (4)$$

hence

$$I(t^\beta) = \int_0^\infty e^{-kt^\beta} H(k) dk, \quad (5)$$

but one also has

$$I(t^\beta) = \int_0^\infty e^{-kt} H_\beta(k) dk. \quad (6)$$

The objective is to relate $H_\beta(k)$ with $H(k)$. For this purpose, and assuming that $I(t^\beta)$ has no singularities for non-negative values of the argument, application of equations (2), and (4–6) with $c = 0$, yields directly the sought-for relation

$$H_\beta(k) = \frac{2}{\pi} \int_0^\infty \int_0^\infty e^{-u\omega^\beta \cos(\beta\pi/2)} \cos[u\omega^\beta \sin(\beta\pi/2)] H(u) \cos(k\omega) du d\omega \quad k > 0. \quad (7)$$

Equations (1) and (3) lead to analogous relations, respectively,

$$H_\beta(k) = \frac{1}{\pi} \int_0^\infty \int_0^\infty e^{-u\omega^\beta \cos(\beta\pi/2)} \{ \cos[u\omega^\beta \sin(\beta\pi/2)] \cos(k\omega) + \sin[u\omega^\beta \sin(\beta\pi/2)] \sin(k\omega) \} H(u) du d\omega, \quad (8)$$

$$H_\beta(k) = \frac{2}{\pi} \int_0^\infty \int_0^\infty e^{-u\omega^\beta \cos(\beta\pi/2)} \sin[u\omega^\beta \sin(\beta\pi/2)] H(u) \sin(k\omega) du d\omega \quad k > 0. \quad (9)$$

3. Inverse Laplace transform for $\beta \leq 1$

For $I(t) = \exp(-t)$, one has $H(k) = \delta(k - 1)$, and it follows from equation (7) that the inverse Laplace transform of $\exp(-t^\beta)$ ($0 < \beta \leq 1$) can be written as [1]

$$H_\beta(k) = L_\beta(k) = \frac{2}{\pi} \int_0^\infty e^{-\omega^\beta \cos(\beta\pi/2)} \cos[\omega^\beta \sin(\beta\pi/2)] \cos(k\omega) d\omega \quad k > 0. \tag{10}$$

This function is the one-sided (asymmetric) Lévy probability density function $L_\beta(k)$. Using equation (10) and reversing the order of integration in equation (7), the inverse Laplace transform of $I(t^\beta)$ is obtained as

$$H_\beta(k) = \int_0^\infty u^{-1/\beta} L_\beta(u^{-1/\beta}k) H(u) du \quad 0 < \beta \leq 1, \tag{11}$$

which is a special case of equation (7) for $0 < \beta \leq 1$. A different derivation of equation (11) is given by Uchaikin and Zolotarev [2]. For $\beta = 1$, equation (11) gives of course $H(k)$, as $L_1(k) = \delta(k - 1)$.

If $I(t) = \exp(-t^\alpha)$, then $I(t^\beta) = \exp(-t^{\alpha\beta})$, and equation (11) becomes

$$L_{\alpha\beta}(k) = \int_0^\infty u^{-1/\beta} L_\beta(u^{-1/\beta}k) L_\alpha(u) du, \tag{12}$$

that can be rewritten either as

$$L_\beta(k) = \int_0^\infty u^{-1/\alpha} L_\alpha(u^{-1/\alpha}k) L_{\beta/\alpha}(u) du \quad \beta \leq \alpha \leq 1 \tag{13}$$

or as

$$L_\beta(k) = \int_0^\infty u^{-\alpha/\beta} L_{\alpha/\beta}(u^{-\alpha/\beta}k) L_\alpha(u) du \quad \alpha \leq \beta \leq 1, \tag{14}$$

where α and β no longer refer to the $I(t)$ given immediately before equation (12). For $\alpha = 1/2$, equation (13) becomes

$$L_\beta(k) = \int_0^\infty u^{-2} L_{1/2}(u^{-2}k) L_{2\beta}(u) du = \frac{k^{-3/2}}{2\sqrt{\pi}} \int_0^\infty u e^{-u^2/4k} L_{2\beta}(u) du \quad \beta \leq \frac{1}{2}, \tag{15}$$

hence, for instance, a simple integral representation for $L_{1/4}(k)$ is obtained,

$$L_{1/4}(k) = \frac{k^{-3/2}}{4\pi} \int_0^\infty u^{-1/2} e^{-1/4(1/u+u^2/k)} du. \tag{16}$$

Equation (16) can be rewritten as

$$L_{1/4}(k) = \frac{k^{-5/4}}{8\pi} \int_0^\infty u^{-3/4} e^{-1/4(1/\sqrt{ku}+u)} du, \tag{17}$$

which is a form that explicitly displays the asymptotic behavior for large k .

4. Application to the Mittag-Leffler relaxation function

The Mittag-Leffler function $E_\alpha(z)$ is defined by [3–5]

$$E_\alpha(z) = \sum_{n=0}^\infty \frac{z^n}{\Gamma(\alpha n + 1)}, \tag{18}$$

where z is a complex variable and $\alpha > 0$ (for $\alpha = 0$ the radius of convergence of equation (18) is finite, but one may define that $E_0(z) = 1/(1 - z)$). The Mittag-Leffler function is a generalization of the exponential function, to which it reduces for $\alpha = 1$, $E_1(z) = \exp(z)$. For $0 < \alpha < 1$ it interpolates between a pure exponential and a hyperbolic function, $E_0(z) = 1/(1 - z)$. Other simple forms are, for instance, $E_{1/2}(z) = \exp(z^2)\text{erfc}(-z)$ and $E_2(z) = \cosh(\sqrt{z})$.

There has been a surge of interest in the Mittag-Leffler and related functions in connection with the description of relaxation phenomena in complex systems [6–15]. In this work, and having in view the applications of this function to relaxation phenomena, the discussion will be restricted to $E_\alpha(-x)$ that corresponds to a relaxation function when x is a non-negative real variable (usually standing for the time) and $0 < \alpha \leq 1$.

A representation of $H_\alpha(k)$ involving the Lévy one-sided distribution was obtained by Pollard [16],

$$H_\alpha(k) = H_\alpha^1(k) = \frac{1}{\alpha} k^{-(1+1/\alpha)} L_\alpha(k^{-1/\alpha}). \tag{19}$$

In this way, insertion of equation (19) into equation (11) gives the inverse Laplace transform of $E_\alpha(-x^\beta)$, with $0 < \beta \leq 1$,

$$H_\alpha^\beta(k) = \int_0^\infty u^{\alpha/\beta} L_\alpha(u) L_\beta(ku^{\alpha/\beta}) du. \tag{20}$$

In particular,

$$H_\alpha^\alpha(k) = \int_0^\infty u L_\alpha(u) L_\alpha(ku) du. \tag{21}$$

The expected results for two limiting cases are recovered from equation (20),

$$H_\alpha^1(k) = \int_0^\infty u^\alpha L_\alpha(u) L_1(ku^\alpha) du = \frac{1}{\alpha} k^{-(1+1/\alpha)} L_\alpha(k^{-1/\alpha}), \tag{22}$$

$$H_1^\beta(k) = \int_0^\infty u^{1/\beta} L_1(u) L_\beta(u^{1/\beta} k) du = L_\beta(k). \tag{23}$$

Also from equation (20), and taking into account that

$$e^{-t^\beta} = \int_0^\infty e^{-kt} L_\beta(k) dk, \tag{24}$$

a compact integral representation for $E_\alpha(-x^\beta)$ is obtained,

$$E_\alpha(-x^\beta) = \int_0^\infty e^{-u^{-\alpha} x^\beta} L_\alpha(u) du, \tag{25}$$

that for $\beta = 1$ reduces to

$$E_\alpha(-x) = \int_0^\infty e^{-u^{-\alpha} x} L_\alpha(u) du. \tag{26}$$

Equation (26) can be rewritten as

$$E_\alpha(-x) = \int_0^\infty e^{-kx} \frac{1}{\alpha} k^{-(1+1/\alpha)} L_\alpha(k^{-\frac{1}{\alpha}}) dk, \tag{27}$$

in agreement with equation (19), that can also be used to obtain equation (25) by proceeding backwards from equation (27).

5. Application to the asymptotic power law relaxation function

The asymptotic power law [17,18]

$$I_\beta(t) = \frac{1}{1 + t^\beta} \tag{28}$$

with $\beta \leq 1$, was suggested as an alternative to the stretched exponential relaxation function, equation (24), for the description of peptide folding kinetics [18]. The inverse Laplace transform for $\beta = 1$ is clearly

$$H_1(k) = e^{-k}. \tag{29}$$

Use of equation (11) yields directly the inverse Laplace transform of $I_\beta(t)$,

$$H_\beta(k) = \int_0^\infty u^{-1/\beta} e^{-u} L_\beta(u^{-1/\beta} k) du \quad 0 < \beta \leq 1, \tag{30}$$

which is an alternative form to the integral representation [1]

$$H_\beta(k) = \frac{2}{\pi} \int_0^\infty \frac{u^\beta \cos(\beta\pi/2) + 1}{u^{2\beta} + 2u^\beta \cos(\beta\pi/2) + 1} \cos(ku) du. \tag{31}$$

6. Conclusions

The relation between $H(k)$, inverse Laplace transform of a relaxation function $I(t)$, and $H_\beta(k)$, inverse Laplace transform of $I(t^\beta)$, was obtained. It was shown that for $\beta < 1$ the function $H_\beta(k)$ can be expressed in terms of $H(k)$ and of the Lévy one-sided distribution $L_\beta(k)$. The obtained results were applied to the Mittag-Leffler and asymptotic inverse power law relaxation functions in order to obtain the respective $H_\beta(k)$. In the case of the Mittag-Leffler function, a compact integral representation of $E_\alpha(-x^\beta)$ was obtained. A simple integral representation for the Lévy one-sided density function $L_{1/4}(k)$ was also obtained.

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