PHYSICAL REVIEW E VOLUME 52, NUMBER 6 DECEMBER 1995

Matrix-inversion method: Applications to Möbius inversion and deconvolution

Qian Xie and Nan-xian Chen
Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, People's Republic of China
*and Institute of Applied Physics, Beijing University of Science and Technology, Beijing 100083, People's Republic of China**
(Received 11 April 1995)

The purpose of this paper is threefold. The first is to show the *matrix-inversion method* as a joint basis for the inversion of two important transforms: the Möbius and Laplace transforms. It is found that the Möbius transform is related to a multiplicative operator while the Laplace transform is related to an additive operator. The second is to show that the *matrix-inversion method* is a useful tool for inverse problems not only in statistical physics but also in applied physics by means of adding two other applications, one the derivation of the Fuoss-Kirkwood formulas for relaxation spectra in studies of anelasticity and dielectrics and the other the reconstruction of real signal in signal processing. The third is to indicate the potentiality of the *matrix-inversion method* as a rough algorithm for numerical solution of the convolution integral equation. The numerical examples given include the inversion of Laplace transform and the signal reconstruction with a Gaussian point spread kernel.

PACS number(s): 05.50.+q, 05.30.Jp, 02.10.Sp, 02.10.Lh

I. INTRODUCTION

The origin of this paper can be traced to a paper by Chen [1], who discovered some physical applications of the old Möbius inversion transform (MIT) from number theory [2]. In that paper, which stimulated extensive interest [3–8], Chen achieved his solutions of three important problems in statistical physics with the use of the MIT. The first problem is to invert the phonon density of states from the specific heat as a function of temperature, which was first raised by Montroll [9]. The second is the inverse blackbody radiation problem, which was first proposed by Bojarski [10]. The third is a physical interpretation for the MIT: to invert a pairwise potential from the cohesive energy as a function of vertex spacing for an infinite linear atomic chain. Both the first and second results are expressed by an infinite summation of the nth order Laplace inversion transform (LIT) modulated by the Möbius function, which simply equals -1, 0, $+1$. Similar formulas have been obtained in the analysis of the dust temperature distributions in star-forming condensations [6] and the determination of the temperature distribution of the material shells of distorted black holes from their Hawking signals [7]. However, before applying Chen's inversion formulas to real problems in which the data to be inverted are always discrete, one has to fit the data with carefully selected analytical functions and use the table of Laplace transform (LT) to find the corresponding solutions.

One may have seen that the MIT and LIT are the keys to obtain the solutions in Ref. [1]. However, one may have not thought of an interesting question: is there any similarity between these two transforms, though they are seemingly quite different?

The answer of this paper is affirmative. A recently proposed method, the *matrix-inversion method* (MIM) [11], acts as a connection between the two transforms. It is found that within the framework of the MIM, the formulations for the two transforms are quite similar except that the MIT is related to a multiplicative operator and the LIT is related to an additive operator. In fact, the MIM may be a useful tool for treating inverse problems not only in statistical physics but also in applied physics. To manifest this, we use it to rederive the Fouss-Kirkwood formulas for relaxation spectra and obtain an alternative formula for reconstructing the real signal in signal processing. On the other hand, we show that the MIM provides a simple approach to the numerical inversion of the LT as well as the numerical reconstruction of real signal with a Gaussian point spread kernel. It helps one to get rid of the inconvenience for dealing with discrete data, which occurs when only using the inversion formulas in Ref. [1], by means of presenting a procedure of discretization for the LIT. In a word, it may represent a different possibility for the numerical solution of the convolution integral equation.

II. MATRIX-INVERSION METHOD

The MIM is dedicated to solving the following function equation:

$$P(x) = \sum_{n=1}^{\infty} A_n \hat{T}(n) Q(x), \tag{1}$$

where $\hat{T}(1), \hat{T}(2), \ldots, \hat{T}(n), \ldots$ is an operator progression and $A_1, A_2, \ldots, A_n, \ldots$ is a number progression. Usually,

*Mailing address.

the first operator is a unit operator, $\hat{T}(1) = \hat{I}$. Carlsson, Gelatt, and Ehrenreich (CGE) have put forward a procedure to solve Eq. (1) [12]. They wrote Eq. (1) in terms of a linear operator $\hat{L}$,

$$P(x) = \hat{L}Q(x) = \sum_{n=1}^{\infty} \hat{R}(n)Q(x) = \hat{R}(1)\left[1 + \sum_{n=2}^{\infty} \hat{R}^{-1}(1)\hat{R}(n)\right] Q(x) , \quad (2)$$

where $\hat{R}(n) = A_n\hat{T}(n)$. Therefore

$$\begin{aligned} Q(x) &= \hat{L}^{-1}P(x) \\ &= \left[1 + \sum_{n=2}^{\infty} \hat{R}^{-1}(1)\hat{R}(n)\right]^{-1} \hat{R}^{-1}(1)P(x) \\ &= \left[1 - \sum_{n=2}^{\infty} \hat{R}^{-1}(1)\hat{R}(n) + \sum_{n,m=2}^{\infty} \hat{R}^{-1}(1) \right. \\ &\quad \left. \times\hat{R}(n)\hat{R}^{-1}(1)\hat{R}(m) - \cdots\right] \hat{R}^{-1}(1)P(x). \quad (3) \end{aligned}$$

However, in the original work of CGE, only the case of one kind of operators that are defined by $\hat{R}(n)f(x) = (w_n/2)f(s_nx)$ (related to a lattice sum) is illustrated. Applications to other kinds of operators such as the differential operator are not pointed out. Furthermore, the CGE technique disregards the translational symmetry of crystal lattices. As a result of this drawback, the formulation and the inverse coefficients are not obvious.

To introduce the MIM, let us first define an additive operator and a multiplicative operator: An operator is additive if $\hat{T}(a)\hat{T}(b) = \hat{T}(a+b)$; it is multiplicative if $\hat{T}(a)\hat{T}(b) = \hat{T}(ab)$, where the real numbers a, b denote the operator parameters.

For example, the scale-change operator defined by $\hat{T}(\alpha)F(x) = F(\alpha x)$ is a multiplicative operator, whereas that defined by $\hat{T}(\alpha)F(x) = F(e^{\alpha}x)$ is an additive operator. The derivative operators $\hat{D}(n) = d^n/dx^n$ are additive operators. An operator is additive or multiplicative means that we have the possibility to find a series of its kins which together with itself form a semigroup, whose operation is namely addition or multiplication.

In the case that $\hat{T}(n)$ are either additive or multiplicative, operating $\hat{T}(1)$, $\hat{T}(2)$, $\ldots, \hat{T}(n)$, $\ldots$ in turn on the right-hand side of Eq. (1) yields a series of function equations, which can be written in matrix notation as

$$(\hat{T}(1)P(x), \hat{T}(2)P(x), \ldots, \hat{T}(k)P(x), \ldots)^T = \mathbf{A}(\hat{T}(1)Q(x), \hat{T}(2)Q(x), \ldots, \hat{T}(k)Q(x), \ldots)^T . \quad (4)$$

The infinite-dimensional matrix $\mathbf{A}$ is the representation of an operator which stands for some kind of transformation from the function space spanned by $\{\hat{T}(1)Q(x), \hat{T}(2)Q(x), \ldots, \hat{T}(n)Q(x), \ldots\}$ to that spanned by $\{\hat{T}(1)P(x), \hat{T}(2)P(x), \ldots, \hat{T}(n)P(x), \ldots\}$.

If $\hat{T}(n)$ are additive, $\mathbf{A}$ is a Toeplitz matrix,

$$\mathbf{A} = \begin{pmatrix} A_1 & A_2 & A_3 & A_4 & A_5 & \cdots \\ 0 & A_1 & A_2 & A_3 & A_4 & \cdots \\ 0 & 0 & A_1 & A_2 & A_3 & \cdots \\ 0 & 0 & 0 & A_1 & A_2 & \cdots \\ 0 & 0 & 0 & 0 & A_1 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} . \quad (5)$$

On the other hand, if $\hat{T}(n)$ are multiplicative, we call $\mathbf{A}$ a Möbius matrix,

$$\mathbf{A} = \begin{pmatrix} A_1 & A_2 & A_3 & A_4 & A_5 & \cdots \\ 0 & A_1 & 0 & A_2 & 0 & \cdots \\ 0 & 0 & A_1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & A_1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & A_1 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} . \quad (6)$$

The characteristic feature of a Möbius matrix is that every two adjacent nonvanishing elements A_i and A_{i+1} in the nth row are uniformly separated by n-1 zeros. As a result, the jth element in the mth column is $A_{m/j}$, when $j|m$ (j divides m); and 0, otherwise.

No matter whether $\mathbf{A}$ is a Toeplitz or Möbius matrix, its inverse matrix $\mathbf{B} = \mathbf{A}^{-1}$ does exist, provided the diagonal element A_1 is nonvanishing. So we have

$$(\hat{T}(1)Q(x), \hat{T}(2)Q(x), \ldots, \hat{T}(k)Q(x), \ldots)^T = \mathbf{B}(\hat{T}(1)P(x), \hat{T}(2)P(x), \ldots, \hat{T}(k)P(x), \ldots)^T . \quad (7)$$

It is noteworthy that the formulas of Eq. (4) and Eq. (7) are symmetrical. The inverse matrix $\mathbf{B}$ possesses the same structure as $\mathbf{A}$. That is to say, if $\mathbf{A}$ is a Toeplitz matrix, then $\mathbf{B}$ is also a Toeplitz matrix; while if $\mathbf{A}$ is a Möbius matrix, then $\mathbf{B}$ is a Möbius matrix as well. In the case of a Toeplitz matrix, this property leads to a discrete convolution as

$$\sum_{k=1}^{n} A_k B_{n+1-k} = \delta_{n1}. \quad (8)$$

In the case of a Möbius matrix, it leads to a recursion relation as

$$\sum_{k|n} A_k B_{n/k} = \delta_{n1} . \quad (9)$$

The δ's in Eqs. (8) and (9) refer to the Kronecker delta symbol. We shall show in the following sections that Eqs. (8) and (9) are the keys to determining the inversion coefficients B_n in both the cases. From Eq. (7) the inversion result can be seen to be

$$Q(x) = \sum_{n=1}^{\infty} B_n\hat{T}(n)P(x). \quad (10)$$

In the following we show that the convolution integral equation, which frequently appears in physical and technological sciences, can be attributed to the former case.

A convolution integral equation as

$$P(x) = \int_{-\infty}^{+\infty} Q(y)K(y-x)dy \qquad (11)$$

can be rewritten as the following form if $Q(y)$ can be expanded into a Taylor series around x:

$$P(x) = \sum_{n=0}^{\infty} A_n Q^{(n)}(x), \qquad (12)$$

where

$$A_n = \frac{1}{n!}\int_{-\infty}^{+\infty} t^n K(t)dt \; . \qquad (13)$$

The operators in this case being the derivative operators: $\hat{D}(n)$, are additive. By derivative action upon Eq. (12) with respect to x step by step, we can reach a Toeplitz matrix formulation. Therefore the inverted result, the function $Q(x)$, can be expressed by

$$Q(x) = \sum_{n=0}^{\infty} B_n P^{(n)}(x), \qquad (14)$$

where the coefficient B_n can be determined by a discrete convolution relation

$$\sum_{k=0}^{n} A_k B_{n-k} = \delta_{n0}. \qquad (15)$$

Thus the basic idea of the MIM applied to solving a convolution integral equation has been shown. The inversion of integral equation is ascribed to that of a Toeplitz matrix. This then leads to a recursion formula, Eq.(15), from which the inversion coefficients can be determined. Actually, Eq. (15) establishes a connection between the characteristic functions of the two progressions, $\{A_m\}$ and $\{B_m\}$, as

$$\sum_{n=0}^{\infty} A_n z^n = \frac{1}{\sum\limits_{n=0}^{\infty} B_n z^n} \; . \qquad (16)$$

This equality is very useful for determining the inversion coefficients B_n.

The reader may have realized that an advantage of the MIM for integral equation lies in its unusual treatment on the integration limits. As we have known, before the discretization of an integral equation with an infinite integral interval, one has to at first cut off the interval to a finite one. However, since the function in the integrand is unknown, we do not know where to truncate, nor do we know the influence of an arbitary truncation on the solution. But in the present method, this difficulty is avoided. The truncation takes place only during the integration of Eq. (13), and since the kernel function $K(t)$ is exactly known all the time, the integrand in Eq. (13) can be evaluated to any precision as needed. That is to say, the inversion coeffients can be determined very accurately. The cost for this advantage is that $P(x)$ should be differentiable at any order.

III. GENERALIZED MÖBIUS INVERSION FORMULA

Given a function $P(x)$ that is related to another function $Q(x)$ by

$$P(x) = \sum_{n=1}^{\infty} Q(n^\alpha x), \qquad (17)$$

where α is an arbitary nonzero real number. We have in this case $A_n = 1$ for all $n \in \mathbf{N}$. The operators, defined by $\hat{T}(n)Q(x) = Q(n^\alpha x)$, are multiplicative. According to the MIM, we obtain

$$Q(x) = \sum_{n=1} B_n P(n^\alpha x), \qquad (18)$$

with B_n determined by

$$\sum_{k|n} B_{n/k} = \sum_{k|n} B_k = \delta_{n1} \; . \qquad (19)$$

Equation (19) implies that B_n is, namely, the Möbius function in arithmetic number theory:

$$B_k = \mu(k) = \begin{cases} 1 & k=1 \\ (-1)^r & k \text{ is a product of } r \text{ distinct primes} \\ 0 & \text{otherwise.} \end{cases} \qquad (20)$$

Thus we have

$$P(x) = \sum_{n=1}^{\infty} Q(n^\alpha x) \Longleftrightarrow Q(x) = \sum_{n=1}^{\infty} \mu(n) P(n^\alpha x). \qquad (21)$$

The cases of $\alpha = \pm 1$ can be found in Schroeder's book [2].

With the same idea, we can easily figure out two alternative versions for the MIT,

$$P(x) = \sum_{n=1}^{\infty} Q(x^{\pm n}) \Longleftrightarrow Q(x) = \sum_{n=1}^{\infty} \mu(n) P(x^{\pm n}) \qquad (22)$$

and

$$P(x) = \sum_{n=1}^{\infty} Q[(2n-1)^\alpha x] \Longleftrightarrow Q(x) = \sum_{n=1}^{\infty} \mu(2n-1) P[(2n-1)^\alpha x], \tag{23}$$

since the operators in the above equations are both multiplicative. The latter was previously obtained by using the Kronecker δ expansion for the Möbius function [13]. From Eq. (22), a special case of a known result for Lambert series can be deduced,

$$\frac{x}{1-x} = \sum_{n=1}^{\infty} x^n \Longleftrightarrow x = \sum_{n=1}^{\infty} \mu(n) \frac{x^n}{1-x^n} \quad (|x| < 1). \tag{24}$$

An interesting example of the above transform appears when we take the left-hand side as the Bose-Einstein distribution for phonons or photons with zero chemical potential,

$$f_{BE}\left(\frac{\hbar\omega}{kT}\right) = \sum_{n=1}^{\infty} f_{Boltz}\left(\frac{n\hbar\omega}{kT}\right) \Longleftrightarrow f_{Boltz}\left(\frac{\hbar\omega}{kT}\right) = \sum_{n=1}^{\infty} \mu(n) f_{BE}\left(\frac{n\hbar\omega}{kT}\right), \tag{25}$$

where $f_{BE}(x) = 1/[\exp(x)-1]$ is the Bose-Einstein distribution function, and $f_{Boltz}(x) = \exp(-x)$ is the classical Boltzmann distribution function.

The lattice-inversion method (LIM) can be regarded as an example for the nonunity case: $A_n \neq 1$. Over a sc or fcc lattice with the lattice constant as a, the lattice sum of a function $f(x)$ can be expressed as

$$F(R_1) = \sum_{l_1,l_2,l_3=0}^{\infty}{}' f(\sqrt{l_1^2 + l_2^2 + l_3^2} R_1), \tag{26}$$

where R_1 is the nearest-neighbor distance, $R_1 = a$ for sc or $R_1 = a/\sqrt{2}$ for fcc, and the prime on the summation excludes the case that $l_1 = l_2 = l_3 = 0$. Obviously, Eq. (26) can be rewritten as

$$F(R_1) = \sum_{n=1}^{\infty} w(n) f(\sqrt{n} R_1), \tag{27}$$

provided we introduce a weight function $w(n)$ which vanishes when the natural number n cannot be decomposed into a sum of three square non-negative integers $l_1^2+l_2^2+l_3^2$ and equals the number of atoms on the sphere with the radius $\sqrt{l_1^2 + l_2^2 + l_3^2} R_1$ otherwise. By using the MIM, the inversion of Eq. (27) is obtained as

$$f(R_1) = \sum_{n=1}^{\infty} m(n) F(\sqrt{n} R_1), \tag{28}$$

where $m(n)$ is the generalized Möbius function for sc or fcc lattice, which is governed by the following recursion formula:

$$\sum_{k|n} w(k) m(n/k) = \sum_{k|n} w(n/k) m(k) = \delta_{n1}. \tag{29}$$

This is exactly the result presented in Ref. [14], but the method presented here is clearer.

As for other lattices, such as bcc and diamond structure, since the corresponding operator does not explicitly form a semigroup, the MIM cannot be directly used. Some trick is needed to modify the multiplicative operator progression into a semigroup which essentially covers the original operator progression, if one wants to obtain inversion formulas similiar to Eqs. (28) and (29).

The LIM has been shown to be a very useful tool for materials simulation. In an atomistic view, many properties such as cohesive energy, elastic constants, and so on are contributed by all the atoms arrayed in the crystal lattice. Conventionally, it is an effective way to assign potential functions (such as pair potentials) to every individual atom and use them to calculate properties of materials. Therefore, the determinations of such individual functions become the key problem. As a usual treatment, one supposes parametrized forms for them and by careful fitting to available data of properties determines the parameters. However, the fit procedure will become more difficult once more distant neighbors are involved in. If only a few neighbors are considered, a cut-off function is needed to smooth the potential function at the truncated sphere; otherwise the potential derivative at the truncated point will become infinite. Now the LIM presents a way to get rid of the inconvenience of treating many neighbors, by removing the parametrization procedure from the individual functions to their corresponding lattice sums and inverting the individual functions from the parametrized lattice sums [15]. This way looks more natural because most of the materials properties are related more closely to the lattice sums than to the individual functions. This idea has been applied to atomistic simulation. For example, it was used to construct first-principles pair potentials from *ab initio* cohesive energies versus lattice constants [16–18]. In the semiempirical embedded-atom method [19], it was used to determine the pair potential and the electron density from a universal cohesion equation and the Thomas-Fermi screening equation for electron density [20]. In addition, it provides a useful scheme for building the pair potential between a couple of distinct atoms from a specified binary alloy superstructure as a reference, which otherwise is usually constructed from the two respective pair potentials between pairs of identical atoms through averaging methods [21].

IV. APPLICATION TO THE INVERSION OF LAPLACE TRANSFORM

The LT has been a widely used tool for technologies such as circuit theory and network analysis. It has been also frequently employed in applied physics. For example, in the study of anelastic relaxation of solids, the relation between the creep function and the relaxation spectrum under constant stress can be attributed to a LT [22]. Another example is that in the investigation of the inverse problem of depth profiling with photoacoustic spectroscopy, the optical absorption coefficient is shown to be related to the surface temperature distribution through a LT after some simplifications [23]. Both the problems seek to invert an unknown function from the experimentally measureable functions. The third example is that the LT is a useful method for analyzing the problem of hydrogen permeation through a multilayered material in electrochemical systems [24]. All these examples raise the necessity of practical algorithms for the LIT.

The studies of the LIT by mathematicians have formed a long history. A well-known scheme is the Bromwich formula, which is similar in formulation to the LT. Bellman *et al.* wrote a specialized book to discuss the numerical inversion of the LT [25]. Because of its complications, the numerical studies for the LIT still remains an attractive research objective in recent years. For instance, Cunha and Viloche presented a numerical inversion method based on the Fourier series of Laguerre functions [26]; Brianzi and Frontini presented another regularized inversion algorithm [27]. In this section, we show that the MIM presents a different possibilty of numerical calculation for the LIT.

The Laplace transform

$$\overline{\phi}(p) = \int_0^{\infty} e^{-pt}\phi(t)dt \qquad (30)$$

can be translated into

$$P^L(x) = \sum_{m=0}^{\infty} A_m^L \frac{d^m}{dx^m} Q^L(x) \ , \qquad (31)$$

with $t = e^y$, $p = e^{-x}$, $P^L(x) = \overline{\phi}(e^{-x})e^{-\lambda x}$, $Q^L(y) = \phi(e^y)e^{(1-\lambda)y}$, $K^L(u) = e^{\lambda u}\exp(-e^u)$, and

$$A_m^L = \frac{1}{m!}\int_{-\infty}^{+\infty} t^m e^{\lambda t}\exp(-e^t)dt, \qquad (32)$$

where λ is a positive parameter introduced to guarantee the existence of the integrand of Eq. (32). The characteristic function of the progression $\{A_m^L\}$ can be found to be

$$\sum_{m=0}^{\infty} A_m^L z^m = \int_{-\infty}^{+\infty} e^{(\lambda+z)t}\exp(-e^t)dt$$
$$= \int_0^{+\infty} t^{\lambda+z-1}e^{-t}dt = \Gamma(\lambda+z) \ , \qquad (33)$$

where $\Gamma(z)$ is the gamma function. According to the MIM, we have

$$Q^L(x) = \sum_{m=0}^{\infty} B_m^L \frac{d^m}{dx^m} P^L(x), \qquad (34)$$

where the inversion coefficients B_m^L may be determined from its characteristic function

$$\sum_{m=0}^{\infty} B_m^L z^m = \frac{1}{\Gamma(\lambda+z)}. \qquad (35)$$

Completing some simple substitutions, we obtain the solution as

$$\phi(x) = \sum_{m=0}^{\infty} x^{\lambda-1} B_m^L \left(x\frac{d}{dx}\right)^m \left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right] . \qquad (36)$$

Note that we have used $d^n/dx^n = (e^x d/de^x)^n$.

The MIM can be used directly to invert an analytical function. A few examples are given to indicate this application. For simplicity, in the following treatment, $\lambda = 1$ is chosen as the optimal parameter (in the Appendix, we prove that the inversion result is strictly free from the parameter λ).

(1) $\overline{\phi}(p) = 1$,

$$\phi(x) = \sum_{m=0}^{\infty} B_m^L \left(x\frac{d}{dx}\right)^m \left(\frac{1}{x}\right)$$
$$= \sum_{m=0}^{\infty} B_m^L (-1)^m \frac{1}{x}$$
$$= \lim_{\epsilon\to -1} \frac{1}{\Gamma(1+\epsilon)x} = \delta(x). \qquad (37)$$

(2) $\overline{\phi}(p) = \Gamma(\alpha+1)/p^{\alpha+1}$,

$$\phi(x) = \Gamma(\alpha+1)\sum_{m=0}^{\infty} B_m^L \left(x\frac{d}{dx}\right)^m [x^\alpha]$$
$$= \Gamma(\alpha+1)\left[\sum_{m=0}^{\infty} B_m^L \alpha^m\right] x^\alpha = x^\alpha. \qquad (38)$$

(3) $\overline{\phi}(p) = b/(p^2+b^2)$,

$$\phi(x) = \sum_{m=0}^{\infty} B_m^L \left(x\frac{d}{dx}\right)^m \left[\frac{bx}{1+(bx)^2}\right]$$
$$= \sum_{m=0}^{\infty} B_m^L \left(x\frac{d}{dx}\right)^m [(bx)-(bx)^3+(bx)^5-\cdots]$$
$$= (bx) - \frac{1}{3!}(bx)^3 + \frac{1}{5!}(bx)^5 - \cdots = \sin(bx). \qquad (39)$$

Now we turn to the determination of coefficients A_m^L and B_m^L from Eqs. (33) and (35). Although the Weierstrass expression for the inverse of the Γ function has long existed, we find that it is inconvenient in finding the coefficients. We find that the Taylor's expansion for the Γ function is a substitution for the determination of A_m^L and B_m^L. First, we have

$$\sum_{m=0}^{\infty} A_m^L z^m = \Gamma(1+z) = \Gamma(1) + \Gamma'(1)z + \frac{\Gamma''(1)}{2!}z^2$$
$$+ \cdots + \frac{\Gamma^{(m)}(1)}{m!}z^m + \cdots . \qquad (40)$$

Note that there are

$$\Gamma'(x) = \psi(x)\Gamma(x) , \quad (41)$$

where $\psi(x)$ is the psi function

$$\psi(x) = -\gamma - \frac{1}{x} + \sum_{k=1}^{\infty}\left(\frac{1}{k} - \frac{1}{k+x}\right) \quad (42)$$

and

$$\psi^{(n)}(x) = (-1)^{n+1} n! \sum_{k=0}^{\infty} \frac{1}{(k+x)^{n+1}}, \quad (43)$$

where γ is the Euler's constant

$$\gamma = \lim_{n\to\infty}\left(1 + \frac{1}{2} + \cdots + \frac{1}{n} - \ln n\right) = 0.577\,215\,6\ldots.$$

On the ground of the above formulas, one can derive the recursion formulas for A_m^L and B_m^L, respectively,

$$(m+1)A_{m+1}^L = -\gamma A_m^L + \sum_{i=1}^{m}(-1)^{i+1}\zeta(i+1)A_{m-i}^L, \quad (44)$$

$$(m+1)B_{m+1}^L = \gamma B_m^L + \sum_{i=1}^{m}(-1)^{i}\zeta(i+1)B_{m-i}^L, \quad (45)$$

where $A_0^L = B_0^L = 1$, and $\zeta(n)$ is the Riemann ζ function. From Eqs. (44) and (45), A_m^L and B_m^L can be determined. For instance, $A_1^L = \Gamma'(1) = \phi(1)\Gamma(1) = -\gamma$, $A_2^L = [-\gamma A_1^L + (-1)^2\zeta(2)A_0^L]/2 = [\gamma^2 + \zeta(2)]/2$, $A_3^L = -[\gamma^3/2 + 3\gamma\zeta(2)/2 + \zeta(3)]/3, \ldots$, and $B_1^L = \gamma$, $B_2^L = [\gamma^2 - \zeta(2)]/2$, $B_3^L = [\gamma^3/2 - 3\gamma\zeta(2)/2 + \zeta(3)]/3, \ldots$.

The coefficients A_m^L can also be calculated using Eq. (32). We list the first dozen coefficients of A_m^L and B_m^L in Table I. The listed data show that B_m^L decreases quickly when m increases. Hence, it may be plausible to truncate Eq. (36) for an approximate inversion. Figure 1 illustrates the results of numerical inversion for three selected functions. It is shown that the approximate solutions are in good agreement with the exact solutions.

V. DERIVATION OF THE FUOSS-KIRKWOOD FORMULA FOR RELAXATION SPECTRA

In studies of dielectric and anelastic relaxation, it is of importance to invert a relaxation spectrum from an experimentally measurable property such as permittivity and compliance response functions via their connection as integral equations. For example, the anelastic dynamic response functions, sometimes called the storage compliance and the loss compliance [22], can be expressed by

$$J_1(\omega) = J_U + \int_{-\infty}^{+\infty} \frac{G(\ln\tau)d(\ln\tau)}{1+\omega^2\tau^2}, \quad (46)$$

$$J_2(\omega) = \int_{-\infty}^{+\infty} \frac{\omega\tau G(\ln\tau)d(\ln\tau)}{1+\omega^2\tau^2}. \quad (47)$$

By letting $\omega = e^{-x}$ and $\tau = e^{y}$ with $H_1(x) = J_1(e^{-x})$ and $H_2(x) = J_2(e^{-x})$, Eqs. (46) and (47) can be translated into

$$H_1(x) = J_U + \int_{-\infty}^{+\infty} \frac{G(y)dy}{1+\exp[2(y-x)]}, \quad (48)$$

$$H_2(x) = \int_{-\infty}^{+\infty} \frac{\exp(y-x)G(y)dy}{1+\exp[2(y-x)]}. \quad (49)$$

The first-order derivative of Eq. (48) with respect to x is

$$H_1'(x) = 2\int_{-\infty}^{+\infty} \frac{\exp[2(y-x)]}{\{1+\exp[2(y-x)]\}^2} G(y)dy. \quad (50)$$

The above equation can be reexpressed within the MIM as

$$H_1'(x) = \sum_{m=0}^{\infty} A_m G^{(m)}(x). \quad (51)$$

It immediately follows that

$$G(x) = \sum_{m=0}^{\infty} B_m H_1^{(m+1)}(x). \quad (52)$$

To find the inversion coefficients B_m, it can be first shown that

$$\sum_{m=0}^{\infty} A_m z^m = \sum_{m=0}^{\infty} \frac{2}{m!}\int_{-\infty}^{+\infty} \frac{(zt)^m e^{2t}}{(1+e^{2t})^2}dt = \int_0^{\infty} \frac{t^{z/2}}{(1+t)^2}dt = B\left(1-\frac{z}{2}, 1+\frac{z}{2}\right) = \frac{\Gamma(1-\frac{z}{2})\Gamma(1+\frac{z}{2})}{\Gamma(2)} = \frac{z}{2}\Gamma\left(1-\frac{z}{2}\right)\Gamma\left(\frac{z}{2}\right) = \frac{z}{2}\frac{\pi}{\sin(\frac{\pi}{2}z)}, \quad (53)$$

TABLE I. The first 12 coefficients of A_m^L and B_m^L for the LT and LIT, calculated from Eq. (32). The number in brackets corresponds to a power of 10.

n	A_n^L	B_n^L	n	A_n^L	B_n^L
0	0.100000000[+01]	0.100000000[+1]	6	0.993149115[+00]	-.962197153[-2]
1	-.577215665[+00]	0.577215665[+00]	7	-.996001760[+00]	0.721894325[-2]
2	0.989055995[+00]	-.655878072[+00]	8	0.998105694[+00]	-.116516759[-2]
3	-.907479076[+00]	-.420026350[-1]	9	-.999025268[+00]	-.215241675[-3]
4	0.981728087[+00]	0.166538611[+00]	10	0.999515656 [+00]	0.128050287[-3]
5	-.981995069[+00]	-.421977346[1]	11	-.999756597[+00]	-.201348764[-4]

where $\mathcal{B}(x,y)$ is the $\mathcal{B}$ function. Second, according to Eq. (16) we have

$$\sum_{m=0}^{\infty} B_m z^m = \frac{2\sin(\frac{\pi}{2}z)}{\pi z}. \tag{54}$$

Hence the inversion coefficients B_n are

$$B_n = \begin{cases} 0, & n = 2m+1 \\ (-1)^m(\frac{\pi}{2})^{2m}/(2m+1)!, & n = 2m. \end{cases} \tag{55}$$

Therefore

$$G(x) = \frac{2}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m}{(2m+1)!}\left(\frac{\pi}{2}\right)^{2m+1}\frac{\partial^{2m+1}}{\partial x^{2m+1}}H_1(x). \tag{56}$$

Equation (56) is, namely,

$$\begin{aligned} G(x) &= \frac{2}{\pi}\mathrm{Im}\left[\exp\left(i\frac{\pi}{2}\frac{\partial}{\partial x}\right)\right]H_1(x) \\ &= \frac{1}{\pi i}\left[H_1\left(x+i\frac{\pi}{2}\right) - H_1\left(x-i\frac{\pi}{2}\right)\right]. \end{aligned} \tag{57}$$

By analogy, in the other case of Eq. (49), we have

$$\begin{aligned} \sum_{m=0}^{\infty} A_m z^m &= \int_{-\infty}^{+\infty}\frac{e^{zt}e^t dt}{1+e^{2t}} \\ &= \frac{1}{2}\int_0^{\infty}\frac{t^{(z-1)/2}dt}{1+t} \\ &= \frac{1}{2}\mathcal{B}\left(\frac{1-z}{2},\frac{1+z}{2}\right) \\ &= \frac{\Gamma(\frac{1-z}{2})\Gamma(\frac{1+z}{2})}{2\Gamma(1)} = \frac{1}{2}\frac{\pi}{\cos(\frac{\pi}{2}z)} \end{aligned} \tag{58}$$

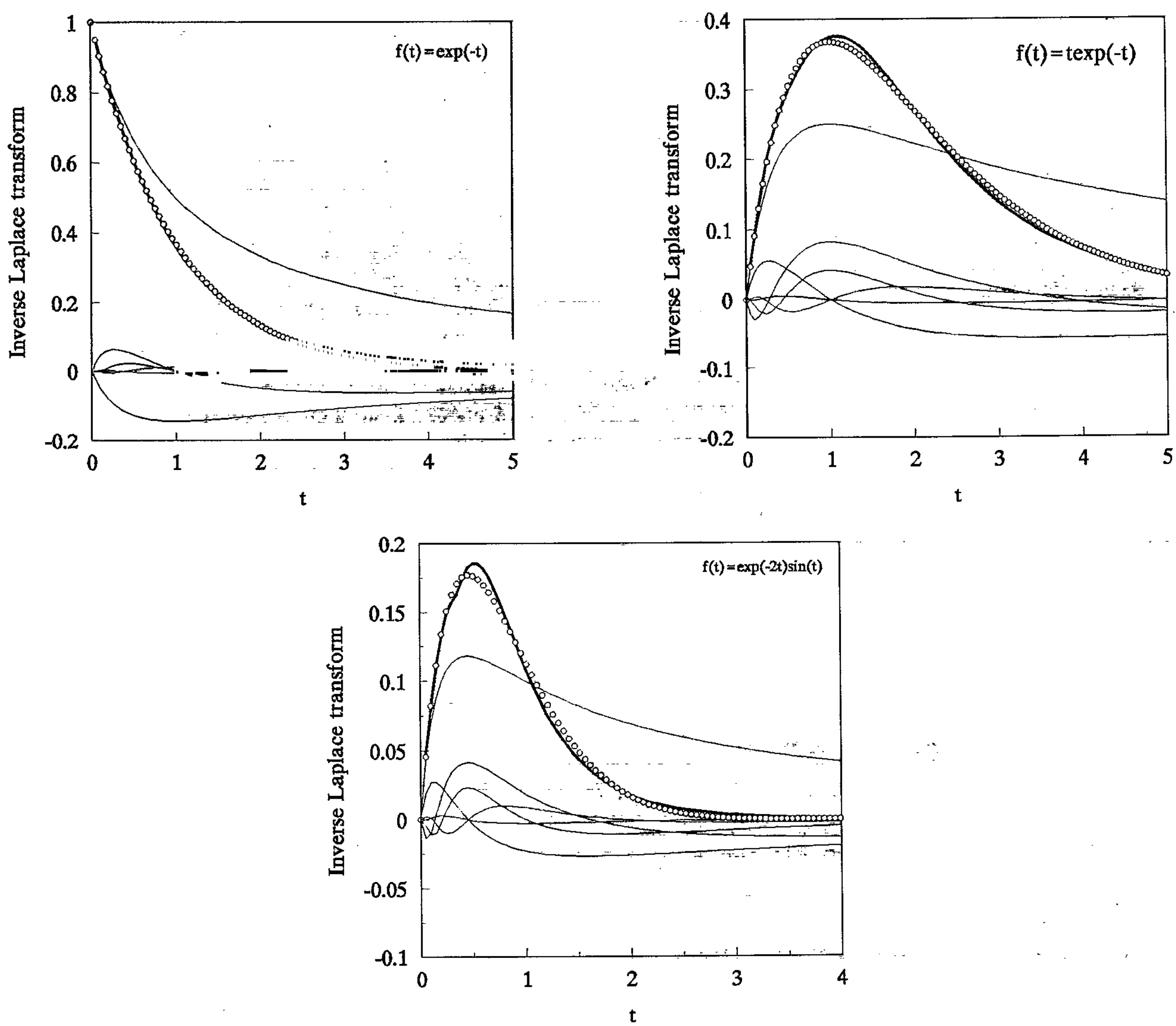

FIG. 1. The numerical results of LIT for three selected functions (cut off to the tenth order). The solid line is the approximate solution, and the thin lines are the terms of approximations from the first order to the sixth order. The open circles denote the exact solution. (a) $\exp(-t) \Longleftrightarrow 1/(p+1)$; (b) $t\exp(-t) \Longleftrightarrow 1/(p+1)^2$; (c) $\exp(-2t)\sin(t) \Longleftrightarrow 1/[1+(p+2)^2]$.

and

$$\sum_{m=0}^{\infty} B_m z^m = \frac{2}{\pi}\cos\left(\frac{\pi}{2}z\right). \quad (59)$$

So one obtains

$$G(x) = \frac{2}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m}{(2m)!}\left(\frac{\pi}{2}\right)^{2m}\frac{\partial^{2m}}{\partial x^{2m}}H_2(x), \quad (60)$$

i.e.,

$$G(x) = \frac{2}{\pi}\mathrm{Re}\left[\exp\left(i\frac{\pi}{2}\frac{\partial}{\partial x}\right)\right]H_2(x)$$

$$= \frac{1}{\pi}\left[H_2\left(x+i\frac{\pi}{2}\right) + H_2\left(x-i\frac{\pi}{2}\right)\right]. \quad (61)$$

Equations (57) and (61) have been obtained by Fuoss and Kirkwood by utilizing the analytic continuation onto the whole of the complex plane [22].

VI. RECONSTRUCTION OF REAL SIGNAL FROM A MEASUREMENT

The data measured by an instrument are always not the actual signal generated in experimental processes. The relationship of a real signal and a measurement is often assumed to obey the following convolution equation in the noise-free limit

$$g(x,y) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} K(x-\xi, y-\eta) \times f(\xi,\eta)d\xi d\eta\ , \quad (62)$$

where f is the actual signal, and g is the measured data. In many cases, the kernel is found to be the Gaussian point spread function

$$K(\xi,\eta) = \frac{1}{2\pi\sigma^2}\exp\left(-\frac{\xi^2+\eta^2}{2\sigma^2}\right), \quad (63)$$

which is able to mimic many processes such as random media degradations, flash radiography, x-ray picture and recovery of turbulent degraded images [28]. Since the Gaussian kernel function is separable, we can write Eq. (62) as

$$g(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} A_1(m)A_2(n)\frac{d^m}{dx^m}\frac{d^n}{dy^n}f(x,y), \quad (64)$$

where

$$A_1(k) = A_2(k) = \frac{1}{k!}\int_{-\infty}^{+\infty}\frac{t^k}{\sqrt{2\pi}\sigma}\exp\left(-\frac{t^2}{2\sigma^2}\right)dt. \quad (65)$$

Therefore we obtain

$$\sum_{k=0}^{\infty} B_1(k)z^k = \sum_{k=0}^{\infty} B_2(k)z^k = \exp\left(-\frac{\sigma^2 z^2}{2}\right) = \sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\left(\frac{\sigma^2}{2}\right)^k z^{2k}. \quad (66)$$

Thus we obtain an inversion result as

$$f(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^{m+n}}{m!n!}\left(\frac{\sigma^2}{2}\right)^{m+n}\frac{d^{2m}}{dx^{2m}}\frac{d^{2n}}{dy^{2n}}g(x,y). \quad (67)$$

Let us consider a test for the above formula. For simplicity, we only take the one-dimensional case into account. According to Eq. (62), an impulse signal $\delta(x-x_0)$ will yield a measured signal in form of a Gaussian function. On the contrary, we can try to reconstruct the real signal via Eq. (67),

$$\delta(x-x_0) = \frac{1}{\sqrt{2\pi}\sigma}\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}\left(\frac{\sigma^2}{2}\right)^m\frac{d^{2m}}{dx^{2m}} \times\left\{\exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]\right\}. \quad (68)$$

Although it may not be wise to use the above formula to simulate the δ function, it should be pointed out that such a simulation can help us to learn how precise we can reach when the method is used in other cases. This can be illustrated in Fig. 2(a). The result may be satisfactory with the truncation at sixth order, but if more terms are added, it would be better than the results shown in Fig. 2(a). As further demonstrations, it is shown in Figs. 2(b) and 2(c) the numerical reconstructions of a three-impulse signal and a double-rectangle signal using Eq. (67).

VII. DISCUSSION

We have shown in the above text that the present MIM contains two kinds of symmetrical transforms which cover important problems such as the MIT and LIT. Actually, both the two cases can be also attributed to the Möbius transform on a partially ordered set (POS) according to Rota [29],

$$P(\alpha) = \sum_{\alpha\preceq\beta}\lambda(\alpha,\beta)Q(\beta) \Longleftrightarrow Q(\alpha) = \sum_{\alpha\preceq\beta}\mu(\alpha,\beta)P(\beta), \quad (69)$$

where the symbol $\preceq$ denotes a binary relation among the elements of the set, and the Möbius function for the POS is defined by

$$\sum_{\alpha\preceq\beta\preceq\gamma}\mu(\alpha,\beta)\lambda(\beta,\gamma) = \delta(\alpha,\gamma), \quad (70)$$

where $\delta(\alpha,\gamma)$ is the Kronecker δ function. When the POS degenerates into a unitary semigroup with addition operation, the POS Möbius transform returns to the additive case of the MIM; when it degenerates into that with multiplication operation, the POS Möbius transform returns to the multiplicative case of the MIM. Though Rota's POS Möbius transform has been applied to the simplification of the cluster-variation method [30,31], its applications to other physical problems are rare. This perhaps is due to its mathematical form which may be unfamiliar for physicists. In a sense, since the MIM is relatively simple, it may help one to understand the Möbius transform on the POS.

Another problem to be discussed here is the noise and regularization. In the above sections we have treated the toy problems in the absence of noise. However, it should be pointed out that since the inversion of the Fredholm integral equation of the first kind is inherently an ill-posed problem, a regularization procedure is needed to improve the solutions of practical problems which are inevitably contaminated by noise. Many attempts have been made to handle the ill-posedness, such as Tikhonov's regularization theory [32] and the method of singular value decomposition [33,34]. Recently, a noteworthy algorithm based on the general theory of amplitude-phase retrieval was put forward and used to solve the inverse blackbody radiation problem [35]. Although different from all the above methods, the present approach is numerically unstable, because the differentiation of noisy signals is highly ill-posed. Nevertheless, since the MIM turns the solution of convolution integral equation into a series of differentiations, one has to regularize only a derivative equation regardless of the kernel function.

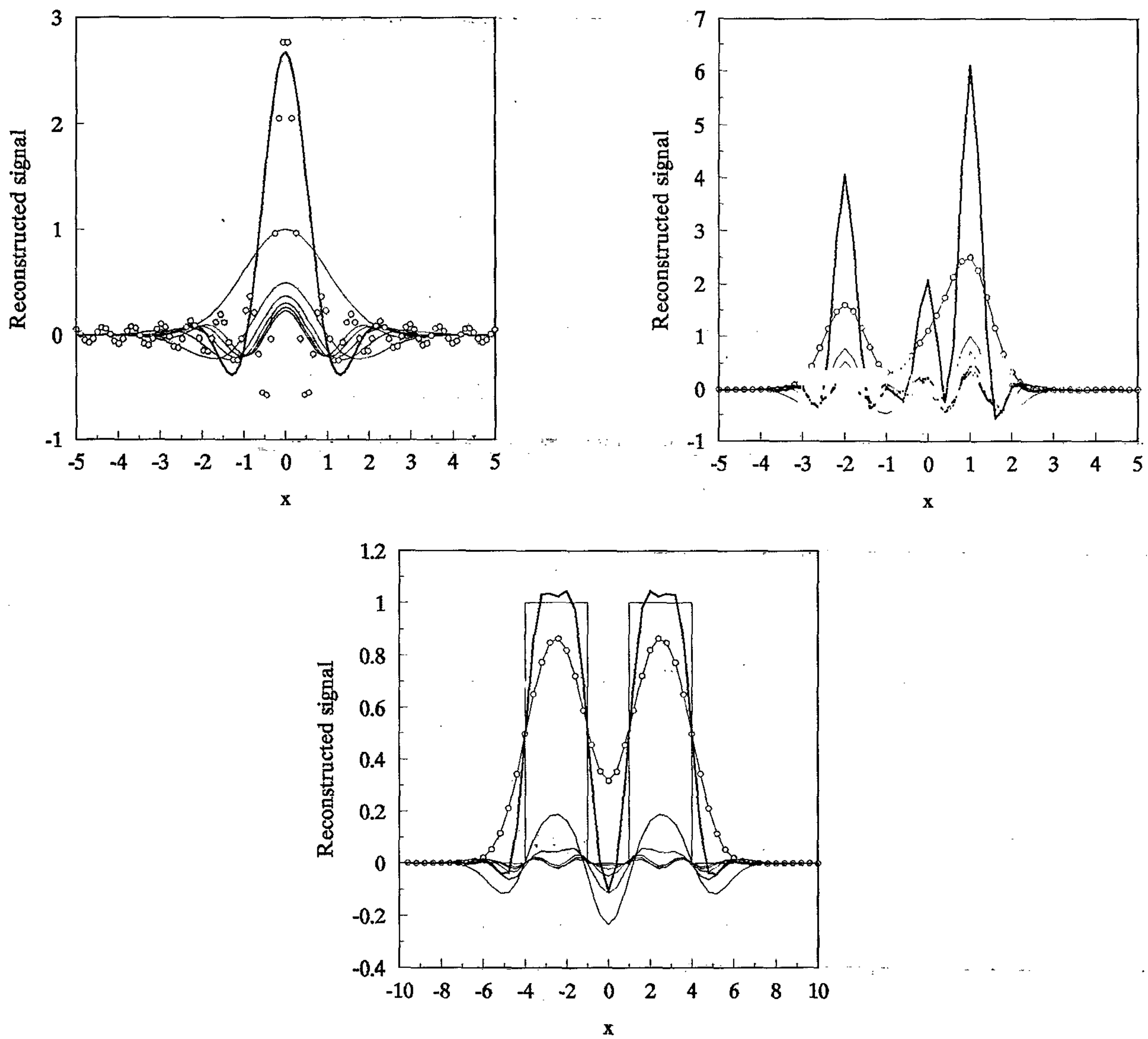

FIG. 2. Three examples of signal reconstruction using Eq. (67) (cut off at the sixth order). The solid line denotes the sum of the lower six lines, which in sequence represent the terms from the first order to the sixth order. (a) A one-impulse signal [the open circles denote the approach function $\sin(\alpha x)/\pi x$]. (b) A three-impulse signal $2\delta(x+2)+\delta(x)+3\delta(x-1)$ (the open circles are the discrete input points). (c) A double-rectangle signal $\theta(x-1)\theta(4-x)+\theta(-1-x)\theta(x+4)$ (the open circles are the discrete input points).

ACKNOWLEDGMENTS

The authors would like to thank Professor E.Q. Rong and Dr. W.Q. Zhang at Beijing University of Science and Technology for their very helpful suggestions. They are indebted to the referee for pointing out some grammatical and stylistic mistakes in the original manuscript. Q.X. is also grateful to Miss X.D. Zhao for her stimulating discussion on the regularization method. This work was supported in part by the National Natural Science Foundation of China and in part by the National Advanced Materials Committee of China.

APPENDIX

By derivative action on Eq. (36) with respect to λ, we have

$$\frac{\partial\phi(x)}{\partial\lambda}=\sum_{m=0}^{\infty}\left\{x^{\lambda-1}\ln x B_m^L\left(x\frac{d}{dx}\right)^m\left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right]\right.$$
$$\left.+x^{\lambda-1}\frac{\partial B_m^L}{\partial\lambda}\left(x\frac{d}{dx}\right)^m\left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right]+x^{\lambda-1}B_m^L\left(x\frac{d}{dx}\right)^m\left[-x^{-\lambda}\ln x\overline{\phi}\left(\frac{1}{x}\right)\right]\right\}. \tag{A1}$$

Note the equality

$$\left(x\frac{d}{dx}\right)^m\left[x^{-\lambda}\ln x\overline{\phi}\left(\frac{1}{x}\right)\right]=m\left(x\frac{d}{dx}\right)^{m-1}\left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right]+\ln x\left(x\frac{d}{dx}\right)^m\left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right]\ (m\geq 1)\ . \tag{A2}$$

We have

$$\frac{\partial\phi(x)}{\partial\lambda}=\sum_{m=0}^{\infty}\left\{x^{\lambda-1}\left[\frac{\partial B_m^L}{\partial\lambda}-(m+1)B_{m+1}^L\right]\left(x\frac{d}{dx}\right)^m\left[x^{-\lambda}\overline{\phi}\left(\frac{1}{x}\right)\right]\right\}\ . \tag{A3}$$

On the other hand

$$\frac{\partial}{\partial\lambda}\left[\frac{1}{\Gamma(\lambda+z)}\right]=\frac{\partial}{\partial z}\left[\frac{1}{\Gamma(\lambda+z)}\right], \tag{A4}$$

namely,

$$\sum_{m=0}^{\infty}\frac{\partial B_m^L}{\partial\lambda}z^m=\sum_{m=0}^{\infty}(m+1)B_{m+1}^L z^m, \tag{A5}$$

i.e.,

$$\frac{\partial B_m^L}{\partial\lambda}=(m+1)B_{m+1}^L. \tag{A6}$$

By inserting Eq. (A6) into Eq. (A3), we can see that

$$\frac{\partial}{\partial\lambda}\phi(x)=0. \tag{A7}$$

This result means that the solution is free from the parameter λ.

[1] N.X. Chen, Phys. Rev. Lett. **64**, 1193 (1990).
[2] M.R. Schroeder, *Number Theory in Science and Communication* (Springer-Verlag, Berlin, 1984).
[3] J. Maddox, Nature (London) **344**, 377 (1990).
[4] B.D. Hughes *et al.*, Phys. Rev. A **42**, 3643 (1990).
[5] S.Y. Ren and J.D. Dow, Phys. Lett. A **154**, 215 (1991).
[6] T.L. Xie *et al.*, Astrophys. J. **371**, L81 (1991); **402**, 216 (1993).
[7] H. Rosu, Nuovo Cimento B **108**, 1333 (1993).
[8] B.W. Ninham *et al.*, Physica A **186**, 441 (1992).
[9] E.W. Montroll, J. Chem. Phys. **10**, 218 (1942).
[10] N.N. Bojarski, IEEE Trans. Antennas Propag. **AP-30**, 778 (1982).
[11] Q. Xie and N.X. Chen, Phys. Rev. E **52**, 351 (1995).
[12] A.E. Carlsson, C.D. Gelatt, and H. Ehrenreich, Philos. Mag. A **41**, 241(1980).

[13] Q. Xie and M.C. Huang, Phys. Lett. A **184**, 119 (1993).
[14] N.X. Chen *et al.*, Phys. Lett. A **184**, 347 (1994); **195**, 135 (1994).
[15] Q. Xie and M.C. Huang, Phys. Status Solidi B **186**, 393 (1994).
[16] N.X. Chen and G.B. Ren, Phys. Rev. B **45**, 8177 (1992); **47**, 593 (E) (1993).
[17] A. Mookerjee *et al.*, J. Phys. Condens. Matter **4**, 2439 (1992).
[18] Q. Xie, W. Xu, and M.C. Huang, Chin. Phys. Lett. **12**, 12 (1995).
[19] M.S. Daw and M.I. Baskes, Phys. Rev. Lett. **50**, 1245 (1983); Phys. Rev. **B29**, 6443 (1984).
[20] Q. Xie and N.X. Chen, Phys. Rev. B **51**, 15 856 (1995).
[21] Q. Xie and M.C. Huang, J. Phys. Condens. Matter **6**, 11 015 (1994).
[22] A.S. Nowick and B.S. Berry, *Anelastic Relaxation in Crystalline Solids* (Academic Press, New York, 1972).
[23] R.J.W. Hodgson, J. Appl. Phys. **76**, 7524 (1994).
[24] Y. Ogata, T. Sakka, and M. Iwasaki, J. Appl. Electrochem. **25**, 41 (1995).
[25] R. Bellman, R.E. Kalaba, and J.A. Lockett, *Numerical Inversion of the Laplace Transform* (Elsevier, Amsterdam, 1966).
[26] C. Cunha and F. Viloche, Inverse Prob. **9**, 57 (1993).
[27] P. Brianzi and M. Frontin, Inverse Prob. **7**, 355 (1991).
[28] R.S. Anderssen, F.R. de Hoog, and M.A. Lukas, *The Application and Numerical Solution of Integral Equations* (Sijthoff & Noordhoff, The Netherlands, 1980).
[29] G.C. Rota, Z. Wahrsch. **2**, 340 (1964).
[30] G. An, J. Stat. Phys. **52**, 727 (1988).
[31] J. Morita, J. Stat. Phys. **59**, 819 (1990).
[32] A.N. Tikhonov and V.Y. Arsenin, *Solution of Ill-Posed Problems* (Winston, Washington, D.C. 1977).
[33] P.C. Hansen, Inverse Probl. **10**, 895 (1994).
[34] M. Bertero, P. Boccacci, F. Malfanti, and E.R. Pike, Inverse Probl. **10**, 1059 (1994), and references therein.
[35] X. Tan, G.Z. Yang, B.Y. Gu, and B.Z. Dong, J. Opt. Soc. Am. A **11**, 1068 (1994).