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Chen's inversion formula

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Nan-xian Chen [Phys. Rev. Lett. **64**, 1193 (1990)] has generalized a formula of classical algebraic number theory to continuous variables and noted some useful consequences of the generalization. We present an alternative view of this analysis, based on the Mellin transformation and Riemann's zeta function.

From time to time, apparently obscure results of classical mathematics suddenly find new physical applications. Recently, Chen¹ has generalized to continuous variables by a limiting argument the Möbius inversion formula which states that if

$$F(n) = \sum_{d|n} f(d) \tag{1}$$

then

$$f(n) = \sum_{d|n} \mu(d)F(n/d). \tag{2}$$

In Eqs. (1) and (2), $d|n$ means that $1 \leq d \leq n$ and the integer d is a factor of the positive integer n . The Möbius function $\mu(n)$ is defined by the formula

$$\mu(n) = \begin{cases} 1, & n = 1, \\ (-1)^r, & \text{if } n \text{ has } r \text{ distinct prime factors,} \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

Chen's generalization of Eqs. (1) and (2) is equivalent to the assertion that

$$\alpha(x) = \sum_{n=1}^{\infty} \beta(nx), \quad x > 0 \tag{4}$$

implies that

$$\beta(x) = \sum_{n=1}^{\infty} \mu(n)\alpha(nx), \quad x > 0. \tag{5}$$

This assertion can be given a rigorous proof directly without the need to apply any limiting argument to the discrete formulas (1) and (2). The Mellin transform of a

function is defined by the formula

$$\tilde{\alpha}(s) = \int_0^{\infty} x^{s-1} \alpha(x) dx. \tag{6}$$

For the properties of the Mellin transform, reference may be made to a treatise of Titchmarsh.² If we take the Mellin transform of both sides of Eq. (4), restricting the range of the complex variable s appropriately, we find on interchanging orders of integration and summation that

$$\tilde{\alpha}(s) = \zeta(s) \tilde{\beta}(s), \tag{7}$$

where Riemann's ζ function is defined by the series

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \tag{8}$$

for $\text{Re}(s) > 1$, and by analytic continuation elsewhere. Equation (7) is rigorously correct provided that the integrals defining the Mellin transforms of α and β converge absolutely at least in some strip $1 < a < \text{Re}(s) < b$. The reader will have no difficulty translating this requirement into a hypothesis on the dominant asymptotic behavior of the original functions at the origin and at infinity. Similarly, the Mellin transform of Eq. (5) gives

$$\tilde{\beta}(s) = \tilde{\alpha}(s) \sum_{n=1}^{\infty} \mu(n) n^{-s}, \tag{9}$$

with obvious similar restrictions on $\text{Re}(s)$, and Chen's result, as presented in Eqs. (4) and (5) above, reduces to the assertion that

$$\zeta(s)^{-1} = \sum_{n=1}^{\infty} \mu(n) n^{-s}, \tag{10}$$

for $\text{Re}(s) > 1$. A direct proof of Eq. (10) will be found in another treatise of Titchmarsh, page 3.³ The proof is a one-line consequence of the well-known result proven on pages 1 and 2 of Titchmarsh³ that

$$\zeta(s) = \prod_p (1 - p^{-s})^{-1}, \quad \text{Re}(s) > 1, \quad (11)$$

where the product is taken over all prime numbers.

The Riemann ζ function arises in surprisingly many contexts, for example, in connection with a class of random walks processes,⁴ and the Mellin transform has a primary role in asymptotic analysis which is still not well known in physics, though it has at least begun to receive adequate coverage in textbooks.⁵ We shall reexamine two of the physical examples considered by Chen from the point of view of Mellin transform methods. Chen's third application, to Ewald summation, is a direct application of Eqs. (4) and (5), and merits no further discussion here. In our discussion of the examples, the following well-documented properties of the Γ function and the Riemann ζ function⁶ are used:

$$\Gamma(s) = \int_0^\infty e^{-x} x^{s-1} dx = a^s \int_0^\infty e^{-ax} x^{s-1} dx, \quad (12)$$

$$\text{Re}(s) > 0, \quad \text{Re}(a) > 0,$$

$$\begin{aligned} \zeta(s)\Gamma(s) &= \int_0^\infty \frac{x^{s-1}}{\exp(x)-1} dx \\ &= a^s \int_0^\infty \frac{x^{s-1}}{\exp(ax)-1} dx, \end{aligned} \quad (13)$$

$$\text{Re}(s) > 1, \quad \text{Re}(a) > 0,$$

$$\zeta(s) = 2^s \pi^{s-1} \sin(\pi s/2) \zeta(1-s) \Gamma(1-s). \quad (14)$$

The Γ function never vanishes, and is holomorphic except for simple poles at $0, -1, -2, \dots$, while the Riemann ζ function is holomorphic except for a simple pole at 1, and has its zeros at $-2, -4, -6, \dots$, and in the strip $0 < \text{Re}(s) < 1$, infinitely many of which lie on the line $\text{Re}(s) = \frac{1}{2}$. The most famous unsolved problem in complex analysis is the proof or disproof of Riemann's hypothesis that $\zeta(s)$ has no zeros in the strip $0 < \text{Re}(s) < 1$, other than those on the line $\text{Re}(s) = \frac{1}{2}$.

The key to the relation between our presentation and Chen's is the observation that if

$$f(x) = \sum_{n=1}^\infty \mu(n) n^{-\lambda} \phi(n^{\pm 1} x), \quad (15)$$

then

$$\tilde{f}(s) = \zeta(\lambda \pm s)^{-1} \tilde{\phi}(s). \quad (16)$$

Inverse blackbody radiation. The inverse problem of blackbody radiation, though of long standing, appears to retain some interest.^{7,8} In this problem, the function $W(\nu)$ is taken as known, and $a(u)$ is to be found, where

$$W(\nu) = \frac{2h\nu^3}{c^2} \int_0^\infty \frac{a(u)}{\exp(u\nu)-1} du. \quad (17)$$

If we take the Mellin transform of both sides of Eq. (17),

we find using Eq. (13) that

$$\tilde{W}(s) = \frac{2h}{c^2} \zeta(s+3) \Gamma(s+3) \tilde{a}(-s-2). \quad (18)$$

If we now introduce the change of variables $z = -s-2$ and subsequently rename z as s , we find that

$$\begin{aligned} \tilde{a}(s) &= \frac{c^2}{2h} \frac{\tilde{W}(-s-2)}{\zeta(1-s) \Gamma(1-s)} \\ &= \frac{c^2}{2h} \frac{\tilde{W}(-s-2) 2^s \pi^{s-1} \sin(\pi s/2)}{\zeta(s)}. \end{aligned} \quad (19)$$

Either of the expressions for $\tilde{a}(s)$ in Eq. (19) may be used as a point of departure for generating asymptotic expansions of $a(u)$. (We illustrate the procedure below in the discussion of another of Chen's examples.) To recover the results derived by Kim and Jaggard⁸ and rederived by Chen,⁹ we use Eqs. (15) and (16) with $\lambda=1$ and the minus sign selected, to give

$$a(x) = \sum_{n=1}^\infty \frac{\mu(n)}{n} \phi(x/n), \quad (20)$$

where

$$\tilde{\phi}(s) = \frac{c^2}{2h} \frac{\tilde{W}(-s-2)}{\Gamma(1-s)}. \quad (21)$$

If the analytic structure of W is known, the function ϕ can be recovered from Eq. (21) using the inversion integral

$$\phi(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-s} \tilde{\phi}(s) ds. \quad (22)$$

The result of Kim and Jaggard, which is fundamentally no simpler than that exhibited in Eqs. (20)-(22), follows from noting that Eq. (21) is equivalent to the statement that

$$\int_0^\infty \frac{c^2 W(\nu)}{2h\nu^3} \nu^{-s} d\nu = \int_0^\infty \Gamma(1-s) t^{s-1} \phi(t) dt. \quad (23)$$

Using the integral representation (12) and interchanging orders of integration, we find that

$$\int_0^\infty \frac{c^2 W(\nu)}{2h\nu^3} \nu^{-s} d\nu = \int_0^\infty \nu^{-s} \int_0^\infty e^{-\nu t} \phi(t) dt, \quad (24)$$

and inverting the transform over ν we deduce that $c^2 W(\nu)/(2h\nu^3) = L\{\phi(t); t \rightarrow \nu\}$, where L denotes the Laplace transform operator.

Phonon density of states. Chen considers the problem of obtaining the phonon density of states $g(\nu)$ from the formula

$$c(u) = \int_0^\infty \frac{(u\nu)^2 \exp(u\nu) g(\nu)}{[\exp(u\nu)-1]^2} d\nu. \quad (25)$$

Here $u = h/kT$, with h denoting Planck's constant, k Boltzmann's constant, and T the absolute temperature, as usual. Up to a multiplicative constant, the function c corresponds to the specific heat of lattice vibration, and is regarded as a known function. The inversion of this formula is a problem of modest antiquity, with an important inves-

tigation having been made in 1959 by Weiss.¹⁰ If we take a Mellin transform of this equation and interchange orders of integration, the integral over u is easily evaluated using Eq. (13), if one rewrites Eq. (13) as an integral representation of $\zeta(s)\Gamma(s)a^{-s}$ and differentiates with respect to a . We find that

$$\begin{aligned} \bar{c}(s) &= \Gamma(s+2)\zeta(s+1) \int_0^\infty g(v)v^{-s}dv \\ &= \Gamma(s+2)\zeta(s+1)\bar{g}(1-s). \end{aligned} \tag{26}$$

This equation can be used as a starting point of asymptotic analysis. If we introduce the change of variables $z = 1 - s$ and subsequently rename z as s , we find that

$$\bar{g}(s) = \frac{\bar{c}(1-s)}{\Gamma(3-s)\zeta(2-s)}. \tag{27}$$

From the inversion integral (22), the small- v expansion of $g(v)$ is determined by the singularity structure of $\bar{g}(s)$ on the left-hand side of the integration contour. Since the denominator in Eq. (27) does not vanish on this side of the contour, we need only determine the singularities of the numerator. If we assume a standard low-temperature expansion of the specific heat in odd powers of T , we may write

$$c(u) \sim \sum_{n=1}^\infty c_n u^{-2n-1} \text{ as } u \rightarrow \infty, \tag{28}$$

so that $\bar{c}(1-s)$ has simple poles of residue c_n at $s = -2n(n=1,2,\dots)$. At these points the denominator in Eq. (27) is simply

$$\Gamma(2n+3)\zeta(2n+2) = (2n+2)!\zeta(2n+2).$$

We easily recover Weiss' low-frequency expansion¹⁰

$$g(v) \sim \sum_{n=1}^\infty \frac{c_n v^{2n}}{(2n+2)!\zeta(2n+2)}. \tag{29}$$

If we desire an alternative formal inversion formula, inspection of Eqs. (15) and (16) at once suggests the expansion

$$g(v) = \sum_{n=1}^\infty \frac{\mu(n)}{n^2} \psi(v/n), \tag{30}$$

to remove the ζ function. We find that we need only select ψ such that

$$\bar{\psi}(1-s) = \bar{c}(s)/\Gamma(s+2). \tag{31}$$

As in the example of inverse blackbody radiation above, we can easily turn this into a relation involving Laplace transforms, with $c(u)/u^2 = L\{t^2\psi(t); t \rightarrow u\}$.

The analysis in Chen's original paper, with its reliance on algebraic number theory, has attracted some interest as a potential example of a treasure trove of, yet to be applied, obscure mathematical results.¹¹ This may indeed be so, but it is hoped that the present discussion shows clearly why the Möbius function arises in the examples considered. In essence, in all cases studied by Chen, the Mellin transform of the unknown function has a Riemann ζ function on the denominator. It is the expansion of the reciprocal ζ function which produces the Möbius function. This expansion is actually used without comment at one point in Chen's paper as a minor technical result, but we regard it as central to the method. The great advantage of the Mellin transform method is that it places us quickly in touch with the powerful techniques of complex variable theory, and may produce a more obvious way to proceed in cases more complicated than those considered by Chen.

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³E. C. Titchmarsh, *The Theory of the Riemann Zeta Function* (Clarendon, Oxford, 1951).
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⁵See, e.g., R. Wong, *Asymptotic Approximations of Integrals* (Academic, New York, 1989).
⁶Equation (12) is the usual definition of the Γ function; Eq. (13)

comes from the defining series (8) on replacing n^{-s} with the integral representation of the Γ function; seven different proofs of Eq. (14) are given in Ref. 3.
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