Unified solution of the inverse capacity problem

Chen Nan-xian and Rong Er-qian
*China Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China and Institute of Applied Physics, University of Science and Technology Beijing, Beijing 100083, China**
(Received 18 August 1997)

The inverse specific heat problem has played a significant role in physics. But there is no satisfactory solution for this inherently ill-posed inverse problem. The present work shows a concise and unified solution based on the Möbius inversion technique and the Poisson-Abel process. This solution can explain both Debye's and Einstein's approximations very well. All the mathematical deductions are shown in the Appendixes; they are deduced in an elementary way for physicists. [S1063-651X(98)02302-2]

PACS number(s): 05.90.+m, 65.40.+g, 02.10.Lh, 02.30.Sa

I. INTRODUCTION

When establishing the thermodynamics for a system, the key point is to determine the energy spectrum of the quasiparticle based on the Hamiltonian operator. Once the energy spectrum is known, all the thermodynamic quantities can be given by integration. The corresponding inverse problem is to determine the energy spectrum from the thermodynamic quantities. The specific heat of lattice vibrations can be expressed as

$$C_v(T)=rk\int_0^\infty \frac{(h\nu/kT)^2 e^{h\nu/kT}}{(e^{h\nu/kT}-1)^2}\, g(\nu)d\nu, \tag{1}$$

where h and k represent the Planck and Boltzmann constants, respectively, and r is the number of atoms per unit cell, and $g(\nu)$, the phonon density of states, is normalized to $3Nr$:

$$\int_0^\infty g(\nu)d\nu=3Nr. \tag{2}$$

The problem is to recover the $g(\nu)$ based on the experimentally measurable $C_\nu(T)$. This problem was proposed and approximately solved by Einstein in 1907 and Debye in 1912 using trial and error. Their contribution was crucial to the development of the concept of early quantum theory [1]; it has also been very important in the field of condensed matter physics.

The problem of heat capacities of solids is considered anomalous in classical physics. The problem was to determine the energy quantization from the heat capacity curve [1]. Einstein proposed a harmonic model with single frequency (Fig. 1), which was a significant contribution to early quantum theory at the beginning of this century [2]. Soon after that, Debye suggested the continuous medium model for the low-temperature limit (Fig. 2) [3]. In 1942, this problem was proposed again by Montroll [4] due to the importance of phonon density of states for thermodynamic properties of solids, lattice dynamics, electron-phonon interactions, and the optical-phonon spectrum. Lifshitz proposed the inverse specific heat problem independently in 1954 [5]. Montroll and Lifshitz arrived at virtually identical solutions to this problem despite the fact that the two worked in complete isolation as a result of World War II. It was repeated by Chambers in 1961 [6] and Dai, Xu, and Dai in 1990 [7]. Also, Lifshitz obtained a formal solution by Mellin transform [5]. In 1959, Weiss gave a general formula of the phonon density of states for low-frequency limit [8]. Recently, Hughes, Frankel, and Ninham again used Mellin transform to obtain an integral representation of solution with the Weiss formula [9]. Most of the works mentioned above focus on the integral representation of the exact solution. As a result, these solutions are difficult to interpret in terms of intuition in physics.

This work introduces the Möbius inversion formula [10,11] to obtain a concise and unified solution for this interesting inverse problem. This solution makes the discussion for various physical situations easier and much more convenient. Two general formulas for both high-frequency limit and low-frequency limit are given directly, and the Debye model and the Einstein model appear as two zero-order approximations. For convenience, Sec. II provides a brief review of previous work. Section III shows the concise and unified closed form solution in a series representation. The general formula for the low-frequency limit is given in Sec. IV, the general formula for the high-frequency limit is given

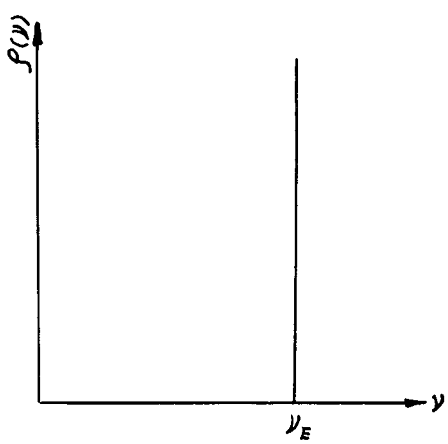

FIG. 1. Einstein approximation.

*Mailing address.

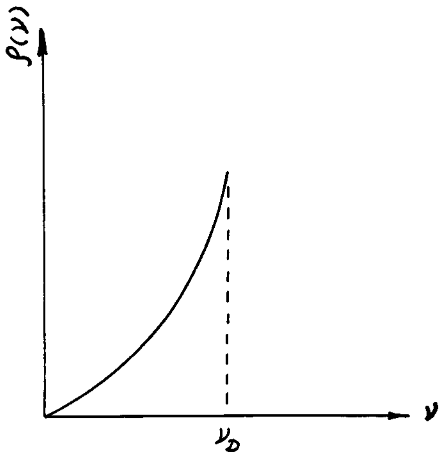

FIG. 2. Debye approximation.

in Sec. V. Section VI is the Conclusion and Discussion. A concise deduction of Möbius transform and some divergent series related to the Riemann ζ function are introduced in Appendices A and B.

II. REVIEW OF MONTROLL-LIFSHITZ FORMULA

Let us introduce new variables x and y such that

$$e^x=\frac{h\nu}{k}, \quad e^y=T. \tag{3}$$

Then Eq. (1) becomes

$$C(y)=\int_{-\infty}^{\infty}\Phi(y-x)G(x)dx=\Phi(y)*G(y), \tag{4}$$

where

$$C(y)=\frac{he^{-\delta y}}{rk^2}\,C_v(e^y) \tag{5}$$

and

$$G(x)=e^{(1-\delta)x}g\left(\frac{ke^x}{h}\right), \tag{6}$$

and the integral kernel is given as

$$\Phi(u)=\frac{e^{-(\delta+2)u}e^{e^{-u}}}{(e^{e^{-u}}-1)^2}. \tag{7}$$

The parameter δ is chosen such that

$$0\leqslant\delta\leqslant 3 \tag{8}$$

in order to satisfy

$$\lim_{u\to\pm\infty}\Phi(u)=0. \tag{9}$$

Using Fourier deconvolution, one has

$$\hat{G}(k)=\frac{\hat{C}(k)}{\hat{\Phi}(-k)} \tag{10}$$

and

$$\hat{\Phi}(-k)=\int_{-\infty}^{\infty}\frac{e^{isk}e^{e^s}e^{(\delta+2)s}ds}{(e^{e^s}-1)^2}=(1+\delta+ik)\zeta(1+\delta+ik)\times\Gamma(1+\delta+ik). \tag{11}$$

Therefore a solution in the integral form is obtained as

$$g(\nu)=\frac{1}{\nu}\int_{-\infty}^{\infty}\frac{(h\nu)^{ik\nu}\hat{C}(k)dk}{(1+\delta+ik)\zeta(1+\delta+ik)\Gamma(1+\delta+ik)}. \tag{12}$$

This is the Montroll-Lifshitz formula for the inverse specific heat problem. This formula has an integral form with the kernel on the complex plane, and is difficult to use when discussing various concrete situations. Lifshitz mentioned the formal expression of the solution based on Mellin transform in his work [5], which has recently been presented by Hughes, Frankel, and Ninham [9]

$$M[g](s)=\frac{M[C](1-s)}{\Gamma(3-s)\zeta(2-s)}. \tag{13}$$

Nevertheless, it is still difficult to relate this solution to the various physical situations.

III. UNIFIED SOLUTION FOR INVERSE SPECIFIC HEAT PROBLEM

For solving Eq. (1), let us introduce ''coldness'' as $u=h/kT$, thus Eq. (1) becomes [12]

$$C_v\left(\frac{h}{ku}\right)=rk\int_0^{\infty}\frac{(u\nu)^2e^{u\nu}}{(e^{u\nu}-1)^2}\,g(\nu)d\nu. \tag{14}$$

By using Taylor's expansion, one can find that

$$\begin{aligned}C_v(h/ku)&=rk\sum_{n=1}^{\infty}\int_0^{\infty}n(u\nu)^2e^{-nu\nu}g(\nu)d\nu\\&=rku^2\sum_{n=1}^{\infty}n\int_0^{\infty}\nu^2g(\nu)e^{-n\nu u}d\nu\\&=rku\sum_{n=1}^{\infty}(nu)L[\nu^2g(\nu);\nu\to nu],\end{aligned}$$

where $L[\ ]$ represents the Laplace transform. Therefore

$$uL[\nu^2g(\nu);\nu\to u]=\sum_{n=1}^{\infty}\mu(n)\,\frac{C_v(h/nku)}{rknu},$$

where we have used the Möbius transform (see Appendix A), which states if

$$F(x)=\sum_{n=1}^{\infty}f(nx), \tag{15}$$

then

$$f(x)=\sum_{n=1}^{\infty} \mu(n)F(nx). \tag{16}$$

Thus it is given that

$$g(\nu)=\frac{1}{rk\nu^2}\sum_{n=1}^{\infty} \mu(n)L^{-1}\left[\frac{C_v(h/nku)}{nu^2};u\rightarrow\nu\right]. \tag{17}$$

Unlike Einstein's or Debye's approximation, this is an exact closed form solution. The spirit of most previous works is to solve the inverse problem based on the method for direct problems, i.e., the trial and error method. This work is slightly different.

IV. GENERAL FORMULA FOR LOW-TEMPERATURE LIMIT

If we assume a standard low-temperature expansion of the specific heat in odd powers of T, we may write

$$C_v(T)=a_3T^3+a_5T^5+a_7T^7+\cdots \quad \text{as} \quad T\rightarrow 0 \tag{18}$$

or

$$C_v(h/ku)=\sum_{n=2}^{\infty} a_{2n-1}(h/k)^{2n-1}u^{-(2n-1)} \quad \text{as} \quad u\rightarrow\infty. \tag{19}$$

Hence,

$$g(\nu)=\frac{1}{rk\nu^2}\sum_{n=1}^{\infty} \mu(n)\sum_{m=2}^{\infty} a_{2m-1}\left(\frac{h}{nk}\right)^{(2m-1)}L^{-1}\times\left[\frac{u^{-(2m-1)}}{nu^2};u\rightarrow\nu\right]$$

$$=\frac{1}{rk\nu}\sum_{m=2}^{\infty}\left[\sum_{n=1}^{\infty}\frac{\mu(n)}{n^{2m}}\right]a_{2m-1}\left(\frac{h}{k}\right)^{2m-1}L^{-1}\times\left[\frac{1}{u^{2m+1}};u\rightarrow\nu\right]$$

or

$$g(\nu)=\frac{1}{rk\nu}\sum_{m=2}^{\infty}\frac{a_{2m-1}(h\nu/k)^{2m-1}}{(2m)!\zeta(2m)}.$$

By using $\zeta(2m)=(-1)^{m+1}\{(2\pi)^{2m}/2[(2m)!]\}B_{2m}$, we have

$$g(\nu)=\frac{1}{rk\nu}\sum_{m=2}^{\infty}\frac{a_{2m-1}(h\nu/k)^{2m-1}}{(2m)!\zeta(2m)}. \tag{20}$$

This is completely the same as Weiss's formula for the low-temperature limit [8]. Taking only the first term, the expression above simply gives the Debye model as

$$g(\nu)=\left[\left(\frac{h}{k}\right)^3\frac{1}{4!\zeta(4)}\frac{1}{rk}a_3\right]\nu^2=\frac{90a_3h^3}{\pi^2rk^4}\nu^2. \tag{21}$$

V. GENERAL FORMULA FOR HIGH-TEMPERATURE LIMIT

Now let us show how to get a general formula for the high-frequency limit. If the temperature is high enough, we have

$$C(T)=a_0-\frac{a_2}{T^2}+\frac{a_4}{T^4}-\frac{a_6}{T^6}+\cdots \tag{22}$$

or

$$\frac{C(h/ku)}{u^2}=\frac{1}{u^2}\left[a_0-\frac{a_2(ku)^2}{h^2}+\frac{a_4(ku)^4}{h^4}-\frac{a_6(ku)^6}{h^6}+\cdots\right]. \tag{23}$$

Hence,

$$\frac{C(h/ku)}{u^2}=\frac{a_0}{u^2}-\frac{a_2k^2}{h^2}+\frac{a_4k^4u^2}{h^4}-\frac{a_6k^6u^4}{h^6}+\cdots,$$

$$\frac{C(h/2ku)}{2u^2}=\frac{a_0}{2u^2}-\frac{2a_2k^2}{h^2}+\frac{2^3a_4k^4u^2}{h^4}-\frac{2^5a_6k^6u^4}{h^6}+\cdots,$$

$$\frac{C(h/3ku)}{3u^2}=\frac{a_0}{3u^2}-\frac{3a_2k^2}{h^2}+\frac{3^3a_4k^4u^2}{h^4}-\frac{3^5a_6k^6u^4}{h^6}+\cdots,$$

$$\frac{C(h/nku)}{nu^2}=\frac{a_0}{nu^2}-\frac{na_2k^2}{h^2}+\frac{n^3a_4k^4u^2}{h^4}-\frac{n^5a_6k^6u^4}{h^6}+\cdots$$

$$=\sum_{m=0}^{\infty}(-1)^m a_{2m}(k/h)^{2m}u^{2(m-1)}n^{2(m-1)}.$$

According to Eq. (17),

$$g(\nu)=\frac{1}{rk\nu^2}\sum_{n=1}^{\infty}\mu(n)L^{-}\left[\frac{C_v(h/nku)}{nu^2};u\rightarrow\nu\right]$$

$$=\frac{1}{rk\nu^2}\sum_{n=1}^{\infty}\mu(n)L^{-1}\left[\frac{a_0}{nu^2}\right]-\frac{1}{rk\nu^2}\sum_{n=1}^{\infty}\mu(n)L^{-1}\left[\frac{na_2k^2}{h^2}\right]+\frac{1}{rk\nu^2}\sum_{n=1}^{\infty}\mu(n)L^{-1}\left[\frac{n^3a_4k^4u^2}{h^4}\right]-\cdots$$

$$=\frac{1}{rk\nu^2}\left\{\left[\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\right]L^{-1}\left[\frac{a_0}{u^2}\right]-\left[\sum_{n=1}^{\infty}n\mu(n)\right]L^{-1}\left[\frac{a_2k^2}{h^2}\right]+\left[\sum_{n=1}^{\infty}n^3\mu(n)\right]L^{-1}\left[\frac{a_4k^4u^2}{h^4}\right]-\cdots\right\}$$

$$=\frac{1}{rk\nu^2}\left\{\frac{1}{\zeta(1)}L^{-1}\left[\frac{a_0}{u^2}\right]-\frac{1}{\zeta(-1)}L^{-1}\left[\frac{a_2k^2}{h^2}\right]+\frac{1}{\zeta(-3)}L^{-1}\left[\frac{a_4k^4u^2}{h^4}\right]-\cdots\right\}.$$

Considering $\zeta(1)=\infty$, we have

$$g(\nu)=\frac{1}{rk\nu^2}\sum_{n=1}^{\infty}\frac{a_{2n}}{\zeta(1-2n)}\left(\frac{k}{h}\right)^{2n}\delta^{(2n-2)}(\nu). \quad (24)$$

This is the general representation of Eq. (17) for the high-frequency limit. In the above deduction, the relation for generalized functions,

$$L^{-1}[u^m;u\to\nu]=\delta^{(m)}(\nu), \quad (25)$$

was used in which $\{\delta^{(m)}(\nu)\}$ are derivatives of the generalized even function $\delta(\nu)$. Also, a definition of Riemann's ζ function

$$\frac{1}{\zeta(s)}=\sum_{n=1}^{\infty}\frac{\mu(n)}{n^s} \quad (s\geqslant 1) \quad (26)$$

has been extended to s being negative integers. At this point it can be considered as a symbolic operation, since the summation in Eq. (26) is divergent. However, we find that the result for the high-temperature limit or the high-frequency limit is certainly reasonable from the physical point of view. It seems quite ridiculous that we had extended Eq. (26) to

$$\frac{1}{\zeta(s)}=\sum_{n=1}^{\infty}\frac{\mu(n)}{n^s} \quad (s=-1,-2,-3,\ldots)$$
$$=\sum_{n=1}^{\infty}\mu(n)n^s \quad (s=1,2,3,\ldots). \quad (27)$$

This apparently unreasonable effectiveness can be understood as the result of a generalized function (see Appendix B).

A. Einstein's single peak approximation

Einstein's approximation would be the most important check for our general high-frequency formula. In this case, Eq. (24) can be rewritten as

$$g(\nu)=\frac{k}{rh^2\nu^2}\frac{a_2}{[-\zeta(-1)]}\left[\delta(\nu)+\frac{\nu_E^2}{2}\delta^{(2)}(\nu)+\cdots\right]$$
$$=\frac{k}{rh^2\nu^2}\frac{a_2}{[-\zeta(-1)]}\delta(\nu-\nu_E)$$
$$=\frac{12ka_2}{rh^2\nu_E^2}\delta(\nu-\nu_E). \quad (28)$$

Thus the Einstein frequency can be given directly as

$$\nu_E=\frac{k}{h}\left(\frac{2a_4[-\zeta(-1)]}{a_2\zeta(-3)}\right)^{1/2}=\frac{k}{h}\left(\frac{20a_4}{a_2}\right)^{1/2}. \quad (29)$$

This indicates that the Einstein frequency is only dependent on the second and third expansion coefficients in Eq. (22). In the solution (29), we have considered that [13] and $a_{2m}>0$, and

$$\zeta(1-2m)=-B_{2m}/2m.$$

From $B_2=1/6$, $B_4=-1/30$, $B_6=1/42$, $B_8=-1/30$, $B_{10}=5/66,\ldots$ we have

$$\zeta(-1)=-1/12,\quad \zeta(-3)=1/120,\quad \zeta(-5)=-1/252,$$
$$\zeta(-7)=1/240,\quad \zeta(-9)=-1/132,\ldots\ . \quad (30)$$

In fact, Einstein's solution $\delta(\nu-\nu_E)$ corresponds to the heat capacity spectrum [7]

$$\frac{x^2e^x}{(e^x-1)^2}=1-\frac{x^2}{12}+\frac{x^4}{240}-\frac{x^6}{6084}+\cdots \quad (x=T_E/T). \quad (31)$$

Substituting this expression into Eq. (29), we obtain

$$\nu_E=\frac{k}{h}\left(\frac{20T_E^4/240}{T_E^2/12}\right)^{1/2}=\frac{kT_E}{h}. \quad (32)$$

This shows the success of the general formula (22) for the high-frequency limit.

B. Two peak approximation

If there are two δ peaks at ν_+ and ν_- in phonon spectra, then it is given that

$$\frac{\nu_+^2+\nu_-^2}{2!}=2\frac{a_4\zeta(-1)}{-a_2\zeta(-3)}\left(\frac{k}{h}\right)^2=\mathbf{A} \quad (33)$$

and

$$\frac{\nu_+^4+\nu_-^4}{4!}=\frac{2a_6\zeta(-1)}{a_2\zeta(-5)}\left(\frac{k}{h}\right)^4=\mathbf{B}. \quad (34)$$

Hence, we have

$$\nu_+^2+\nu_-^2=2A \quad (35)$$

or

$$\nu_+^4+\nu_-^4+2\nu_+^2\nu_-^2=4A^2. \quad (36)$$

Thus

$$2\nu_+^2\nu_-^2=4A^2-24B \quad (37)$$

or

$$(\nu_+^2-\nu_-^2)^2=48B-4A^2. \quad (38)$$

Therefore

$$\nu_+^2-\nu_-^2=\pm 2\sqrt{12B-A^2}. \quad (39)$$

Finally, we have

$$\nu_\pm=(A\pm\sqrt{12B-A^2})^{1/2}. \quad (40)$$

Based on Eq. (40) with the experimental fitting parameters in the general formula (22), the peak width for high frequency in the phonon frequency spectrum can be estimated by calculating $\nu_+-\nu_-$, and hence the main characterization of optical branches can be obtained. A more complicated situation can be discussed in a similar way.

VI. CONCLUSION AND DISCUSSION

The apparently obscure Möbius inversion formula has been applied successfully to the inverse specific heat problems, which have played a very important role in the development of physics, and which have been studied by Einstein, Debye, Montroll, Landau, Lifshitz, Chambers, and so on. Now this quite interesting and difficult problem is solved unexpectedly by the Möbius technique in this concise manner. This cannot be considered as an isolated and occasional situation [14]. The wide use of the number theory technique reflects the arrival of the digital information age, and the quantum age. In addition, a power series representation for the Riemann ζ function has been extended to negative integer points in a Poisson-Abel process, which is very useful for physical applications. This might become a typical technique to deal with some inherently ill-posed inverse problems instead of some numerical methods such as the maximum entropy method and the regularization method.

ACKNOWLEDGMENTS

The authors would like to thank Wang Yuan and Wei Yu-chuan for their helpful discussion. This work is supported partly by the Chinese National Science Foundation, and partly by the National Advanced Materials Committee of China.

APPENDIX A: A CONCISE DEDUCTION OF THE MÖBIUS TRANSFORM

From

$$\begin{aligned} F(x) &= f(x)+f(2x)+f(3x)+\cdots+f(nx)+\cdots \\ &= T_1 f(x)+T_2 f(x)+\cdots+T_n f(x)+\cdots \\ &= (T_1+T_2+\cdots+T_n+\cdots)f(x), \end{aligned} \tag{A1}$$

we have

$$\begin{aligned} f(x) &= \frac{1}{T_1+T_2+\cdots+T_n+\cdots} F(x) \\ &= \frac{1}{\Pi_p(T_1+T_p+T_{p^2}+T_{p^3}+\cdots)} F(x). \end{aligned} \tag{A2}$$

Thus it is given that

$$f(x)=\frac{1}{\Pi_p[1/(T_1-T_p)]} F(x)=\left[\prod_p (T_1-T_p)\right]F(x). \tag{A3}$$

Therefore we have

$$\begin{aligned} f(x) &= \left[T_1+\sum_{\{p_1p_2p_3,\ldots,p_r\}} (-1)^r T_{p_1}T_{p_2}T_{p_3}\cdots T_{p_r}\right]F(x) \\ &= F(x)+\sum_{\{p_1p_2p_3,\ldots,p_r\}} (-1)^r F(p_1p_2p_3\cdots p_r x). \end{aligned} \tag{A4}$$

Let us denote the last expression as

$$f(x)=\sum_{n=1}^{\infty} I(n)T_nF(x)=\sum_{n=1}^{\infty} I(n)F(nx), \tag{A5}$$

where

$$\mu(n)\equiv I(n)=\begin{cases} 1, & n=1 \\ (-1)^r, & n=p_1p_2,\ldots,p_r \\ 0 & \text{otherwise.} \end{cases} \tag{A6}$$

In this deduction, we did not make any assumption about the Möbius function; instead, we used the definition of the Möbius function found in standard textbooks.

APPENDIX B: SOME SPECIAL RELATIONS BETWEEN $\zeta(s)$ AND $\mu(n)$

For the reader's convenience, some mathematical notes are attached in this section. First, we define two convergent series as [15]

$$f(x,s)=\sum_{n=1}^{\infty} \mu(n)n^s x^n, \quad s>1 \text{ and } x\in(0,1), \tag{B1}$$

and

$$q(x,s)=\sum_{n=1}^{\infty} n^s x^n, \quad s>1 \text{ and } x\in(0,1). \tag{B2}$$

The evaluation of the generalized function

$$\sum_{n=1}^{\infty} n^s \quad (s>1)$$

and

$$\sum_{n=1}^{\infty} \mu(n)n^s \quad (s>1)$$

can be defined as the Poisson-Abel principal value or Poisson-Abel generalized sum as

$$\sum_{n=1}^{\infty} n^s=\lim_{x\to 1} q(x,s) \tag{B3}$$

and

$$\sum_{n=1}^{\infty} \mu(n)n^s=\lim_{x\to 1} f(x,s). \tag{B4}$$

From now on, all the divergent series will be considered as Poisson-Abel generalized sums without explanation.

1. Relation between $\zeta(s)$ and $\mu(n)$ [3]

The Riemann ζ function is defined as

$$\zeta(s)=\sum_{n=1}^{\infty} \frac{1}{n^s}, \quad s>1. \tag{B5}$$

The relation of $\zeta(s)$ and $\mu(n)$ has been proved to be

$$\frac{1}{\zeta(s)}=\sum_{n=1}^{\infty}\frac{\mu(n)}{n^s},\quad s>1. \tag{B6}$$

2. A special relation between two divergent sums

In Eqs. (B5) and (B6), both series

$$\sum_{n=1}^{\infty}\frac{1}{n^s}\quad\text{and}\quad\sum_{n=1}^{\infty}\frac{\mu(n)}{n^s}$$

are convergent if $s>1$, and both are divergent if $s\leqslant 1$. But there is an important and unreasonable effective relation between the two divergent sums. That is,

$$\left[\sum_{n=1}^{\infty}n^s\right]^{-1}=\sum_{n=1}^{\infty}\mu(n)n^s,\quad s>0. \tag{B7}$$

This pseudotheorem can be proved the same way as before provided that the Poisson-Abel process is used. In fact, for $s>0$ we have

$$\begin{aligned}&\lim_{0<x\to 1^-}\left[\sum_{n=1}^{\infty}\mu(n)n^s x^n\right]\left[\sum_{m=1}^{\infty}m^s x^m\right]\\&=\lim_{0<x\to 1^-}\left[\sum_{m,n=1}^{\infty}\mu(n)(mn)^s x^{n+m}\right]\\&=\sum_{k=1}^{\infty}\left[\lim_{0<x\to 1^-}\sum_{n|k}\mu(n)x^{n+k/n}\right]k^s=1.\end{aligned} \tag{B8}$$

3. Other two pseudotheorems on $\zeta(s)$

The first theorem states that

$$\sum_{\mathbf{n=1}}^{\infty}\mathbf{n^s}=\begin{cases}0, & s=2k\\ \zeta(1-2k), & s=2k-1>0\end{cases} \tag{B9}$$

and the second one states that

$$\sum_{n=1}^{\infty}\mu(n)n^{2k-1}=\frac{1}{\zeta(1-2k)},\quad k=1,2,3,\ldots. \tag{B10}$$

Proof. Taking the integral representation of $\Gamma(s)$ for arbitrary s as

$$\frac{1}{\Gamma(z)}=\frac{-1}{2\pi i}\int_{\infty}^{(0+)}e^{-t}(-t)^{-z}dt \tag{B11}$$

in which the integral path is from infinity on the real axis, surrounding the origin counterclockwise once, and back to infinity on the real axis as in Fig. 3. Now let us consider the case of $z=m+1$, where m is a positive integer. Introducing the variable

$$t=(n+1)x, \tag{B12}$$

we obtain that

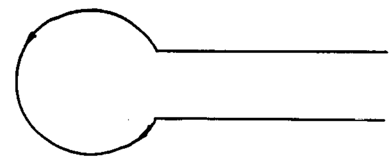

FIG. 3. Integral loop.

$$\begin{aligned}1&=\frac{-\Gamma(z)}{2\pi i}\int_{\infty}^{(0+)}e^{-t}(-t)^{-z}dt\\&=\frac{-\Gamma(m+1)}{2\pi i}\int_{\infty}^{(0+)}e^{-(n+1)x}[x(n+1)]^{-(m+1)}(n+1)dx\\&=\frac{-m!}{2\pi i}\int_{\infty}^{(0+)}e^{-(n+1)x}(n+1)^{-m}x^{-(m+1)}dx\end{aligned} \tag{B13}$$

$$\to(n+1)^m=\frac{-m!}{2\pi i}\int_{\infty}^{(0+)}e^{-(n+1)x}x^{-(m+1)}dx. \tag{B14}$$

Taking the summation, we get that

$$\begin{aligned}&\lim_{0<y\to 1^-}\sum_{n=0}^{\infty}(n+1)^m y^{n+1}\\&=\frac{-m!}{2\pi i}\int_{\infty}^{(0+)}x^{-(m+1)}\sum_{n=0}^{\infty}e^{-(n+1)x}dx\\&=\frac{-m!}{2\pi i}\int_{\infty}^{(0+)}x^{-(m+1)}e^{-x}\sum_{n=0}^{\infty}e^{-nx}dx\\&=\frac{-m!}{2\pi i}\int_{\infty}^{(0+)}x^{-(m+1)}\frac{e^{-x}}{1-e^{-x}}dx.\end{aligned} \tag{B15}$$

The integration in the right-hand side has a pole of rank $(m+2)$ at $x=0$. Thus

$$\begin{aligned}&\frac{1}{2\pi i}\int_{\infty}^{(0+)}x^{-(m+1)}\frac{e^{-x}}{1-e^{-x}}dx\\&=\mathrm{Res}_{x=0}\left[x^{-(m+1)}\frac{e^{-x}}{1-e^{-x}}\right]\\&=\frac{1}{(m+1)!}\frac{\partial^{(m+1)}}{\partial x^{(m+1)}}\left[\frac{xe^{-x}}{e^x-1}\right]x=0.\end{aligned} \tag{B16}$$

Based on the generating function of Bernoulli numbers B_n,

$$\frac{t}{e^t-1}=\sum_{n=0}^{\infty}\frac{t^n}{n!}B_n, \tag{B17}$$

we have

$$\lim_{0<x\to 1^-}\sum_{n=0}^{\infty}(n+1)^m x^{n+1}=-m!\frac{B_{m+1}}{(m+1)!}=\frac{-B_{m+1}}{m+1}. \tag{B18}$$

Therefore for any natural number m

$$\lim_{0<x\to 1^-}\sum_{n=1}^{\infty} n^m x^n = \begin{cases} 0, & m=2k>0 \\ \zeta(1\text{-}2k), & m=2k\text{-}1>0. \end{cases} \tag{B19}$$

Notice that $B_{2k-1}=0$. Thus the first theorem is proved.

Combining Eq. (B7) with Eq. (B9), we get that

$$\lim_{0<x\to 1^-}\sum_{n=1}^{\infty} \mu(n) n^{2k-1} x^n = \frac{1}{\zeta(1-2k)}, \quad k=1,2,3,\cdots . \tag{B20}$$

That is the reason for the interesting equation (27).

[1] R. Resnick and D. Halliday, *Basic Concepts in Relativity and Early Quantum Theory*, 2nd ed. (Wiley, New York, 1985).

[2] A. Einstein, Ann. Phys. (Leipzig) **22**, 180 (1907).

[3] P. Debye, Ann. Phys. (Leipzig) **39**, 789 (1912).

[4] E. W. Montroll, J. Chem. Phys. **10**, 218 (1942).

[5] I. M. Lifshitz, Zh. Eskp. Teor. Fiz **26**, 551 (1954).

[6] R. G. Chambers, Prog. Phys. Soc. **78**, 941 (1961).

[7] X. X. Dai, X. W. Xu, and J. Q. Dai, Phys. Lett. A **147**, 445 (1990).

[8] G. Weiss, Prog. Theor. Phys. **22**, 520 (1959).

[9] B. D. Hughes, N. E. Frankel, and B. W. Ninham, Phys. Rev. A **42**, 3643 (1990).

[10] M. R. Schroeder, *Number Theory in Science and Communication*, 2nd English ed., corrected printing (Springer, Berlin, 1990).

[11] G. H. Hardy and E. M. Wright, *An Introduction to the Theory of Numbers* (Oxford, 1968).

[12] N. X. Chen, Phys. Rev. Lett. **64**, 1193 (1990); N. X. Chen, Y. Chen, and G. Y. Li, Phys. Lett. A **149**, 357 (1990).

[13] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1980).

[14] *Proceedings of Symposia in Applied Mathematica*, edited by A. Burr (American Mathematical Society, Providence, Rhode Island, 1991), Vol. 46.

[15] L. K. Hua, *Starting with the Unit Circle* (Springer-Verlag, New York, 1981), Chap. 8.