Modified Möbius Inverse Formula and Its Applications in Physics

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A new theorem of inverse formula is introduced for a kind of infinite series. Thus some new results for important inverse problems in physics are presented in this paper. These are the inverse problems for obtaining the photon density of states, the inverse blackbody radiation problem for remote sensing, and the solution for inverse Ewald summation. Of more importance, it shows the possibility of the application of number theory to physical problems.

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(1) A new inverse formula.— According to the Möbius inverse formula,[1] if $f(n)$ is any number-theoretic function and

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

then

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

where the sum runs over all the factors of n including 1 and n, and $\mu(n)$ is the Möbius function in number theory:

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

For example, $\mu(1)=1$, $\mu(2)=-1$, $\mu(3)=-1$, $\mu(4)=0$, $\mu(5)=-1$, $\mu(6)=1$, $\mu(7)=-1$, $\mu(8)=0$, $\mu(9)=0$, $\mu(10)=1$, $\mu(11)=-1$, $\mu(12)=0$, $\mu(13)=-1$, $\mu(14)=1$, $\mu(15)=1$, etc.

Now, we try to replace the number-theoretic functions $F(n)$ and $f(n)$ by the common functions $A(\omega)$ and $B(\omega)$, respectively, with the continuous variable ω. In this case, ω is divided into n intervals, and n tends to infinity. Notice that

$$\sum_{d|n} f(d)=\sum_{(n/d)|n} f(n/d) \tag{4}$$

and

$$f(n/d)\to B(\omega/d) \text{ and } F(n/d)\to A(\omega/d). \tag{5}$$

Also, when we are talking about $n\to\infty$, n is an infinite set of numbers instead of a single number. Therefore the summation over $d\,|\,n$ in Eqs. (1) and (2) would be changed into summation from 1 to infinity since all the integers can be considered as factors of the infinite set of n. From the above, a new theorem instead of Eqs. (1) and (2) is given by the following.

If

$$A(\omega)=\sum_{n=1}^{\infty} B(\omega/n) \tag{6}$$

then

$$B(\omega)=\sum_{n=1}^{\infty} \mu(n)A(\omega/n). \tag{7}$$

This theorem is very useful for different kinds of physical problems. The rigorous proof of the theorem is shown in the Appendix.

(2) A new formula for phonon density of states.— The specific heat of lattice vibration is expressed as[2]

$$C_v(T)=rk\int_0^\infty \frac{(h\nu/kT)^2 e^{h\nu/kT}}{(e^{h\nu/kT}-1)^2} g(\nu)d\nu, \tag{8}$$

where h is the Planck constant and k is the Boltzmann constant, and the phonon density of states is normalized to $3N$:

$$\int_0^\infty g(\nu)d\nu=3N. \tag{9}$$

Equation (8) holds for a crystalline lattice with r atoms per unit cell. The problem is how to solve the integral equation for significantly different $g(\nu)$ based on very similar curves of specific heat $C_v(T)$. It has received attention for a long time, and has not been solved up to date.[3-6]

Introducing a new parameter "coldness" as $u=h/kT$, it follows that

$$C_v\left(\frac{h}{ku}\right)=rk\int_0^\infty \frac{(u\nu)^2 e^{u\nu}}{(e^{u\nu}-1)^2} g(\nu)d\nu. \tag{10}$$

By using Taylor's expansion, one can find that

$$C_v(h/ku)=rk\sum_{n=1}^{\infty}\int_0^\infty n(u\nu)^2 e^{-nu\nu} g(\nu)d\nu. \tag{11}$$

Let $\omega=n\nu$, then

$$\begin{aligned}C_v(h/ku)&=rk\sum_{n=1}^{\infty}\int_0^\infty (u\omega/n)^2 e^{-u\omega} g(\omega/n)d\omega\\ &=rku^2\int_0^\infty e^{-u\omega}\sum_{n=1}^{\infty}(\omega/n)^2 g(\omega/n)d\omega\\ &=rku^2 L[G(\omega)],\end{aligned} \tag{12}$$

where

$$G(\omega)=\sum_{n=1}^{\infty}(\omega/n)^2 g(\omega/n) \qquad (13)$$

and $L[\,]$ is the Laplace operator. Based on the new theorem presented in Sec. 1, by replacing $A(\omega)$ and $B(\omega)$ by $G(\omega)$ and $\omega^2 g(\omega)$, respectively, one can obtain

$$g(\omega)=(1/\omega^2)\sum_{n=1}^{\infty}\mu(n)G(\omega/n)\,. \qquad (14)$$

From Eq. (12), it is given that

$$g(v)=\left[\frac{1}{rkv^2}\right]\sum_{n=1}^{\infty}\mu(n)L_n^{-1}\left[\frac{C_v(h/ku)}{u^2}\right], \qquad (15)$$

where the inverse Laplace L_n^{-1} inverts the u space to v/n space. Equation (15) describes a new method based on which one can obtain $g(v)$ from experimental data of $C_v(T)$. It is an exact closed form solution for this important inverse problem. The formula is simple to apply and can be used if specific-heat measurements of reasonable accuracy are available.

Particularly, in the low-temperature region, experiments show that

$$\begin{aligned}C_v(T)&=a_3T^3+a_5T^5+a_7T^7+\cdots\\&=\sum_{n=2}^{\infty}a_{2n-1}(h/k)^{2n-1}u^{-(2n-1)}\,.\end{aligned} \qquad (16)$$

Hence

$$\begin{aligned}G(v)&=(1/rk)\sum_{n=2}^{\infty}(h/k)^{2n-1}a_{2n-1}L^{-1}[u^{-(2n-1)}]\\&=(1/rk)\sum_{n=2}^{\infty}(h/k)^{2n-1}a_{2n-1}v^{2n}/(2n)!\,.\end{aligned} \qquad (17)$$

Therefore,

$$\begin{aligned}g(v)&=(1/v^2)\sum_{n=1}^{\infty}\mu(n)G(v/n)\\&=\frac{1}{rkv^2}\sum_{i=2}^{\infty}\left[\frac{h}{k}\right]^{2i-1}\frac{a_{2i-1}}{(2i)!}\sum_{n=1}^{\infty}\mu(n)\left[\frac{v}{n}\right]^{2i}\\&=\frac{1}{rkv}\sum_{i=2}^{\infty}\left[\frac{hv}{k}\right]^{2i-1}\frac{a_{2i-1}}{(2i)!\zeta(2i)}\,,\end{aligned} \qquad (18)$$

where ζ is the Riemann function which can be expressed through the Bernoulli numbers. Only this result for the low-temperature limit was given by Weiss before,[4] and the method here is more concise and general. Taking only the first term in Eq. (18), the expected Debye's approximation,

$$g(v)\propto v^2\,, \qquad (19)$$

is obtained.

(3) An exact solution for inverse blackbody radiation.—The inverse blackbody radiation problem has been given much attention in recent literature.[7-12] The problem is to determine the area distribution $a(T)$ of a blackbody from the measured total radiation power spectrum $W(v)$ of the blackbody, where v is the frequency. The relation between $W(v)$ and $a(T)$ is given by Planck's law as

$$W(v)=\frac{2hv^3}{c^2}\int_0^{\infty}\frac{a(T)dT}{e^{hv/kT}-1}\,, \qquad (20)$$

where h and k are the same as in Eq. (8), and c is the velocity of light.

The inverse blackbody radiation problem thus consists of solving the integral equation (20) for the area temperature distribution $a(T)$. It is important in the field of remote sensing. Bojarski[7] introduced two variables "absolute coldness" u and "area-coldness distribution" $a(u)$ so that

$$u=h/kT \quad\text{and}\quad a(u)du=-a(T)dT\,, \qquad (21)$$

then Eq. (20) can be rewritten as

$$W(v)=\frac{2hv^3}{c^2}\int_0^{\infty}\frac{a(u)}{e^{uv}-1}du\,, \qquad (22)$$

where $uv>0$. By using a series expansion of the denominator of the integrand the integral equation (22) can be rewritten as

$$W(v)=\frac{2hv^3}{c^2}\int_0^{\infty}e^{-uv}\sum_{n=1}^{\infty}\left[\frac{1}{n}\right]a\left[\frac{u}{n}\right]du\,. \qquad (23)$$

Let

$$f(u)=\sum_{n=0}^{\infty}(1/n)a(u/n) \qquad (24)$$

and

$$g(v)=\frac{c^2}{2hv^3}W(v)\,. \qquad (25)$$

From Eqs. (23)-(25), $f(u)$ is simply the inverse Laplace transformation of $g(v)$, i.e.,

$$f(u)=L^{-1}[g(v)]\,. \qquad (26)$$

From Eq. (24), we have

$$uf(u)=\sum_{n=1}^{\infty}(u/n)a(u/n)\,. \qquad (27)$$

Now, by using the modified Möbius formula [Eq. (7)], replacing $A(\omega)$ and $B(\omega)$ by $uf(u)$ and $ua(u)$, one can obtain

$$ua(u)=\sum_{n=1}^{\infty}\mu(n)(u/n)f(u/n)\,, \qquad (28)$$

$$a(u)=\sum_{n=1}^{\infty}[\mu(n)/n]f(u/n)\,, \qquad (29)$$

or

$$a(u)=f(u)-\tfrac{1}{2}f(\tfrac{1}{2})-\tfrac{1}{5}f(\tfrac{1}{5})+\tfrac{1}{6}f(\tfrac{1}{6})-\tfrac{1}{7}f(\tfrac{1}{7})+\tfrac{1}{10}f(\tfrac{1}{10})-\tfrac{1}{11}f(\tfrac{1}{11})-\tfrac{1}{13}f(\tfrac{1}{13})+\tfrac{1}{14}f(\tfrac{1}{14})+\tfrac{1}{15}f(\tfrac{1}{15})+\cdots. \quad (30)$$

This is an exact closed form for solving the inverse blackbody radiation problem. Equation (30) was first presented by Kim and Jaggard without using the simple expression [Eq. (29)].[9] If only the first term is taken into account, it corresponds to the Wien approximation.[7,8]

(4) Conclusion and discussion.— A quite useful result in physics from the modified inverse Möbius formula indicates the potential application of number theory to physical problems not only for the integer eigenvalue spectrum in quantum mechanics, but also for the different kinds of inverse problems in other branches in physics. For example, one may consider the Ewald summation

$$V(x)=v(x)+v(2x)+v(3x)+\cdots \quad (31)$$

in a one-dimensional lattice, and the inverse problem is to find $v(x)$ from experimentally known $V(x)$. By using the method in the Appendix, we may find

$$v(x)=V(x)-V(2x)-V(3x)-V(5x)+V(6x)-V(7x)+V(10x)+\cdots, \quad (32)$$

which is first presented in this paper, and would be useful for the atomic-potential design. All of these inverse problems mentioned have fundamental significance in physics.

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Appendix.— To obtain convergence for the series, we add a very common condition,

$$|B(x)| \le cx^{1+\epsilon} \quad (x>0), \quad (A1)$$

where c and ϵ are two positive constants. Let us look at the right-hand side of Eq. (7);

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\mu(n)B(\omega/mn). \quad (A2)$$

Obviously,

$$|\mu(n)B(\omega/mn)| \le c(\omega/mn)^{1+\epsilon}. \quad (A3)$$

Hence, this series is absolutely convergent since

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}c(\omega/mn)^{1+\epsilon} \quad (A4)$$

converges. From the twofold-series theory, the terms in Eq. (A2) can be combined arbitrarily. Therefore,

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\mu(n)B(\omega/mn)=\sum_{n=1}^{\infty}\mu(n)\sum_{m=1}^{\infty}B(\omega/mn)=\sum_{k=1}^{\infty}\left[\sum_{mn=k}^{\infty}\mu(n)\right]B(\omega/mn). \quad (A5)$$

Finally, we have

$$\sum_{n=1}^{\infty}\mu(n)\left[\sum_{m=1}^{\infty}B(\omega/mn)\right]=B(\omega), \quad (A6)$$

since

$$\sum_{mn=k}\mu(n)=\sum_{n|k}\mu(n)=\delta_{k1}. \quad (A7)$$

For most problems in physics, condition (A1) is well satisfied. If we set $|A(x)| \le cx^{1+\epsilon}$, the inverse theorem can be proven in a similar way.

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