PHYSICAL REVIEW E

STATISTICAL PHYSICS, PLASMAS, FLUIDS, AND RELATED INTERDISCIPLINARY TOPICS

THIRD SERIES, VOLUME 62, NUMBER 3 PART A SEPTEMBER 2000

RAPID COMMUNICATIONS

The Rapid Communications section is intended for the accelerated publication of important new results. Since manuscripts submitted to this section are given priority treatment both in the editorial office and in production, authors should explain in their submittal letter why the work justifies this special handling. A Rapid Communication should be no longer than 4 printed pages and must be accompanied by an abstract. Page proofs are sent to authors.

Exact solution of the specific-heat–phonon spectrum inversion from the Möbius inverse formula

DengMing Ming,[1] Tao Wen,[1] JiXin Dai,[1,2] Xianxi Dai, [1,3] and William E. Evenson[3]

[1]*Group of Quantum Statistics and Methods of Theoretical Physics, Department of Physics, Fudan University, Shanghai 200433, People's Republic of China*

[2]*Department of Chemistry, New York University, New York, New York 10003*

[3]*Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602*

(Received 3 April 2000)

The application of the Möbius inversion formula to the specific-heat–phonon spectrum inversion problem (SPI) initially appeared promising [N .X. Chen, Phys. Rev. Lett. **64**, 1193 (1990); J. Maddox, Nature (London) **344**, 377 (1990)]. However, no one has previously been able to obtain the exact Debye spectrum with the correct cut-off factor and frequency dependence from the Möbius formula. The main difficulty arises from the fact that the Möbius function $\mu(n)$ is not completely known for large n in practice. In this paper, some exact solutions of SPI are obtained by using the Möbius inversion formula, most importantly the Debye spectrum as a special case, and the problem of the unknown Möbius function $\mu(n)$ for large n is avoided. It is shown that the Möbius inversion formula can be useful for exact solutions to spectral inversion problems.

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

I. INTRODUCTION

The lattice specific heat $C_V(T)$ can be expressed by

$$C_V(T)=k_B\int_0^\infty\left(\frac{h\nu}{k_BT}\right)^2\frac{e^{h\nu/k_BT}}{(e^{h\nu/k_BT}-1)^2}g(\nu)d\nu, \qquad (1.1)$$

where h and k_B represent the Planck and Boltzmann constants, respectively, and $g(\nu)$, the phonon density of states, is normalized to $3Nr$:

$$\int_0^\infty g(\nu)d\nu=3Nr, \qquad (1.2)$$

where r is the number of degrees of freedom per molecule. The inverse problem is to determine $g(\nu)$ from the measured lattice specific heat $C_V(T)$. This problem has received intensive theoretical study due to the importance of the phonon density of states for the thermodynamic properties of solids, lattice dynamics, electron-phonon interactions, the microscopic mechanism of superconductivity, etc.

In 1989, Dai, Xu, and Dai introduced techniques for eliminating divergences and used the Fourier transform to obtain an exact solution formula with a parameter s [1,2]. Existence and uniqueness theorems were also proved. The formulas of Montroll [3] and Lifshitz [4] are special cases for $s=1$. Another special case is given by Carlsson, Gelatt, and Ehrenreich [5].

A class of exact solutions for concrete systems in SPI (including the Einstein and Debye spectra) and in the related black-body radiation inverse problem were obtained by Dai's exact solution formula [1,2,6,7]. Recently, the exact solution formula [2] was also applied to carry out specific heat inversion for a real system such as YBCO [8]. The parameter s for eliminating divergence is shown to be very important for asymptotic behavior control. Most of the above work focused on an exact solution in closed form: an integral representation of the exact solution.

In 1990, Chen [9] introduced a modified Möbius inversion formula which stated that if $B(\omega)$ satisfies a common condition,

$$|B(\omega)|<c\omega^{1+\varepsilon} \quad (\omega>0), \qquad (1.3)$$

where c and ε are two positive constants, and

$$A(\omega)=\sum_{n=1}^{\infty} B(\omega/n), \tag{1.4}$$

then

$$B(\omega)=\sum_{n=1}^{\infty} \mu(n)A(\omega/n). \tag{1.5}$$

The Möbius function $\mu(n)$ is equal to zero when n includes repeated factors, or equal to $(-1)^r$ when n is a product of r distinct primes. Specifically, $\mu(1)=1$. By using this inversion formula and denoting $u=h/k_BT$, he obtained a formal solution of the integral equation (1.1),

$$g(\nu)=\frac{1}{k_B\nu^2}\sum_{n=1}^{\infty} \mu(n)\mathcal{L}^{-1}\left\{\frac{C_V(h/k_Bu)}{u^2},\ u\to\frac{\nu}{n}\right\}, \tag{1.6}$$

where $\mathcal{L}^{-1}$ stands for inverse Laplace transform. Chen's method received much attention [10–12], since he introduced methods from number theory, including the Möbius inversion formula [13], to study inverse problems in physics.

It is important to notice that Chen's formal solution formula (1.6) involves an infinite number of inverse Laplace transforms. This makes it rather difficult to apply in practice. (See, for example, the work of Bertero *et al.* [14], who have carefully studied the instability problems of inverse Laplace transforms.) Furthermore, to determine the values of the Möbius function $\mu(n)$ for large n is an extremely difficult and unsolved problem, seriously complicating any attempt to discuss the convergence of the solution and existence and uniqueness theorems.

In Ref. [15], the Einstein spectrum was obtained using the Möbius inversion formula. Chen and Rong also used a ''standard'' low-temperature expansion of the specific heat to find the phonon spectrum by Chen's formula. They obtained a spectrum of the form $g(\nu)\sim\nu^2$ but with no cut-off factor and Debye frequency, which implied that one still cannot obtain the complete Debye spectrum with a correct cut-off factor and Debye frequency from the Möbius inversion formula in SPI. A question then arises as to whether the Möbius formula can be used in practice to produce exact solutions for nontrivial physical models other than the Einstein spectrum. In fact, to our knowledge no one has previously obtained exact solutions for any concrete physical models in SPI by using the Möbius inversion formula.

This Rapid Communication uses the Möbius inversion formula to derive the exact solution for SPI for a general model, in which the Debye spectrum is included as a special case. A correct phonon density of states will be derived from the complete expression of the specific heat.

II. EXACT SOLUTION FOR SPI FROM MÖBIUS INVERSION FORMULA

Considering the historic importance of Debye's work [16], we start from the following specific heat $C_V(T)$, which includes the Debye specific heat as a special case:

$$C_V(T)=3Nrk_B\left((n+1)D_n(x_0)-\frac{nx_0}{e^{x_0}-1}\right),\quad x_0=\frac{h\nu_0}{k_BT},$$
$$n=1,2,3\ \ldots, \tag{2.1}$$

where ν_0 is the cut-off frequency of lattice vibrations, N is the number of molecules, r is the number of degrees of freedom per molecule, and $D_n(x)$ is the integral

$$D_n(x)=\frac{n}{x^n}\int_0^x\frac{z^n}{e^z-1}dz. \tag{2.2}$$

Formula (2.1) is the well-known Debye specific heat interpolation formula of dimension n [16].

We evaluate $D_n(x)$ in a series of exponential functions as follows:

$$\begin{aligned}D_n(x)&=\frac{n}{x^n}\sum_{k=1}^{\infty}\int_0^x z^ne^{-kz}dz\\&=nn!\left(\frac{\zeta(n+1)}{x^n}-\sum_{k=1}^{\infty}\frac{1}{k^{n+1}}\sum_{l=0}^{n}\frac{k^l}{l!}\frac{e^{-kx}}{x^{n-l}}\right),\end{aligned} \tag{2.3}$$

where $\zeta(z)$ is the Riemann zeta-function,

$$\zeta(z)=\sum_{n=1}^{\infty}\frac{1}{n^z}\ \Re z>1. \tag{2.4}$$

The reciprocal of $\zeta(z)$ is [17]

$$\frac{1}{\zeta(z)}=\sum_{n=1}^{\infty}\frac{\mu(n)}{n^z}\ \Re z>1\quad, \tag{2.5}$$

where $\mu(n)$ is the Möbius function.

Denoting $u=h/k_BT=\ x_0/\nu_0$, one has

$$\begin{aligned}\frac{C_V(h/k_Bu)}{u^2}&=\frac{3Nrk_B}{u^2}\left\{n(n+1)!\left(\frac{\zeta(n+1)}{u^n\nu_0^n}\right.\right.\\&\quad\left.\left.-\sum_{k=1}^{\infty}\frac{1}{k^{n+1}}\sum_{l=0}^{n}\frac{k^l}{l!}\frac{e^{-kx_0}}{u^n\nu_0^{n-l}}\right)-nx_0\sum_{k=1}^{\infty}e^{-kx_0}\right\}\\&=\frac{3Nrk_B}{\nu_0^n}n(n+1)!\left(\frac{\zeta(n+1)}{u^{n+2}}\right.\\&\quad\left.-\sum_{k=1}^{\infty}\frac{1}{k^{n+1}}\sum_{l=0}^{n+1}\frac{(k\nu_0)^l}{l!}\frac{e^{-k\nu_0u}}{u^{n+2-l}}\right).\end{aligned} \tag{2.6}$$

Noting that [18]

$$\mathcal{L}^{-1}\left\{\frac{e^{-\alpha p}}{p^n},\ p\to x\right\}=\frac{(x-\alpha)^{n-1}\theta(x-\alpha)}{(n-1)!}, \tag{2.7}$$

where $\theta(x)$ is the Heaviside step function which is defined as

$$\theta(x)=\begin{cases}0 & x<0\\ 1 & x>0.\end{cases} \tag{2.8}$$

Thus,

$$\mathcal{L}^{-1}\left\{\frac{C_V(1/u)}{u^2},\ u\to\nu\right\}$$

$$=3Nrk_B\nu_0^2 n\left\{(n+1)!\zeta(n+1)\frac{\nu^{n+1}}{\Gamma(n+2)\nu_0^{n+2}}\right.$$

$$\left.-\sum_{k=1}^{\infty}\frac{(n+1)!}{k^{n+1}}\sum_{l=0}^{n+1}\frac{k^l}{l!}\frac{(\nu-k\nu_0)^{n+1-l}\theta(\nu-k\nu_0)}{\Gamma(n+2-l)\nu_0^{n+2-l}}\right\}$$

$$=\frac{3Nrk_Bn}{\nu_0^n}\left\{\zeta(n+1)\nu^{n+1}-\sum_{k=1}^{\infty}\frac{\theta(\nu-k\nu_0)}{k^{n+1}}\right. \tag{2.9}$$

$$\left.\times\sum_{l=0}^{n+1}\frac{(n+1)!(\nu-k\nu_0)^{n+1-l}(k\nu_0)^l}{l!(n+1-l)!}\right\}$$

$$=\frac{3Nrk_Bn}{\nu_0^n}\left(\zeta(n+1)\nu^{n+1}-\sum_{k=1}^{\infty}\frac{\theta(\nu-k\nu_0)\nu^{n+1}}{k^{n+1}}\right)$$

$$=\frac{3Nrk_Bn}{\nu_0^n}\{\zeta(n+1)\nu^{n+1}-H(\nu)\}, \tag{2.10}$$

where $H(\nu)$ is defined as

$$H(\nu)=\sum_{k=1}^{\infty}\left(\frac{\nu}{k}\right)^{n+1}\theta\left(\frac{\nu}{k}-\nu_0\right), \tag{2.11}$$

and where the relation $\theta(\nu-k\nu_0)=\theta(\nu/k-\nu_0)$ has been used. It is obvious that the above series (2.11) is absolutely convergent. According to the Möbius inversion formula (1.5), replacing $B(\omega)$ by $\nu^{n+1}\theta(\nu-\nu_0)$ [which obviously satisfies the condition (1.3)], and replacing $A(\nu)$ by $H(\nu)$, one finds that

$$\sum_{k=1}^{\infty}\mu(k)H(\nu/k)=\nu^{n+1}\theta(\nu-\nu_0). \tag{2.12}$$

Inserting Eq. (2.10) into Chen's solution formula (1.6) and using Eq. (2.12), one obtains

$$g(\nu)=\frac{1}{rk_B\nu^2}\frac{3Nrk_Bn}{\nu_0^n}\sum_{k=1}^{\infty}\mu(k)\left\{\zeta(n+1)\left(\frac{\nu}{k}\right)^{n+1}-H\left(\frac{\nu}{k}\right)\right\}$$

$$=\frac{3Nn}{\nu_0^n\nu^2}\left\{\zeta(n+1)\frac{\nu^{n+1}}{\zeta(n+1)}-\nu^{n+1}\theta(\nu-\nu_0)\right\}$$

$$=3N\frac{n\nu^{n-1}}{\nu_0^n}\{1-\theta(\nu-\nu_0)\}$$

$$=3N\frac{n\nu^{n-1}}{\nu_0^n}\theta(\nu_0-\nu), \tag{2.13}$$

which gives the phonon spectrum. As a special case of this result, let $n=3$ and $\nu_0=\nu_D$ in formula (2.1), then the Debye spectrum is recovered:

$$g(\nu)=9N\frac{\nu^2}{\nu_D^3}\theta(\nu_D-\nu). \tag{2.14}$$

Supposing $C_V(T)$ is a superposition of the form (2.1),

$$C_V(T)=3Nrk_B\sum_n A_n\left((n+1)D_n(x_{0,n})-\frac{nx_{0,n}}{e^{x_0}-1}\right),$$

$$x_{0,n}=\frac{h\nu_{0,n}}{k_BT}, \tag{2.15}$$

where $0<\nu_{0,1}<\nu_{0,2}<\nu_{0,3}<\dots,$ and $A_n\geqslant 0$, $n=1, 2, 3\ \dots,\ \Sigma_n A_n=1$. According to the principle of superposition, the exact solutions are

$$g(\nu)=3N\sum_n A_n\frac{n\nu^{n-1}}{\nu_{0,n}^n}\theta(\nu_{0,n}-\nu). \tag{2.16}$$

One can now obtain the complete Debye spectrum and the related general spectra (2.16) by the Möbius inversion formula exactly.

It is interesting to note that the smooth Debye specific heat (differentiable infinitely many times) can produce a discontinuous output (the Debye spectrum) from the integral equation. However, according to the theory of Xie and Chen [19], a smooth input *A* should produce a smooth output *B*. Is there a contradiction between the two theories? No, because in the Möbius inversion solution, there are two independent steps: One is the Laplace transformation, which transforms the integral equation into a summation equation. The other is the modified Mobius inversion, which is used to solve this algebraic equation. What Xie and Chen showed is that the smooth input *A* in the second step, will produce a smooth output *B*. This is the same in our work. The key point is that in our work, the input *A*, which is the inverse Laplace transform of the Debye specific heat, is already discontinuous. Then the output *B* is discontinuous too. So these two theories are consistent.

In conclusion, with the aid of some summation techniques and the Möbius inversion formula itself, the Möbius inversion formula in SPI is shown to be useful in finding concrete exact solutions for physical models. One of the key contributions here is that the unknown Möbius function $\mu(n)$ for large n was avoided in practice, and the complete Debye spectrum with correct cut-off factor was recovered. The current result can also be applied to investigate other inversion problems.

ACKNOWLEDGMENTS

This work is in Project Nos. 19834010 and 19975009 and supported by the National Natural Science Foundation of China. One of the authors (X. Dai) would like to thank the Department of Physics and Astronomy at Brigham Young University for their hospitality and its research group in theoretical physics for significant discussions.

[1] X. X. Dai, X. W. Xu, and J. Q. Dai, in *Proceedings of Beijing International Conference on High Tc Superconductivity, September 1989* (World Scientific, Singapore, 1989), pp. 521–524.
[2] X. X. Dai, X. W. Xu, and J. Q. Dai, Phys. Lett. A **147**, 445 (1990).
[3] E. W. Montroll, J. Chem. Phys. **10**, 218 (1942).
[4] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **26**, 551 (1954).
[5] A. E. Carlsson, C. D. Gelatt, and H. Ehrenreich, Philos. Mag. A **41**, 241 (1980).
[6] Xianxi Dai and Jiqiong Dai, Phys. Lett. A **161**, 45 (1991).
[7] Dai Xianxi and Dai Jiqiong, IEEE Trans. Appl. Supercond. **40**, 257 (1992).
[8] Dai Xianxi, Tao Wen, GuiCun Ma, and JiXin Dai, Phys. Lett. A **264**, 68 (1999).
[9] N. X. Chen, Phys. Rev. Lett. **64**, 1193 (1990).
[10] J. Maddox, Nature (London) **344**, 377 (1990).
[11] S. Y. Ren and J. D. Dow, Phys. Lett. A **154**, 215 (1991).
[12] R. P. Millane, Phys. Lett. A **162**, 213 (1992).
[13] G. H. Hardy and E. M. Wright, *An Introduction to the Theory of Numbers*, 5th ed. (Oxford University Press, Oxford, 1979).
[14] M. Bertero, P. Boccacci, F. Malfanti, and E. R. Pike, Inverse Problems **10**, 1059 (1994).
[15] N. X. Chen and Rong Erqian, Phys. Rev. E **57**, 1302 (1998); **57**, 6216 (1998).
[16] P. Debye, Ann. Phys. (Leipzig) **39**, 789 (1912).
[17] E. C. Titchmarsh, *The Theory of the Riemann Zeta-Function* (Clarendon Press, Oxford, 1986).
[18] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, 1980).
[19] Qian Xie and Nan-xian Chen, Phys. Rev. E **52**, 6055 (1995).