Closed-form solution for inverse problems of Fermi systems

Chen Nan-xian
*Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, People's Republic of China and Beijing University of Science and Technology, Beijing 100083, People's Republic of China**

Zhang Chen-fu
Department of Physics, Peking University, Beijing 100875, People's Republic of China

Zhou Mai
Department of Mathematics, Nan-Kai University, Tianjin 300071, People's Republic of China

Ren Guang-bao and Zhao Wen-bin
Institute of Applied Physics, Beijing University of Science and Technology, Beijing 100083, People's Republic of China
(Received 23 November 1992)

A series of applications of a theorem relating the Dirac δ function to the Fermi distribution [Chen, Phys. Rev. A **46**, 3538 (1992)] are presented in this paper. In particular, the inverse problem for determining the density of states of Fermi systems, the determination of relaxation-time distribution from dielectric function spectra, and the inverse isotherm problem for the adsorption energy distribution function are treated with closed-form general solutions. The present method is not only simplified significantly relative to all the previous work, but also has the merit of not making *a priori* assumptions about the solution of the integral equation; hence it is a direct way of evaluating the density of states.

PACS number(s): 05.30.Fk, 82.65.My, 02.30.−f, 02.70.−c

I. INTRODUCTION

Recently, Chen has proposed a relationship between the Dirac δ function and the Fermi distribution [1], which provides a powerful tool to solve a group of integral equations which are important to fermion systems and other branches in applied physics. The present work will explain the method in detail with a series of applications. Essentially, once a relation between the δ function and the kernel of the integral equation is given, the general solution of the equation can be obtained immediately.

II. AN EXPRESSION OF THE δ FUNCTION

It is well known from the elementary generalized function theory that [2,3]

$$\lim_{\epsilon\to 0^+}\frac{1}{x\pm i\epsilon}=\frac{1}{x\pm 0^+}=\mathrm{P}\frac{1}{x}\mp i\pi\delta(x)\ , \tag{1}$$

where P indicates the Cauchy principal value. Therefore, it is given as

$$\begin{aligned}\delta(x-y)&=\frac{1}{2\pi i}\left[\frac{1}{x-y-i0^+}-\frac{1}{x-y+i0^+}\right]\\&=\frac{1}{2\pi i}\left[\frac{1}{1-e^{x-y+i0^+}}-\frac{1}{1-e^{x-y-i0^+}}\right].\end{aligned} \tag{2}$$

Introducing the translational operators $e^{i(\pi-0^+)(\partial/\partial y)}$ and $e^{-i(\pi-0^+)(\partial/\partial y)}$, which represent the translations of π and $-\pi$ along the imaginary axis in a complex plane extended from the y axis, an expression of the δ function is given such that

$$\begin{aligned}\frac{1}{2\pi i}[e^{i(\pi-0^+)(\partial/\partial y)}-e^{-i(\pi-0^+)(\partial/\partial y)}]\frac{1}{1+e^{x-y}}&=\frac{1}{2\pi i}\left[\frac{1}{1-e^{x-[y+i(\pi-0^+)]}}-\frac{1}{1-e^{x-[y-i(\pi-0^+)]}}\right]\\&=\frac{1}{2\pi i}\left[\frac{1}{1-e^{x-y+i0^+}}-\frac{1}{1-e^{x-y-i0^+}}\right]=\delta(x-y)\ .\end{aligned} \tag{3}$$

Notice that the appearance of the above translational operators is equivalent to requiring the extension of y from the real axis to the complex plane z with the cut $(-\infty,0)$. In other words, the real function $1-e^{x-y}$ defined on y has been extended to a complex function $1-e^{x-z}$ defined on the z plane with the cut $(-\infty,0)$, and the corresponding argument of the complex function is restricted to $(-\pi,\pi)$. Based on this understanding, Eq. (3) can be expressed simply as

$$\delta(x-y)=\frac{1}{2\pi i}[e^{-i\pi(\partial/\partial y)}-e^{i\pi(\partial/\partial y)}]\frac{1}{1+e^{x-y}} \tag{4}$$

or

$$\delta(x-y)=\frac{1}{\pi}\text{Im}\left[\exp\left[i\pi\frac{\partial}{\partial y}\right]\frac{1}{1+e^{x-y}}\right] . \tag{5}$$

Executing Taylor's expansion, we have

$$\delta(x-y)=\frac{1}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m\pi^{2m+1}}{(2m+1)!}\frac{\partial^{2m+1}}{\partial y^{2m+1}}\frac{1}{1+e^{x-y}} . \tag{6}$$

From a variety of applications and the above understanding, one may use the Eqs. (4–6) without hesitation. For some problems with a "quasi"-Fermi-distribution, a similar relation is needed:

$$\delta(x-y)=\frac{-1}{\pi}\text{Im}\left[\exp\left[i\pi\frac{\partial}{\partial y}\right]\frac{1}{1+e^{y-x}}\right] . \tag{7}$$

III. A GENERAL SOLUTION OF THE INVERSE PROBLEM FOR THE DENSITY OF STATES OF FERMI SYSTEMS

Now we give an example that applies Eq. (6) to a Fermi system. According to Eq. (6), the temperature-dependent density of states (DOS) near the Fermi level $g(E_F,T)$ can be expressed as

$$\begin{aligned} g(E_F,T)&=\int_{-\infty}^{\infty}dE\, g(E,T)\delta(E-E_F)=\int_0^{\infty}dE\, g(E,T)\delta(E-E_F)\\ &=\int_0^{\infty}dE\, g(E,T)\sum_{m=0}^{\infty}(-1)^m\frac{(\pi kT)^{2m}}{(2m+1)!}\frac{\partial^{2m+1}}{\partial E_F^{2m+1}}F_T(E,E_F)\\ &=\sum_{m=0}^{\infty}(-1)^m\frac{(\pi kT)^{2m}}{(2m+1)!}\frac{\partial^{2m+1}}{\partial E_F^{2m+1}}\int_0^{\infty}dE\, g(E,T)F_T(E,E_F)\\ &=\sum_{m=0}^{\infty}(-1)^m\frac{(\pi kT)^{2m}}{(2m+1)!}\frac{\partial^{2m+1}}{\partial E_F^{2m+1}}n(E_F,T) , \end{aligned} \tag{8}$$

where $n(E_F,T)$ represents the carrier density, i.e.,

$$n(E_F,T)=\int_{-\infty}^{\infty}dE\, g(E,T)\frac{1}{(1+e^{(E-E_F)/kT})} . \tag{9}$$

Notice that for the second expression in Eq. (8), we have considered $E_F>0$. Therefore, Eq. (8) is a closed-form solution of the integral equation (9). In other words, one can determine the density of states of a fermion system based on the measurable carrier density and Fermi level. In fact, the first three approximate solutions can be expressed as

$$g_0(E_F,T)=\frac{\partial n(E_F,T)}{\partial E_F} , \tag{10}$$

$$g_1(E_F,T)=\frac{\partial n(E_F,T)}{\partial E_F}-\frac{\pi^2}{6}(kT)^2\frac{\partial^3 n(E_F,T)}{\partial E_F^3} , \tag{11}$$

and

$$g_2(E_F,T)=\frac{\partial n(E_F,T)}{\partial E_F}-\frac{\pi^2}{6}(kT)^2\frac{\partial^3 n(E_F,T)}{\partial E_F^3}+\frac{\pi^4}{120}(kT)^4\frac{\partial^5 n(E_F,T)}{\partial E_F^5} . \tag{12}$$

In principle, the above expression is suitable for metals controlled by doping impurities.

IV. A GENERAL CLOSED-FORM SOLUTION FOR RELAXATION-TIME SPECTRA

In general, the relaxation-time distribution $Y(\tau)$ of a material and the measurable properties such as the components of the complex permittivity $\epsilon(\omega)=\epsilon'(\omega)+\epsilon''(\omega)$ at frequency ω, can be expressed by [4]

$$\int_0^{\infty}\frac{Y(\tau)d\tau}{1+(\omega\tau)^2}\equiv\frac{\epsilon'(\omega)-\epsilon'_\infty}{\epsilon'_c-\epsilon'_\infty}\equiv Z(\omega) , \tag{13}$$

where ϵ'_c is the low-frequency (in the limit, static) permittivity of the material, and the high-frequency (optical) limit.

The traditional method of solving the above integral equation is to construct an expression of $Y(\tau)$ from general arguments with some parameters determined by experiments [4] based on Eq. (13). Thus, the form of the unknown function has to be decided before doing the calculation. A new technique to calculate the spectra $Y(\tau)$ has been proposed by Ligachev and Filikov [5] recently, but the method is related to both the Mellin transformations, as well as modified Bessel function of the third kind, and so on. Also, their fitting function is restricted [5]. By using Eq. (8), we show a simple and general solution for this problem.

Denote that

$$\tau^2=e^x \text{ and } \omega^2=e^{-y} , \tag{14}$$

then we have

$$2\tau\, d\tau=e^x dx , \tag{15}$$

Substituting Eqs. (14) and (15) into Eq. (13), it is given that

$$Z(e^{-y/2})=\tfrac{1}{2}\int_{-\infty}^{\infty}\frac{Y(e^{x/2})e^{x/2}dx}{1+e^{x-y}} . \tag{16}$$

Therefore,

$$\begin{aligned}\tfrac{1}{2}Y(e^{y/2})e^{y/2}&=\frac{1}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m\pi^{2m+1}}{(2m+1)!}\frac{\partial^{2m+1}}{\partial y^{2m+1}}Z(e^{-y/2})\\ &=\frac{1}{\pi}\text{Im}\left[\exp\left[i\pi\frac{\partial}{\partial y}\right]Z(e^{-y/2})\right] .\end{aligned} \tag{17}$$

The above expression is a general closed-form solution for Eq. (13). Now, let us check the result of Ligachev and Filikov [5] for the case of

$$Z(\omega)=\sum_{j=1}^{N} a_{kj}\exp\left[-\frac{b_{kj}}{2}\left[\frac{\omega}{\omega_j}+\frac{\omega_1}{\omega}\right]\right] . \tag{18}$$

Let us only consider one term in Eq. (18), i.e.,

$$Z(e^{-y/2})\propto\exp\left[b\left[\frac{\omega}{\omega_0}+\frac{\omega_0}{\omega}\right]\right]$$
$$=\exp[-b(e^{(y-y_0)/2}+e^{-(y-y_0)/2})] .$$

Based on Eq. (17), we then have

$$\begin{aligned}Y(\tau)&=\frac{2}{\pi\tau}\mathrm{Im}\{e^{i\pi(\partial/\partial y)}\exp[b(e^{(y-y_0)/2}+e^{-(y-y_0)/2})]\}|_{y=x}\\&=\frac{2}{\pi\tau}\mathrm{Im}\{\exp[ib(e^{(y+i\pi-y_0)/2}+e^{-(y+i\pi-y_0)/2})]\}|_{y=x}\\&=\frac{2}{\pi\tau}\mathrm{Im}\{\exp[ib(e^{(y-y_0)/2}-e^{-(y-y_0)/2})]\}|_{y=x}\\&=\frac{2}{\pi\tau}\sin[b(e^{(y-y_0)/2}-e^{-(y-y_0)/2})]|_{y=x}=\frac{2}{\pi\tau}\sin\left[b\left[\frac{1}{\omega_0\tau}-\omega_0\tau\right]\right] .\end{aligned} \tag{19}$$

This is just the same result as that of Ligachev and Filikov [5], but the present deduction is much simpler and uses only elementary operations.

V. DISTRIBUTION FUNCTIONS WITH A LANGMUIR KERNEL

The concept of adsorption on heterogeneous substrates can be traced to the pioneering work of Langmuir who proposed an expression for the total isotherm. Given the experimentally determined total isotherm Θ_t and a theoretical local isotherm Θ_L, it is necessary to evaluate the distribution function $\rho(\varepsilon,T)$, which satisfies

$$\Theta_t(P,T)=\int_0^\infty\Theta_L(P,T;\varepsilon)\rho(\varepsilon,T)d\varepsilon , \tag{20}$$

and

$$\int_0^\infty\rho(\varepsilon,T)d\varepsilon=1 , \tag{21}$$

where $\varepsilon(\geq 0)$ is the adsorption energy [6], and P and T are the pressure and temperature, respectively.

In general, it is assumed that the local isotherm Θ_L is the well-known Langmuir isotherm [6]

$$\Theta_L(P,T;\varepsilon)=[1+P^{-1}a(T)\exp(-\varepsilon/RT)] , \tag{22}$$

where the meaning of $a(T)$ is clear from a statistical derivation of the Langmuir isotherm [6]. The integral equation (20) now becomes

$$\Theta_t(P,T)=\int_0^\infty[1+P^{-1}a(T)\exp(-\varepsilon/RT)]^{-1}\rho(\varepsilon)d\varepsilon . \tag{23}$$

Let

$$P^{-1}a(T)=e^y \quad\text{or}\quad P=a(T)e^{-y} \tag{24}$$

and

$$x=\varepsilon/RT . \tag{25}$$

Equation (23) then becomes

$$\Theta_t(a(T)e^{-y},T)=RT\int_0^\infty\frac{\rho(RTx)}{[1+e^{y-x}]}dx , \tag{26}$$

$$\rho(\varepsilon)=\rho(RTx)=\frac{-1}{\pi RT}\mathrm{Im}[e^{i\pi(\partial/\partial y)}\Theta_t(y,T)]|_{y=x} . \tag{27}$$

Notice that, unlike $[1+e^{x-y}]^{-1}$ in Eqs. (4)–(6), we are now facing $[1+e^{y-x}]^{-1}$ in (26). This is the reason why a minus sign appears as in Eq. (7).

A. Generalized Freundlich isotherm

This phenomenological law can be expressed as

$$\Theta_t(P,T)=[1+P^{-1}a(T)]^{-c} , \quad 0<c<1 . \tag{28}$$

From Eqs. (33) and (34) and

$$\frac{1}{(1+e^y)^c}=\frac{e^{-cy}}{(1+e^{-y})^c} , \tag{29}$$

we obtain

$$\begin{aligned}\rho(\varepsilon)=\rho(RTx)&=\frac{-1}{2\pi RTi}[e^{i\pi(\partial/\partial y)}-e^{-i\pi(\partial/\partial y)}]\frac{e^{-cy}}{[1+e^{-y}]^c}\Bigg|_{y=x}\\&=\frac{-1}{2\pi ikT}\left\{\frac{e^{-c(y+i\pi)}}{[1+e^{-y-i\pi}]^c}-\frac{e^{-c(y-i\pi)}}{[1+e^{-y+i\pi}]^c}\right\}\Bigg|_{y=x}=\frac{e^{-cy}}{2\pi RT}\frac{e^{ic\pi}-e^{-ic\pi}}{(1-e^{-y})^c}=\frac{\sin\pi c}{\pi RT[\exp(\varepsilon/RT)-1]^c} .\end{aligned} \tag{30}$$

This result agrees completely with that of both Sips [7] and the Wiener-Hopf method [6], in which a much more complicated procedure was performed. Notice that the transform (29) is necessary since $(1-e^y)^c$ is meaningless for $y>0$. If one deduces the procedure as shown in Eqs. (1)–(3), the same result can be obtained with much more confidence.

B. Dubinin-Radushkevich isotherm

The Dubinin-Radushkevich isotherm is given by

$$\Theta_t(P,T)=\exp\{-B[RT\ln(P_0/P)]^2\}\ , \tag{31}$$

where P_0 is the saturation vapor pressure of the adsorbed gas at the ambient temperature AT, and B is a constant. Defining

$$A\equiv B(RT)^2 \quad\text{and}\quad C\equiv\ln[P_0/a(T)]\ , \tag{32}$$

we obtain that

$$\Theta_t(y,T)=\exp[-A(y-C)^2]\ . \tag{33}$$

Using our method, we have

$$\begin{aligned}\rho(\varepsilon)&=\frac{-1}{\pi RT}\mathrm{Im}[e^{i\pi(\partial/\partial y)}e^{-A(y-C)^2}]|_{y=x}=\frac{-1}{\pi RT}\mathrm{Im}[e^{-A[(y+i\pi)-C]^2}]|_{y=x}\\&=\frac{-1}{\pi RT}[e^{-A[(y-C)-i\pi[^2}]|_{y=x}\\&=\frac{-1}{\pi RT}[e^{-A(y-C)^2+A\pi^2+2\pi Ai(y-C)}]|_{y=x}\\&=\frac{1}{\pi RT}e^{-A(C-y)^2+A\pi^2}\sin[2\pi A(C-y)]|_{y=\varepsilon/RT}\\&=\frac{\exp\{-B[\varepsilon^2-(\pi RT)^2]\}\sin(2\pi BRT\varepsilon)}{\pi RT}\ ,\end{aligned} \tag{34}$$

which is identical to the result obtained by the Stieltjes transform technique [7], but here only a very simple operation is applied.

VI. CONCLUSION AND DISCUSSION

The present general method for solving some inverse problems for Fermi system and other systems is presented systematically in this report, but the previous workers [5,6] spent much more effort to obtain the similar piecemeal (sometimes incomplete) results. It can be expected that these new relations might be useful for different physical problems, such as for semiconductor or nuclear systems. Notice that all the differentiations in Eq. (8) are taken at the original Fermi level of the system, and one only needs the data near the initial Fermi level in practice. If the function $n(E_F)$ is smooth enough, one may obtain the density of states $g(E)$ with any value E by using the translation operator, which will be discussed in detail in another paper. Notice that for a numerical calculation with a different fitting technique, the above solution is unique but not a stable one, since the integral Equation (9) essentially is an ill-posed equation. But there is no cause for disappointment since what we have obtained is the most important information near the Fermi level. It should also be indicated that Eqs. (4)–(6) can be modified for application to the degenerated Fermi system, which obeys

$$F_T^{FD}(E,E_F)=\frac{1}{1+\lambda e^{(E-E_F)}/kT}\ , \tag{35}$$

where λ is the degenerate factor. The corresponding expressions should be

$$\frac{1}{\pi kT}\mathrm{Im}\left[\exp\left\{i\pi kT\frac{\partial}{\partial E_F}\right\}\frac{1}{1+\lambda e^{(E-E_F)/kT}}\right]=\delta(E+kT\ln\lambda-E_F)\ . \tag{36}$$

Finally, we would like to mention that the above method would also be suitable for the boson system, which will be uncomplicated and which we will present in another work.

ACKNOWLEDGMENTS

The author gratefully acknowledges helpful suggestions from Z. D. Chen, Department of Mathematics, Beijing University of Science and Technology, and other friends from Peking University and Academia Sinica. Finally, this work was supported in part by the National Foundation of Science in China, and in part by the National Committee of Advanced Materials in China.

*Mailing address.

[1] N. X. Chen, Phys. Rev. A **46**, 3538 (1992).
[2] N. N. Bogoliubov, *Introduction to the Theory of Quantized Fields,* (Interscience Publisher, New York, 1959).
[3] S. Schweber, *An Introduction to Relativistic Quantum Theory,* (Row-Peterson, New York 1961); or C. Itzykson and J. D. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[4] H. Fröhlich, *Theory of Dielectrics,* 2nd ed. (Clarendon, Oxford, 1958).
[5] V. A. Ligachev and V. A. Filikov, Fiz. Tverd. Tela (Leningrad) **33**, 3292 (1991) [Sov. Phys. Solid State **33**, 1857 (1991)].
[6] Uzi Landman and E. W. Montroll, J. Chem. Phys. **64**, 1762 (1976).
[7] R. Sips, J. Chem. Phys. **15**, 490 (1948); **18**, 1024 (1950).