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A note on the closed form solution and the series expansion for the Fermi-Integral $F_{\frac{1}{2}}(E_F/k_BT)$ of the density-of-states function in Semiconductors

P. K. Chakraborty[1], Soma Mukherjee[2] and B. K. Chaudhuri[1,3*]
[1]Centre for Rural and Cryogenic Technology, Jadavpur University, Kolkata -700032, India
[2]Department of Physics, Guru Nanak Institute of Technology, Panihati, Sodepur, Kolkata-700114, India
[3]Department of Physics, National Institute of Technology, Rourkela-769008, Orissa, India

Abstract: ***We have demonstrated from theoretical analysis that the closed form solution of the Fermi Integral is more exact and better than the conventional numerical integration method in the calculation of Fermi energy.***

Keywords: **Density of state, Fermi Integral, Fermi Energy, semiconductor physics**

I. INTRODUCTION

Generally, the Fermi-Integral, $F_j(\eta)$, is defined as [1-3]

$$F_j(\eta)=\frac{1}{\Gamma(j+1)}\cdot\int_{x=0}^{\infty}\frac{x^j dx}{1+\exp(x-\eta)} \tag{1}$$

where j > 0 and it can be an integer or a fraction. For the density-of-states (DOS) function, the value of $j=\frac{1}{2}$. The Fermi-integral, $F_{\frac{1}{2}}(\eta)$, is a well-known integral used in semiconductor devices [3]. Here, $\eta=E_F/k_BT$ and E_F is the Fermi-energy, k_B is the Boltzmann constant and T is absolute temperature. $F_{\frac{1}{2}}(\eta)$ is also known as the Fermi-integral for the density-of-states function and is given from Eq. (1) for $j=\frac{1}{2}$ as [3]:

$$F_{\frac{1}{2}}(\eta)=\frac{2}{\sqrt{\pi}}\cdot\int_{x=0}^{\infty}\frac{x^{\frac{1}{2}}\cdot dx}{1+\exp(x-\eta)} \tag{2}$$

Equation (2) is the special case of Eq. (1) for $j=\frac{1}{2}$.

When E_F is positive or not much lower than (k_BT) at the band edge, i.e., when the material is degenerate, the integral in Eq. (1) has to be evaluated numerically. The numerical values of the integral are, however, available in tabulated [1-3] form. As we know that the numerical integration is an approximate method, we cannot find accurately the value of $\eta\ (=E_F/k_BT)$ by numerical integration. However, it is possible to obtain a closed form solution of the integral (Eq.1), after some algebraic manipulations of the integrand, to a special functional form of Confluent Hypergeometric function of the type [4] Φ (a, b; z) with a = – exp (η), b = (j + 1) and z = 1. The values of Φ (a, b; z) can be obtained from the table [5] of Φ (a, b; z). We can also obtain a series expansion

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of Φ (a, b; z) to an infinite series [4,5] for any values of the arguments; i.e., a, b, and z.

The purpose of the present technical note is to obtain a closed form solution and then a series expansion of the integral Eq. (1), with a special case for $j=\frac{1}{2}$, to an infinite terms. When we evaluate the Fermi-integral (FI) numerically, let us represent it as $F_j(\eta)$. However, when we obtain the closed form solution or a series expansion of FI, we represent the same as $\bar{F}_j(\eta)$, with a special case for $j=\frac{1}{2}$.

The values of the functions $F_{\frac{1}{2}}(\eta)$ and exp (– η). $F_{\frac{1}{2}}(\eta)$ are tabulated in Ref. [1-3] for different values of η; when $F_{\frac{1}{2}}(\eta)$ is calculated numerically. The functions $F_{\frac{1}{2}}(\eta)$ and exp (– η). $F_{\frac{1}{2}}(\eta)$ are plotted in Fig. 1.

The values of the functions $\bar{F}_{\frac{1}{2}}(\eta)$ and exp (–η). $\bar{F}_{\frac{1}{2}}$ calculated from the series expansion method are also plotted in Fig. 1 for the convenience of comparison of the two methods. The graphs in Fig.1 show that the series expansion method of determination of $\eta\left(\text{with}\, j=\frac{1}{2}\right)$ is more appropriate from the point of view of semiconductor device physics, compared to that derived from numerical integration approach.

In the following we shall provide the closed form solution to $\bar{F}_j(\eta)$ with special attention to $j=\frac{1}{2}$, i.e. $\bar{F}_{\frac{1}{2}}(\eta)$: After doing some algebraic manipulations, we can express Eq. (1) as

$$F_j(\eta)=\frac{-\beta}{\Gamma\nu}\int_{x=0}^{\infty}\frac{\exp(-x).x^{\nu-1}dx}{1-\beta\,.\exp(-x)} \tag{3}$$

With $\beta = -\exp(\eta)$ (4)

and $\nu = (j + 1)$ (5)

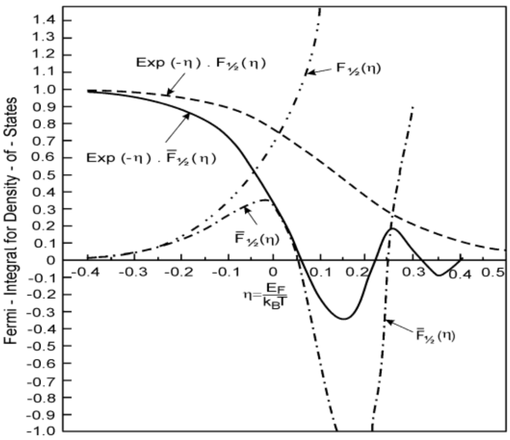

Fig. 1. Variation of Fermi integral density of states (DOS) as a function of reduced temperature $\eta= E_F/k_BT$ (where E_F = Fermi energy, k_B = Boltzmann's constant and T = Absolute temperature)

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The solution of the integration in Eq. (3) can be expressed as [4]:

$$\bar{F}_j(\eta)=\exp(\eta)\cdot\Phi\{-\exp(\eta),(j+1);1\} \qquad (6)$$

where Φ (a, b; z) is the confluent Hypergeometric function, with a = – exp (η), b = (j + 1) and z = 1 (Ref. 4,5). For a given value of $\eta(=E_F/k_BT)$ and j, we can find the value of Φ (a, b; z) from the table [5]. However, for simple calculation of $\bar{F}_j(\eta)$, we can take the series expansion to Φ (a, b; z) as given in Ref. 4,5. Taking the series expansion of Φ (a, b; z), we get [5]

$$\Phi(a,b;z)=1+\frac{a}{b}\frac{z}{1!}+\frac{(a)_2}{(b)_2}\cdot\frac{z^2}{2!}+\frac{(a)_3}{(b)_3}\cdot\frac{z^3}{3!}+\frac{(a)_4}{(b)_4}\cdot\frac{z^4}{4!}+........+\frac{(a)_n}{(b)_n}\cdot\frac{z^n}{n!}+.......... \qquad (7)$$

where, $(a)_0=1$ and $(a)_n=a(a+1)(a+2)(a+3)...(a+n-1)$ (8)

Substituting a = – exp (η), b = (j + 1) and z = 1 in Eqs. (7 and 8), we get

$$\bar{F}_j(\eta)=\exp(\eta).\left[1-\frac{\exp(\eta)}{(j+1)}\cdot\frac{1}{1!}-\frac{\exp(\eta).(1-\exp(\eta))}{(j+1).(j+2)}\cdot\frac{1^2}{2!}-\frac{\exp(\eta).(1-\exp(\eta)).(2-\exp(\eta))}{(j+1).(j+2).(j+3)}\cdot\frac{1^3}{3!}+.......to\infty\right] \qquad (9)$$

Equation (9) is the series expansion of $\bar{F}_j(\eta)$ for any values of j and $\eta(=E_F/K_BT)$. Now, for a given value of j and η, the right hand side of Eq. (9) can be easily calculated and hence we can find $\bar{F}_j(\eta)$ more accurately.

For $j=\frac{1}{2}$, as a special case of Fermi-integral, $\bar{F}_{\frac{1}{2}}(\eta)$, the series expansion of the same can be obtained from Eq. (9) as :

$$\bar{F}_{\frac{1}{2}}(\eta)=\exp(\eta).\left\{1-\frac{2}{3}.\exp(\eta).-\frac{\exp(\eta).(1-\exp(\eta))}{3.5}\frac{2^2}{2!}-\frac{\exp(\eta).(1-\exp(\eta)).(2-\exp(\eta))}{3.5.7}\cdot\frac{2^3}{3!}....\infty\right\} \qquad (10)$$

where $\eta(=E_F/k_BT)$. Equation (10) represents the series expansion of the Fermi-integral, $\bar{F}_{\frac{1}{2}}(\eta)$ for the density-of-states function.

Following observations can be drawn from Fig. 1. As mentioned earlier, $\bar{F}_{\frac{1}{2}}(\eta)$ as well as $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ are computed from Eqn. (10) for both positive and negative values of η and are plotted in Fig. 1. Also $F_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).F_{\frac{1}{2}}(\eta)$ are plotted in Fig. 1 for the same values of η in order to compare the two methods viz. (i) exact methods of calculations from Eq. (10) and (ii) by numerical calculations from Eq. (2). From the graphs for $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ and $\bar{F}_{\frac{1}{2}}(\eta)$, we observe oscillation in the density of state

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function as their values are becoming negative values for the positive values of η; e.g. (+ 0.5 $\leq\eta\leq$ + 2.5) for $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ and (+ 0.53 $\leq\eta\leq$ + 2.5) for $\bar{F}_{\frac{1}{2}}(\eta)$. Also (+ 3.4 $\leq\eta\leq$ + 4.0) values for the graph of $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$. For the negative values of η, i.e., $\eta< 0.0$, both the functions $\bar{F}_{\frac{1}{2}}(\eta)$ as well as $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ are of positive values. Since $\bar{F}_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ are the representations of the density-of-states (DOS), their negative values indicated by the above range of values of η cannot exist. So these ranges of values of η are the forbidden region. Various forbidden regions representing the band-gap of semiconductors are the different Brillioun zones within the lattices.

The graphs for $F_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).F_{\frac{1}{2}}(\eta)$ never show negative values for all values of η both positive and negatives ones. This shows that DOS representations by $F_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).F_{\frac{1}{2}}(\eta)$ do not show the forbidden zones, which are unlikely to the above cases. Hence do not find the presence of band-gap in semiconductors, which in other word means that the representations of the DOS by $F_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).F_{\frac{1}{2}}(\eta)$ (numerical integration method) are not proper. Therefore, we conclude that our representations of DOS by $\bar{F}_{\frac{1}{2}}(\eta)$ and $\exp(-\eta).\bar{F}_{\frac{1}{2}}(\eta)$ (closed form solution method) are better and correct, as compared to the conventional methods of numerical integrations [3].

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AUTHOR BIOGRAPHY

Dr. Paritosh Kumar Chakraborty received the B.E. degree in Electronics from the Indian Institute of Science, Bangalore, India, in 1980 and Ph.D. degree from the Indian Institute of Technology, Kharagpur, India, in 1991. He joined the Department of Electronics and Electrical Communication Engineering, Indian Institute of Technology, Kharagpur, India, as Senior Research Assistant in 1980. He retired from same Department of Electronics and Electrical Communication Engineering, as an Assistant Professor in 2013. Presently, he is working at the Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India as a senior visiting scientist, since 2013. His area of research works are: interband tunneling, resonant tunneling, optical as well as

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carrier transport properties of semiconductors. Also, he is presently concentrating on perturbation techniques to the semiconductors devices Physics.

Dr. Soma Mukherjee is working as Asst Prof. in the Dept. of Physics, Guru Nanak Institute of Technology, Kolkata under Maulana Abul Kalam University of Technology (formerly West Bengal University of Technology) for last 10 years. She completed M.Sc. in Physics and Ph.D in Solid State Physics from Jadavpur University, Kolkata. She did her Post Doctoral work from Indian Association for the Cultivation of Science (IACS), Jadavpur, Kolkata. She has more than 30 publications in different National and International Journals and proceedings to its credit. At present she is life member of Indian Association for the Cultivation of Science and Indian Science Congress Association.

Professor B K Chaudhuri, Ph.D., Sc.(Cal) at present working as visiting Professor at National Institute of Technology, Rourkela, Orissa. Formally, he was the Sr. Professor and Head of the Department of Solid State Physics, Indian Association for the Cultivation of Science, Kolkata -32. Professor Chaudhuri published more than 300 research papers and guided 40 Ph.D students. He worked in Germany and Japan as Alexander von Humboldt Fellow and JSPS Fellow, respectively. He also worked as the visiting Professors at Sun Yet Sen National University, Taiwan; Sheffield University, UK and Tokyo University of Science, Japan.