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Fermi integral and density-of-states functions in a parabolic band semiconductor degenerately doped with impurities forming a band tail

B K CHAUDHURI[1,*], B N MONDAL[2] and P K CHAKRABORTY[3]

[1]Centre for Rural and Cryogenic Technologies, Jadavpur University, Jadavpur, Kolkata 700 032, India
[2]Department of Central Scientific Services, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India
[3]Department of Electronics and Electrical Communication Engineering, Indian Institute of Technology, Kharagpur 721 302, India
*Corresponding author. E-mail: sspbkc@iacs.res.in

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Abstract. We provide the energy spectrum of an electron in a degenerately doped semiconductor of parabolic band. Knowing the energy spectrum, the density-of-states (DOS) functions are obtained, considering the Gaussian distribution of the potential energy of the impurity states, showing a band tail in them e.g., energy spectrum and density-of-states. Therefore, Fermi integrals (FIs) of DOS functions, having band tail, are developed by the exact theoretical calculations of the same. It is noticed that with heavy dopings in semiconductors, the total FI demonstrates complex functions, containing both real and imaginary terms of different FI functions. Their moduli possess an oscillatory function of η (reduced Fermi energy $= E_{\mathrm{f}}/k_{\mathrm{B}}T$, k_{B} is the Boltzmann constant and T is the absolute temperature) and η_e (impurity screening potential), having a series solutions of confluent hypergeometric functions, $\Phi(a, b; z)$, superimposed with natural cosine functions of angle θ. The variation of θ with respect to η indicated a resonance at $\eta = 1.5$. The oscillatory behaviour of FIs show the existence of 'band-gaps', both in the real as well as in the forbidden bands as new band gaps in the semiconductor.

Keywords. Fermi integral; degenerately doped; band tails; semiconductor; density of state; parabolic band.

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1. Introduction

With the advent of MBE, MOCVD, FLL and other experimental techniques for the development of doped semiconductor materials [1], the impact of the theoretical and experimental studies on density-of-state (DOS) functions for the heavily doped semiconductors [1,2] are very promising. Accordingly, the computations of the Fermi energy (E_{f}) or Fermi integrals (FI) in such cases are emerging as a challenging area [3]. To the best of our knowledge, study of FIs with band tail has not been made as yet in literature [4–6]. In the present report, we have developed an exact quantum mechanical approach to calculate the energy spectrum for parabolic band under heavy doping. The energy spectrum possesses a tail, extending within the forbidden band of the semiconductor [7,8]. The DOS functions are calculated from the energy spectrum equation, which also show a tail [7,9].

As we know [3], the FI is involved with the integrations of the product of the DOS functions and the Fermi–Dirac (FD) distribution function [6] for all possible values of E, the electron energy. Therefore, the FIs for the above DOS functions are computed by exact theoretical approaches, involving more mathematical calculations. It is noticed that with heavy dopings in a semiconductor, the total FI demonstrates a complex function, having real and imaginary terms of different FI functions. Their moduli possess oscillating functions of η, η_e, and $k_{\mathrm{B}}T$ having a series solution of the confluent hypergeometric functions, $\Phi(a, b; z)$, superimposed with the natural cosine function of angle, θ. These studies might find applications in transport phenomena in semiconductors with heavy doping and many other electronic properties of materials in condensed matter physics [4], leading to complex phenomena in nanodevices [5] as well as in bulk semiconductor devices [10–12].

Organisation of this paper is as follows: Section 2 provides the theoretical basis of our calculations, where the E–k dispersion relation in the present case of the parabolic band with heavy doping is derived, followed by calculations of DOS function. Thereafter, in §2.1 FIs are computed exactly for the degenerately doped semiconductor showing band tailing in §2.2. Finally, the discussions on the theoretical results are made in §3, followed by conclusions.

2. Theoretical basis

2.1 *Derivation of E–k dispersion relation and the corresponding DOS function for degenerately doped semiconductor forming a band tail*

In order to derive the E–k dispersion relation, in the case of degenerately doped semiconductor, the space-dependent $(\bar{r})$ kinetic energy of an electron can be expressed as [6]

$$E = \frac{\hbar^2 k^2}{2m_c} + V(\bar{r}), \tag{1}$$

where m_c is the effective mass of the electron at the edge of the conduction band (CB), $V(\bar{r})$ is the impurity potential at a local point $(\bar{r})$, E is the total electron energy, $\hbar$ is the reduced Planck's constant and $\bar{k}$ is the wave vector of the electron. The band-tailing in degenerately doped semiconductor can be visualised from the following calculations.

The Gaussian potential energy distribution can be written as [13,14]

$$F(V) = \frac{1}{\sqrt{\pi\eta_e^2}} \exp\left(-\frac{V^2(\bar{r}).}{\eta_e^2}\right), \tag{2}$$

where η_e is the impurity screening potential [7]. It is to be noted that eq. (2) for the impurity potential distribution derived by many authors [13–15], was being widely used since 1963 [7,14]. From eq. (2) we can see that the variance of the parameter η_e is not equal to zero, but its mean value is zero. Further, the impurities are assumed to be uncorrelated and the band mixing has been neglected in the formulation of the energy–momentum spectrum, as given below. The average kinetic energy of the whole system is obtained by averaging the local kinetic energy fluctuation represented by

$$\int_{-\infty}^{E} [E - V(\bar{r})]F(V(\bar{r}))\mathrm{d}V = \frac{\hbar^2 k^2}{2m_c} \int_{-\infty}^{E} F(V(\bar{r}))\,\mathrm{d}V. \tag{3}$$

Thus, using eq. (2) into (3) we can write [7–9]

$$\frac{\hbar^2 k^2}{2m_c} = \gamma(E, \eta_e), \tag{4}$$

where

$$\gamma(E, \eta_e) = \frac{1}{2}E\left[1 + \mathrm{erf}\left(\frac{E}{\eta_e}\right)\right] + \frac{\eta_e}{2\pi^{1/2}} \exp\left(-\frac{E^2}{\eta_e^2}\right) \tag{5}$$

and $\mathrm{erf}(E/\eta_e)$ is the error function [16]

$$\eta_\mathrm{e} = \frac{e^2}{\epsilon_d}\left(4\pi\frac{N_i}{k_D}\right)^{1/2} \tag{6}$$

and

$$k_D^2 = \frac{e^2}{\epsilon_d}\frac{1}{4\pi^2} * \left(\frac{2m_c}{\hbar^2}\right)^{1/2}\left[1 + \mathrm{erf}\left(\frac{E_\mathrm{f}}{\eta_e}\right)\right]. \tag{7}$$

From eq. (4) along with eq. (5), we have the E–k dispersion relation.

It is seen that when $\eta_e \to 0$, i.e., in a non-degenerately doped case of a semiconductor, eqs (4) and (5) become an unperturbed parabolic band.

Because of the error function and exponential functions present in eq. (5), eq. (5) exists in the limit $E \to -\infty$ to $+\infty$. For the region $E \to 0$ to $+\infty$, when the electron energy $E \geq 0$, the nature of eq. (5) remains the same. However, for the region, $E \to -\infty$ to 0 (when the electron energy in the band $E \leq 0$) and substituting, $E_1 = -E$, we have $E_1 \geq 0$. Under this condition, eq. (5) becomes

$$\gamma(-E_1, \eta_e) = -\frac{1}{2}E_1\left\{1 - \mathrm{erf}\left(\frac{E_1}{\eta_e}\right)\right\} + \frac{\eta_e}{2\pi^{1/2}} \exp\left(-\frac{E_1^2}{\eta_e^2}\right). \tag{8}$$

For $E < 0$, the function $\gamma(-E_1, \eta_e)$ (eq. (8)) is positive indicating the presence of band tailing and also we have from eq. (8)

$$\frac{\mathrm{d}}{\mathrm{d}E_1}\gamma(-E_1, \eta_e) = \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{E_1}{\eta_e}\right)\right]. \tag{8a}$$

Equation (8a) is positive. The case, when band tail occurred due to heavy or degenerately doped condition, DOS, $G_D(E)$, is given by eq. (4) as

$$G_D(E,\eta_e) = \frac{1}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} \times \left\{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\right\}. \quad (9)$$

As $\gamma(E,\eta_e)$ exists from $E \to -\infty$ to $+\infty$, $G_D(E,\eta_e)$ also exists from $E \to -\infty$ to $+\infty$, showing tailing.

2.2 *Fermi integral for the degenerately doped semiconductor showing band tailing*

Assuming that the FD statistics is valid for heavily doped semiconductor [6] forming band tail, we can write from eq. (9), the total carrier concentration, N_i, as

$$N_i = \frac{1}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}\int_{-\infty}^{\infty}\frac{G_D(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]}. \quad (10)$$

Again, using eqs (9) and (10), we get

$$N_i = \frac{1}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} \times \int_{E=-\infty}^{\infty}\frac{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]}. \quad (11)$$

Equation (11) can be rewritten as

$$N_D = \frac{N_i}{N_0} = \int_{E=0_+}^{\infty}\frac{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]} \quad (\text{for } E \geq 0_+)$$
$$+ \int_{E=-\infty}^{0_-}\frac{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]} \quad (\text{for } E \leq 0_-)$$

which can be written as

$$N_0 = \frac{1}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}$$
$$N_D = N_{D_1}(E \geq 0_+) + N_{D_2}(E \leq 0_-), \quad (12)$$

where

$$N_{D_1}(E \geq 0_+) = \int_{E=0_+}^{\infty}\frac{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]} \quad (13)$$

and

$$N_{D_2}(E \leq 0_-) = \int_{E=-\infty}^{0_-}\frac{\gamma^{1/2}(E,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(E,\eta_e)\,\mathrm{d}E}{\left[1+\exp\left(\frac{E-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]}. \quad (14)$$

For $E_1 = -E$ as a substitution in eq. (14), we can rewrite it as

$$N_{D_2}(E_1 \geq 0_-) = -\int_{E_1 \geq 0_-}^{\infty}\frac{\gamma^{1/2}(-E_1,\eta_e)\,\frac{\mathrm{d}\gamma}{\mathrm{d}E}(-E_1,\eta_e)\,\mathrm{d}E_1}{\left[1+\exp\left(\frac{-E_1-E_\mathrm{f}}{k_\mathrm{B}T}\right)\right]} \quad (15)$$

and eq. (12) becomes

$$N_D = N_{D_1}(\infty > E \geq 0_+) + N_{D_2}(\infty > E_1 \geq 0_-) \quad (16)$$

as the representation of the total FIs.

Now, we shall evaluate the two integrals N_{D_1} $(E \geq 0_+)$ in eq. (13) and $N_{D_2}(E_1 \geq 0_-)$ in eq. (15) separately and obtain N_D using eq. (16). Doing some algebraic manipulations, we can express N_{D_1} (eq. (13)) as

$$N_{D_1} = -q\eta_e^{3/2}\int_{x=0}^{\infty}\frac{F(x)\,\mathrm{d}x}{\exp(rx)-q}, \quad (17)$$

where

$$x = E/\eta_e,$$
$$-q = \exp\left(\frac{E_\mathrm{f}}{k_\mathrm{B}T}\right) = \exp(\eta)$$

and

$$r = \frac{\eta_e}{k_\mathrm{B}T}$$
$$F(x) = \gamma^{1/2}(x)\,\frac{\mathrm{d}\gamma(x)}{\mathrm{d}(x)} \quad (18)$$

and

$$\gamma(x) = \frac{1}{2}x[1+\mathrm{erf}(x)] + \frac{1}{2\pi^{1/2}}\exp(-x^2) \quad (19)$$
$$\frac{\mathrm{d}\gamma(x)}{\mathrm{d}(x)} = \frac{1}{2}\,[1+\mathrm{erf}(x)]. \quad (20)$$

We have seen earlier that $\gamma(x)$ as well as $\frac{\mathrm{d}\gamma(x)}{\mathrm{d}(x)}$ are continuous function. So, $F(x)$ in eq. (18) is also a continuous function of x. Therefore, its derivatives of any order will exist. Then, we can write

$$F(x) = \sum_{p=1}^{\infty}\frac{x^{p-1}}{(p-1)!}\left\{\left.\frac{\mathrm{d}^{p-1}(F(x))}{\mathrm{d}x^{p-1}}\right|_{x\to 0_+}\right\}. \quad (21)$$

This kind of expansion of $F(x)$ is feasible, because $\frac{\mathrm{d}^{p-1}(F(x))}{\mathrm{d}x^{p-1}}|_{\chi\to 0_+}$ exists. This representation of $F(x)$ is an approximate one and $\frac{d^{p-1}(F(x))}{dx^{p-1}}|_{\chi\to 0_+}$ is a numerical value. Substituting eq. (21) into eq. (17), we find [17]

$$N_{D_1} = -q\eta_e^{3/2}\sum_{p=1}^{\infty}\frac{F(0)^{(p-1)}}{(p-1)!}\int_{x=0}^{\infty}\frac{x^{p-1}dx}{\exp(rx)-q}$$
$$= -q\eta_e^{3/2}\sum_{p=1}^{\infty}\left[\frac{F(0)^{(p-1)}}{(p-1)!}\left\{\Gamma p r^{-p}\Phi(q,p;1)\right\}\right], \quad (22)$$

where $\Phi(q, p; 1)$ is the confluent hypergeometric function [16,17].

Putting,

$$p = j + 1,$$
$$-q = \exp(\eta) = \exp\left(\frac{E_f}{k_B T}\right)$$

and

$$r = \frac{\eta_e}{k_B T}$$

into eq. (22), we get

$$N_{D_1} = \sum_{j=0}^{\infty} C_j(\eta_e, k_B T)\cdot \bar{F}_J(\eta)\,, \quad (23)$$

where

$$C_j(\eta_e, k_B T) = (k_B T)^{3/2}\left\{\left(\frac{k_B T}{\eta_e}\right)^{j-1/2} F_{(0)}^{(j)}\right\} \quad (24)$$

and

$$\bar{F}_J(\eta) = \exp(\eta)\Phi\{-\exp(\eta), (J+1); 1\}\,. \quad (25)$$

We termed $C_j(\eta_e, k_B T)$ as the coefficient of $\bar{F}_J(\eta)$ due to heavy doping conditions.

$F_{(0)}^{(j)} = F_{(x)}^{(j)}|_{x\to 0_+}$ for $j = 0, 1, 2, 3, \ldots$ are the derivative of $F(x)$ of order j (for $j = 0, 1, 2, 3, \ldots$). The derivatives can be carried out either analytically or numerically using the computer, and then evaluated at $x \to 0_+$. However, in the present condition, we have obtained the values of $F_{(0_+)}^{(j)}$, for $j = 0, 1, 2, 3, 4$ and 5, analytically. It is also obvious from eqs (24) and (25) that the coefficient $C_j(\eta_e, k_B T)$ is a real value like $\bar{F}_J(\eta)$. Therefore, $[\frac{N_{D_1}}{(k_B T)^{3/2}}] = D_{(1/2)R}$ is the modified FI of the conventional case and it is a real function of η, η_e and $k_B T$. Thus, we have from eqs (23) and (24)

$$D_{(1/2)R}(\eta, \eta_e, k_B T) = \frac{N_{D_1}}{(k_B T)^{3/2}} = \frac{N_i}{N_0\,(k_B T)^{3/2}}$$
$$= \sum_{j=0}^{\infty}\left(\frac{k_B T}{\eta_e}\right)^{j-\frac{1}{2}} F_{(0)}^{(j)}\left\{\bar{F}_J(\eta)\right\}. \quad (26)$$

It may be noted that $F_{(0)}^{(j)}$ and $\bar{F}_J(\eta)$ are two separate functions. $F_{(0)}^{(j)}$ is a numerical constant and $\bar{F}_J(\eta)$ is a function of η. By the analytical derivatives of $F(x)$ of order j, i.e.,

$$F_{(x)}^{(j)} = \frac{d^j F(x)}{dx^j}$$

and then evaluated $F_{(x)}^{(j)}$ at $x \to 0_+$, for $j = 0, 1, 2, 3, 4$ and 5, we obtain

$$F_{(0)}^{(0)} = 0.265562983$$
$$F_{(0)}^{(1)} = 0.3660464833$$
$$F_{(0)}^{(2)} = 0.5881162699$$
$$F_{(0)}^{(3)} = -0.8575662236$$
$$F_{(0)}^{(4)} = -2.042394238$$
$$F_{(0)}^{(5)} = -3.64719107. \quad (27)$$

It is obvious from above that $F_{(0)}^{(j)}$; $j = 0, 1, 2, 3, 4, 5$, are the numerical values independent of all parameters η, η_e, $k_B T$, but depends only on the nature of the function $F(x)$. We shall now evaluate N_{D_2} $(E_1 \geq 0_-)$ (eq. (15)). Applying eqs (8) and (8a) into eq. (15)), we can write

$$N_{D_2} = \int_{E_1=0}^{\infty} dE_1 \frac{\left\{\frac{1}{2}E_1\left(1-\text{erf}\left(\frac{E_1}{\eta_e}\right)\right) - \frac{\eta_e}{2\pi^{1/2}}\exp\left(-\frac{E_1^2}{\eta_e^2}\right)\right\}^{1/2} * \frac{1}{2}\left(1-\text{erf}\left(\frac{E_1}{\eta_e}\right)\right)}{1+\exp\left(\frac{-E_1-E_f}{k_B T}\right)}. \quad (28)$$

Putting

$$\omega = \frac{E_1}{\eta_e},\quad r = \frac{\eta_e}{k_B T},\quad \eta = \frac{E_f}{k_B T}$$

and

$$-q_1 = \exp(-\eta)$$

into eq. (28), we can rewrite eq. (28) as

$$N_{D_2} = \eta_e^{3/2} \int_{\omega=0}^{\infty} \frac{\exp(r\omega)\, G(\omega)\, \mathrm{d}\omega}{\exp(r\omega) - q_1} \tag{29}$$

where

$$G(\omega) = [W(\omega)]^{1/2} \frac{\mathrm{d}W(\omega)}{\mathrm{d}(\omega)} \tag{30}$$

$$W(\omega) = \left[\frac{1}{2}\omega(1 - \mathrm{erf}(\omega)) - \frac{1}{2\pi^{1/2}}(\exp(-\omega^2))\right] \tag{31}$$

$$\frac{\mathrm{d}W}{\mathrm{d}\omega} = \frac{1}{2}[1 - \mathrm{erf}(\omega)]. \tag{32}$$

Further simplifying (29) we get

$$N_{D_2} = \eta_e^{3/2}[I_{21} + I_{22}], \tag{33}$$

where

$$I_{21} = \int_{\omega=0}^{\infty} G(\omega)\, \mathrm{d}\omega \tag{34}$$

and

$$I_{22} = q_1 \int_{\omega=0}^{\infty} \frac{G(\omega)\, \mathrm{d}\omega}{\exp(r\omega) - q_1}. \tag{35}$$

Substituting eq. (30) into eq. (34) and then integrating and putting the limits, we can get

$$I_{21} = iG_{00}, \tag{36}$$

where G_{00} = the numerical constant = 0.09988524586 and $i = \sqrt{-1}$.

The numerical constant, G_{00}, is a fixed value and is independent of the parameters, η, η_e and $k_B T$. In eq. (35), $G(\omega)$ is given by (30) and it is a continuous function of ω. Therefore, its derivatives of any order will exist. On this assumption, we can expand $G(x)$ as

$$G(x) = \sum_{p=1}^{\infty} \frac{x^{p-1}}{(p-1)!} \left\{\frac{\mathrm{d}^{p-1}}{\mathrm{d}x^{p-1}}[G(x)]\right\}\Bigg|_{x\to 0_-}, \tag{37}$$

$\frac{\mathrm{d}^{p-1}}{\mathrm{d}x^{p-1}}(G(x))$ is the $(p-1)$th derivative of $G(x)$ and then it is evaluated at $x \to 0_-$.

Now, combining eqs (35) and (37), we can write

$$I_{22} = q_1 \sum_{p=1}^{\infty} \left[\left\{\frac{\mathrm{d}^{p-1}}{\mathrm{d}x^{p-1}}(G(x))\Bigg|_{x\to 0_-}\right\} * \int_{x=0}^{\infty} \frac{x^{p-1}}{(p-1)!} \frac{\mathrm{d}x}{(\exp(rx) - q_1)}\right] \tag{38}$$

$$= q_1 \sum_{p=1}^{\infty} r^{-p} \Phi(q_1, p; 1) \cdot \left\{\frac{\mathrm{d}^{p-1}}{\mathrm{d}x^{p-1}}(G(x))\Bigg|_{x\to 0_-}\right\}, \tag{39}$$

where $\Phi(q_1, p; 1)$ is the confluent hypergeometric function [16,17].

Writing $G^{(p-1)}(0)$ as the $(p-1)$th derivative of $G(x)$ and then evaluated at $x \to 0_-$, we have

$$G^{(p-1)}(0) = \frac{\mathrm{d}^{p-1}}{\mathrm{d}x^{p-1}}(G(x))\Bigg|_{x\to 0_-}. \tag{40}$$

By the analytical derivatives of $G(x)$ of order $(p-1)$th, and then evaluated at $x \to 0_-$, we get

$$G^{(0)}(0) = i(0.265562983)$$
$$G^{(1)}(0) = i(-0.5350048035)$$
$$G^{(2)}(0) = i(0.58861162699)$$
$$G^{(3)}(0) = i(0.5579104857)$$
$$G^{(4)}(0) = i(-2.573520205)$$

and

$$G_{00} = i(0.09988524586), \tag{41}$$

where $i = \sqrt{-1}$.

After some algebraic manipulations, we express I_{22}, combining eqs (39), (40) and (41) as

$$I_{22} = -\exp(-\eta) \sum_{j=0}^{\infty} k_j(\eta_{e,}(k_B T)) \times \Phi\{-\exp(-\eta), (j+1); 1\}, \tag{42}$$

where

$$k_j(\eta_{e,} k_B T) = \left\{\left(\frac{k_B T}{\eta_e}\right)^{j+1} G^{(j)}(0)\right\} \tag{43}$$

and $G^{(j)}(0)$, for $j = 0, 1, 2, 3, 4$ are given by eq. (41).

Combining (33), (36), (42) and (43), we get

$$\begin{aligned} N_{D_2} &= i\left\{\eta_e^{3/2} G_{00}\right\} - \eta_e^{3/2} \exp(-\eta) \times \sum_{j=0}^{\infty}\left[\left(\frac{k_B T}{\eta_e}\right)^{3/2}\left[\left(\frac{k_B T}{\eta_e}\right)^{j-1/2}(G^{(j)}(0))\right] * \Phi(-\exp(-\eta), (\mathrm{j}+1); 1)\right] \\ &= (k_B T)^{3/2}\left[\left\{\left(\frac{k_B T}{\eta_e}\right)^{-3/2} iG_{00}\right\} - \exp(-\eta)\left\{\sum_{j=0}^{\infty}\left[\left(\frac{k_B T}{\eta_e}\right)^{j-1/2} G^{(j)}(0)\right] * \Phi(-\exp(-\eta), (j+1); 1)\right\}\right], \end{aligned} \tag{44}$$

where $i = \sqrt{-1}$.

Therefore, using eqs (41) and (44), we get

$$\frac{N_{D_2}}{(k_B T)^{3/2}} = i \cdot D_{(1/2)\,\mathrm{Im}}(\eta, \eta_e, (k_B T)) = S_1 - \exp(-\eta) S_2, \quad (45)$$

where

$$S_1 = \left(\frac{k_B T}{\eta_e}\right)^{-3/2} i G_{00} \quad (46)$$

$$S_2 = \sum_{j=0}^{\infty} \left[\left(\frac{k_B T}{\eta_e}\right)^{j-1/2} G^{(j)}(0) * \Phi(-\exp(-\eta), (j+1); 1) \right] \quad (47)$$

$D_{(1/2)\,\mathrm{Im}} \equiv$ Imaginary functions of degenerately doped FI.

Using eqs (16), (26) and (45) we get

$$\frac{N_D}{(k_B T)^{3/2}} = \frac{N_{D_1}}{(k_B T)^{3/2}} + \frac{N_{D_2}}{(k_B T)^{3/2}} = D_{(1/2)\,\mathrm{R}} + i D_{(1/2)\,\mathrm{Im}} \quad (48)$$

and writing

$$D_{1/2}(\eta, \eta_e, k_B T) = \frac{N_D}{(k_B T)^{3/2}},$$

we have

$$D_{1/2}(\eta, \eta_e, k_B T) = D_{(1/2)\,\mathrm{R}}(\eta, \eta_e, k_B T) + i D_{(1/2)\,\mathrm{Im}}(\eta, \eta_e, k_B T) \quad (49)$$

with $i = \sqrt{-1}$.

Thus, it is seen that the FI, $D_{1/2}(\eta, \eta_e, k_B T)$, for the DOS functions of the degenerately doped semiconductor with band-tailing is of complex nature, with a real ($D_{(1/2)\,\mathrm{R}}$) and an imaginary $D_{1/2\,\mathrm{Im}}$ terms. The DOS being the probability of availability of carriers in a band, it must be a real valued function given by

$$D_{1/2}(\eta, \eta_e, k_B T) = \sqrt{\left(D_{(1/2)\,\mathrm{R}}\right)^2 + \left(D_{(1/2)\,\mathrm{Im}}\right)^2} * \cos(\theta), \quad (50)$$

where

$$\theta = \tan^{-1}\left(\frac{D_{(1/2)\,\mathrm{Im}}}{D_{(1/2)\,\mathrm{R}}}\right) \quad (51)$$

and $D_{1/2}(\eta, \eta_e, k_B T)$ indicates an oscillatory function of $\eta, \eta_e, k_B T$.

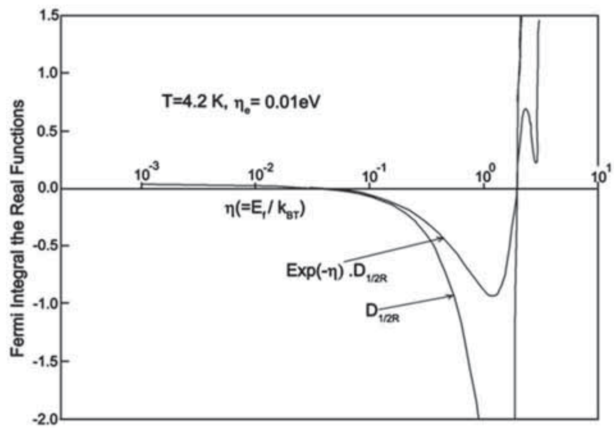

Figure 1. Variations of the Fermi integral of the real functions, $D_{(1/2)\,\mathrm{R}}$, for the DOS of the degenerately doping semiconductor with band-tailing as against η $(=E_f/k_B T)$ at $T = 4.2$ K and $\eta_e = 0.01$ eV.

3. Results and discussions

In figure 1, we have plotted the real part of FI, $D_{(1/2)\,\mathrm{R}}$ as a function of η at $T = 4.2$ K with $\eta_e = 0.01$ eV for the DOS of heavily doped system under the band-tailing condition. Initially, when $\eta = 1.0 \times 10^{-3}$, $D_{(1/2)\,\mathrm{R}}$ maintained small positive value; with the increase of η, FI moves towards negative value. The negative fall-off is in the form of tails and finally reaches to a maximum value. Therefore, with further increase of η, $D_{(1/2)\,\mathrm{R}}$ moved towards positive value showing oscillations. It is clear from figure 1 that the shape of the tail is of exponential nature. Finally, as $D_{(1/2)\,\mathrm{R}}$ moves towards positive values, the transition becomes sharp. As shown in figure 1, the negative values of FIs indicate that there exists a band gap in a semiconductor even with heavy doping, forming band tail. The graphs plotted for $D_{(1/2)\,\mathrm{R}}$ and $\exp(-\eta) D_{(1/2)\,\mathrm{R}}$ showed oscillations.

In figure 2, we have plotted FI for the imaginary functions, $D_{(1/2)\,\mathrm{Im}}$, for the DOS of the heavy doping case under band-tailing condition against η at $T = 4.2$ K and $\eta_e = 0.01$ eV. The graph exhibits two parts, a fixed line with dotted curve, corresponding to $iG_{00} = i(0.09988524586)$ gives $G_{00}(\frac{k_B T}{\eta_e})^{-3/2} = 14.4579983$, $i = \sqrt{-1}$. This constant line indicates that there is a fixed forbidden gap in a semiconductor for an imaginary band. The solid curve has a slowly decreasing value with a sharp well in the graph. This curve moves upwards with increasing η and finally merges with the dotted line for very large values of η. The fall-off of the solid curve indicates that there exists a new band gap within the forbidden zone supporting this result [18].

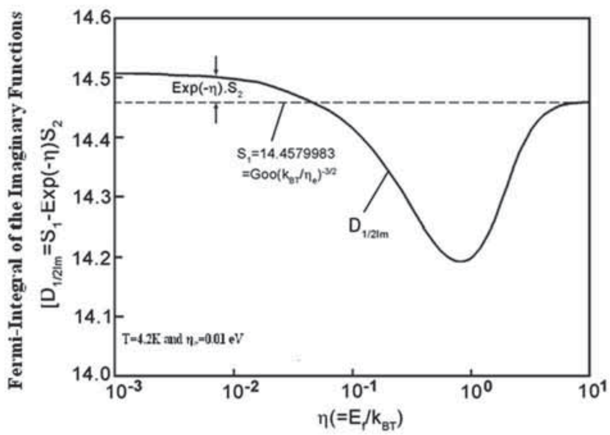

Figure 2. Variations of the Fermi integral of the imaginary functions, $D_{(1/2)\,\mathrm{Im}}$, for the DOS of the degenerately doping semiconductor with band-tailing vs. $\eta\ (=E_\mathrm{f}/k_\mathrm{B}T)$ at $T = 4.2$ K and $\eta_e = 0.01$ eV.

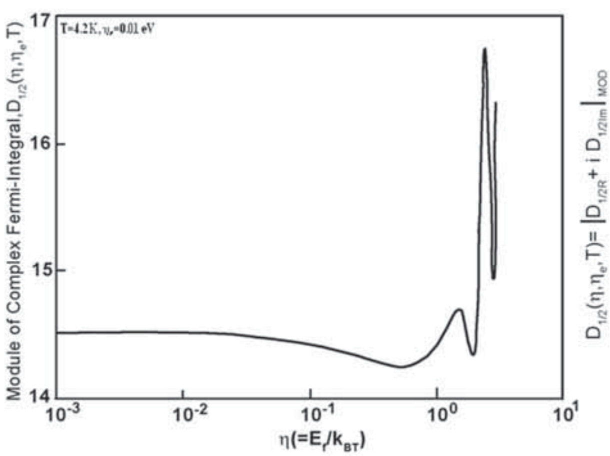

Figure 3. Variations of the modulus of the complex functions $|D_{1/2}\,(\eta, \eta_e, k_\mathrm{B}T)|$ vs. $\eta\ (=E_\mathrm{f}/k_\mathrm{B}T)$ at $T = 4.2$ K and $\eta_e = 0.01$ eV.

In figure 3, modulus of the complex functions, $|D_{1/2}(\eta, \eta_e, T)|$ has been plotted as a function of $\eta\,(= E_\mathrm{f}/k_\mathrm{B}T)$. The graph also exhibits an oscillatory nature. The oscillations are not uniform, as expected, because the nature of variation of the confluent hypergermetric function [16] is superimposed with natural oscillation due to cosine function of angle $\theta\,[= \tan^{-1}(D_{(1/2)\,\mathrm{Im}}/D_{(1/2)\,\mathrm{R}})]$.

Figure 4 shows the plot of the angle θ (in radian) given in eq. (51) as a function of η. This graph shows that θ increases with increase in η and reaches a peak value at $\eta = 1.5$ and finally decreases. The peak value of $\theta = \pi/2$ corresponds to the resonance in θ with $\eta = 1.5$. The resonance indicates that $D_{(1/2)\,\mathrm{Im}}$ and $D_{(1/2)\,\mathrm{R}}$ differ by an angle $\pi/2$ (radian) when $\tan\theta$ tends to very large values.

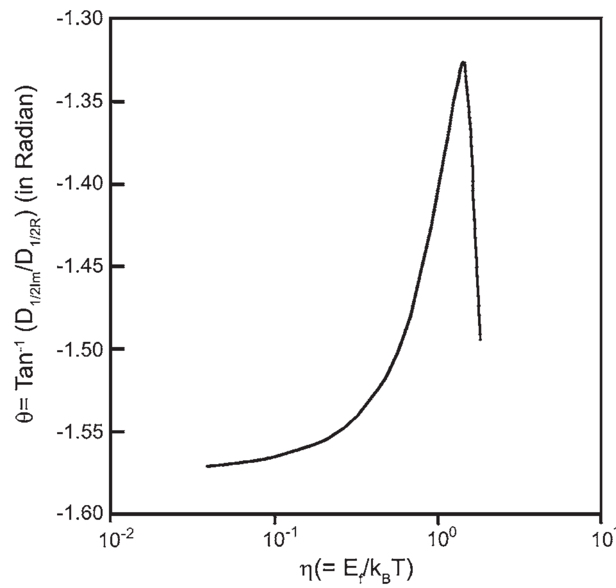

Figure 4. Variations of the angle $\theta = \tan^{-1}(D_{(1/2)\,\mathrm{Im}}/D_{1/2\,\mathrm{R}})$ (in radian) with respect to $\eta\ (=E_\mathrm{f}/k_\mathrm{B}T)$ at $T = 4.2$ K and $\eta_e = 0.01$ eV.

4. Conclusions

We have made exact calculations for the FIs for degenerately doped semiconductors. Such exact calculations provide FI as a complex function in the case of heavily doped semiconductors with band tailing. As the FI is involved with DOS and Fermi–Dirac functions, the present results of our theoretical investigation might provide more accurate explanation of the transport phenomena in semiconductors along with new applications in dynamic magnetic susceptibility, specific heat at low temperature etc., where, DOS as well as the Fermi–Dirac distributions are directly related. The Einstein relation $(=D/\mu$, where D is the diffusion coefficient and μ is the mobility) can be computed from the present model exactly with a complex nature of its variations which will be discussed elsewhere.

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