Fermi-statistics revisited for Degenerately Doping with impurities forming Band-tail

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Keywords: Fermi-statistics, Non-degenerate, Degenerate dopings, Band-tails, Maxwell-Boltzmann's statistics, Semiconductor.

Abstract

Fermi-Dirac (FD) distribution function is generally known as Fermi-Statistics (FS) applicable for non-degenerately doped semiconductors, because in this case, the band structure prevails. As the dopings are increased strongly, the semi-conductor is degenerate and its band-structure is perturbed with the formation of band-tail. It is convinced that the FD distribution function must be revisited for modification under this present condition. In the present attempt, modified Fermi-statistics has been derived for the degenerate semiconductor having band-tail due to Gaussian distribution of the impurity potential. Unlike FS for non-degenerate semi-conductor, which is an exponential function, our present result is general, involving exponential and error functions with series summation solution. In the classical limits, the normal FS and the Maxwell-Boltzmann's (MB) distribution functions can be retrieved for non-degenerate semiconductor from our results. Also, MB distribution function for degenerate dopings are obtained from our approximate results of the general conclusions.

1. Introduction

It is well-known that electrons and holes are free particles in conduction band (CB) and valence-band (VB) under thermal equilibrium with the lattice. At absolute zero temperature, the energy of an electron is at ground state. At a higher temperature, the particles are moving with the thermal energy, when no external fields are applied. So, in thermal equilibrium, the probability of a given energy state, being occupied, will be a function of temperature. Also, by Pauli Exclusion Principle [1], the occupation probability of an electron at an energy state is ½. Therefore, in thermal equilibrium with the lattice, the electron probability distribution function among the available energy levels is named Fermi-Dirac statistics [2-4]. This function, giving the occupancy of the energy levels, (also often called Fermi-Statistics) is [5]:

$$F(E, E_f, T) = \frac{1}{\left\{1+\exp\left[\frac{E(\overline{k})-E_f}{k_B T}\right]\right\}} \quad \text{......... (1)}$$

where, $E(\overline{k})$ is the energy state at the wave-vector, $(\overline{k})$; E_f is the maximum available energy level, called Fermi-energy or Fermi-level, k_B is the Boltzmann's constant, T is the temperature.

In a lightly doped semiconductor, the band structure of a pure material may be assumed to prevail [4]. A semiconductor is said to be lightly doped or non-degenerate, when the condition, $(0.02 \leq (a_D.n_i^{1/3}) < 1.0)$ is satisfied [6], where a_D is the Bohr's radius of the impurity state and n_i is the impurity concentration. For the lightly doped, the potential wells associated with the impurity atoms are isolated from each other and the impurity potential, $V(\bar{r}) \approx 0.0$ at the local point $(\bar{r})$. Therefore, Eq. (1) is valid for the lightly doped semiconductors, when $E(\overline{k})$ remains same as the host materials, and E_f lies within the Forbidden band [4]. Here, we can approximately assume that the wave-function of the outer electrons of the impurity atom covers a large number of atoms of the host crystal. With the increase of impurity dopings, the semiconductor is degenerate for strongly doped condition. In this case, the concentration of impurity dopings satisfies the limits: $(a_D.n_i^{1/3} > 1.0)$ [6]. The nature of impurity levels differ radically in strongly doped and in lightly doped materials and for the former case, the impurity levels are transformed into Gaussian bands [4]. Electrons occupying these bands, take part in transport phenomena [4]. For this, the impurity potential, $V(\bar{r})$ of the wells has some non-zero value and the Gaussian distribution of the impurity potential is given by [7, 8].

$$G(V(\bar{r})) = \frac{\exp\left[-\frac{V^2(\bar{r})}{\eta_e^2}\right]}{\sqrt{\pi\eta_e^2}} \quad \text{......... (2)}$$

where, η_e is the variance of G (V) and is known as impurity screening potential. The amount of impurities doped is decided by the parameter, η_e. For $\eta_e \rightarrow 0$, is the undoped semiconductor.

It has been experimentally observed that band-tail exists in semiconductor devices made of degenerately doped materials [9-12]. This is because of the Gaussian band impurity potential, which interacts with the electrons in the conduction band (CB), so that CB is perturbed forming band tails. For the lightly doped semiconductor, no tail is present and hence the band remains un-perturbed. Therefore, it is expected that the Fermi statistics (FS) must be different for the degenerately doped semiconductor as compared to the same (FS) for un-perturbed band state. To the best of our knowledge, such a study of (FS) has not been done as yet in literatures for degenerate semiconductors. In what follows, we shall provide the derivation of the FS for degenerately doped with perturbation to the semiconductor. The results obtained are general and exact and are involved with exponential and error functions having series summation solution.

2. Derivation of the Fermi-statistics for degenerately doped semiconductors.

Assuming an un-perturbed parabolic band, the volume occupied by the impurities enclosed by the Fermi-surface, is fixed. With the formation of a tail, the total volume covered by the impurities is the sum of the Fermi-surface of the un-perturbed band region and the Fermi-surface bounded by the tail region. So, for an extrinsic semiconductor, the volume of the available occupied states are more that of the volume for the intrinsic semiconductor with non-degenerately doping system. Therefore, it is expected that the probability that the impurities can occupy the energy state with tail is more than that of the no-tail system. For the estimation of this probability, an interaction of the impurity band with the energy state of the FD function must be considered with the Gaussian distribution function and the Schrödinger equation [4];

$$E = V(\bar{r}) + \frac{\hbar^2 k^2}{2m^*} \qquad \text{.........(3)}$$

$$E(\overline{k}) = \frac{\hbar^2 k^2}{2m^*} = E - V(\bar{r}) \qquad \text{......... (4)}$$

where, $\hbar$ is the reduced Planck's constant, m^* is the effective electron mass and E is the total electron energy. Equation (4) is valid for degenerately doped semiconductor, assuming a non-zero value of V $(\bar{r})$. Therefore, the Fermi-statistics for the degenerately doped semiconductor, when the kinetic energy (K.E.) is taken at a local point $(\bar{r})$, is [5-6].

$$F(E(\overline{k}), E_f, T) = \frac{1}{1+\exp[\frac{\left(\frac{\hbar^2 k^2}{2m^*} - -E_f\right)}{k_B T}]} \qquad \text{......... (5)}$$

Electrons move with the K. E. in a semiconductor at thermal equilibrium. Therefore, using Eqs. (4) and (5), we get

$$F(\bar{E}, V, T) = \frac{1}{1+\exp[\frac{(E - E_f) - V(\bar{r})}{k_B T}]} \qquad \text{......... (6)}$$

where, $\bar{E}$ = E- E_f ……… (7)

Therefore, Eq. (6) represents the occupation probability for a degenerately doped system, when the impurities are denoted by V ($\bar{r}$). For different values of V ($\bar{r}$), we have different occupation probability.

Let D ($\bar{E}$,η_e, T) be the total occupation probability of the degenerately doping semiconductor. This can be obtained by taking the convolution of F ($\bar{E}$, V, T), and G (V ($\bar{r}$)), in order to consider the interaction of the energy state and the potential energy.

Thus, we have,

$$D(\bar{E}, \eta_e, T) = \langle F[(\bar{E} - V(\bar{r})), T].\,G(V(\bar{r}))\rangle_{\text{average over } V(\bar{r})}$$

$$= \int_{V=-\infty}^{\infty} F[(\bar{E} - V), T]\,.\,\frac{1}{\sqrt{\pi\eta_e^2}}\,.\,\exp\left(-\frac{V^2}{\eta_e^2}\right).dV$$

$$= \frac{1}{\sqrt{\pi\eta_e^2}}\,.\int_{V=-\infty}^{\bar{E} = E - E_f} \frac{\exp\left(-\frac{V^2}{\eta_e^2}\right).dV}{1+\exp\left[\frac{\bar{E}-V}{k_B T}\right]} \quad \text{……… (8)}$$

It is noticed that the limits of V ($\bar{r}$) exists from -∞ to +∞ and the maximum value of V ($\bar{r}$) is taken as $\bar{E}$ = (E- E_f).

Therefore, Eq. (8) is the representation of the Fermi-Statistics for degenerately doped semiconductor having band-tail.

With the substitution, x= $\frac{\bar{E}-V}{k_B T}$ in Eq. (8) and carrying out some algebraic manipulations, we get,

$$D(\bar{E}, \eta_e, T) = \frac{k_B T/\eta_e}{\sqrt{\pi}} \int_{x=0}^{\infty} \frac{\exp\left[-\left(\frac{\bar{E}}{\eta_e} - \frac{k_B T.x}{\eta_e}\right)^2\right]}{1+\exp(x)} \quad \text{……… (9)}$$

Eq. (9) can be re-written as

$$D(\bar{E}, \eta_e, T) = \frac{k_B T/\eta_e}{\sqrt{\pi}} \sum_{m=1}^{\infty} (-1)^{m-1}.I_m \quad \text{………..(10)}$$

where, m is the number of terms in the series.

$$I_m = \int_{x=0}^{\infty} dx.\exp(-m.x).\exp\left[-\left(\frac{\bar{E} - k_B T.x}{\eta_e}\right)^2\right] \quad \text{……… (11)}$$

The solution of the integration in Eq. (11) is given by [13]

$$I_m = \frac{\sqrt{\pi}}{2}.\left(\frac{\eta_e}{k_BT}\right).\exp\left[-\left(\frac{\bar{E}.m}{k_BT}\right) + \left(\frac{\eta_e}{2k_BT}\right)^2 m^2\right].\ \mathrm{Erfc}\left[-\left\{\frac{\bar{E}}{\eta_e} - \left(\frac{\eta_e}{2k_BT}\right)m\right\}\right] \quad \ldots\ldots\ldots (12)$$

Substituting I_m from Eq. (12) into Eq. (10), the final results are obtained, independent of $V(\bar{r})$, as

$$D(\bar{E}, \eta_e, T) = 1/2 \sum_{m=1}^{\infty}\left\{(-1)^{m-1}.\exp\left[-\left(m.\frac{\bar{E}}{k_BT}\right) + \left(\frac{\eta_e}{2k_BT}\right)^2 m^2\right]*\left[1+\mathrm{erf}\left(\frac{\bar{E}}{\eta_e} - \left(\frac{\eta_e}{2k_BT}\right)m\right)\right]\right\} \quad \ldots\ldots\ldots(13)$$

where, [13]

Erfc(z) = 1- erf(z) ≡ complementary error function

and erf(-z) = -erf(z) ≡ error function, ... (14)

Equation (13) is the required expression containing exponential and error functions (erf(z)) with a series summation solution for Fermi-statistics under degenerately doped system; the degree of degeneracy of the dopings being denoted by η_e.

Several limiting cases:

(a) We have seen earlier that for an un-doped semiconductor, $\eta_e \to 0$. Under this limiting condition, we find from Eq.(13)

$$D(\bar{E}, \eta_e, T) = \frac{\exp\left(-\frac{\bar{E}}{k_BT}\right)}{1+\exp\left(-\frac{\bar{E}}{k_BT}\right)}$$

$$= \frac{1}{\left[1+\exp\left(\frac{E-E_f}{k_BT}\right)\right]} \quad \ldots\ldots\ldots(15)$$

≡ Conventional Fermi-statistics for un-doped case [4].

Therefore, we conclude that $D(\bar{E}, \eta_e, T)$ (Eq.(13)) is the Fermi-statistics for degenerately doped semiconductor.

(b) Equation (13) can be further simplified under limiting condition:

Approximate solution to error function, erf(z), appearing in Eq.(13) can be given by [13] erf(z) ≈ $\{1 - [a_1 t + a_2 t^2 + a_3 t^3].\exp(-z^2)\}$ ……… (16)

z= $[\frac{\bar{E}}{\eta_e} - \left(\frac{\eta_e}{2k_BT}\right).m]$ ……….(17)

t= $\frac{1}{(1+p.z)}$,

and p= 0.47047, a_1= 0.34802, a_2= - 0.09587, a_3= 0.74785

Using Eqs. (16) and (17), we can approximately compute erf(z) for given values of $\bar{E}$,η_e, T and m. The computed erf(z) value can be substituted into Eq.(13) to get the value of D ($\bar{E}$,η_e, T).

(c) Limiting case: Assume that 0<η_e<1.0

$z^2 \approx (\frac{\bar{E}}{\eta_e})^2$ >>1.0

So that $(\frac{\bar{E}}{\eta_e})^2$ >> 1.0 and $\left(\frac{\eta_e}{2k_BT}\right)$ < 1.0

This is the moderately doping case but not the non-degenerate or un-doped condition. Therefore, for the above approximations, we get

and hence erf(z) ≈ 1.0 ……… (18)

Therefore, from Eqs.(13), (16) and (18), with moderately dopings, we obtain:

D ($\bar{E}$,η_e, T)≈ $\sum_{m=1}^{M}\{(-1)^{m-1}$. exp [-($m.\frac{\bar{E}}{k_BT}$) + ($\frac{\eta_e}{2k_BT}.m)^2$] ……… (19)

Equation (19) represents the Fermi-statistics for moderately doping system; here M is the maximum value of m, so that right hand side converges.

(d) Limiting case: $(\frac{\eta_e}{2k_BT})^2$ << 1.0 that is for very low doping condition: we arrive at Eq. (15) from Eq. (19).

Also, with this limiting range of dopings, and for m=1, (the first term in the summation series), we obtain:

D ($\bar{E}$,η_e, T)≈ exp[- ($\frac{E-E_f}{k_BT}$)] ……… (20)

Equation (20) shows that Maxwell-Boltzmann's distribution function (MB) [14], derived from our general results and is valid for non-degenerate semiconductor.

(e) Taking m=1 in Eq.(19) and $(\frac{\eta_e}{2k_BT})$<1.0, the Maxwell-Boltzmann's distribution function with moderately doped condition can be written as

D ($\bar{E}$,η_e, T) ≈ exp[- $\left(\frac{E-E_f}{k_BT}\right) + (\frac{\eta_e}{2k_BT})^2$] ……… (21)

3. Results and discussion

Table 1 shows a comparative study of FS and MB statistics under (i) un-doped and (ii) various moderately doping conditions of semiconductors, for different positive values of $\bar{E}$ = (E- E_f) (in (ev)) and η_e (eV) at T=300°K. Data presented in Table 1 are obtained by computer calculations using different equations, mentioned therein. For FS with moderately dopings, taking various values of $\bar{E}$ and η_e, D ($\bar{E}$,η_e, T) are calculated using Eq. (19). When F($\bar{E}$, T) are calculated using Eq. (15) for several values of $\bar{E}$, independent of η_e. Different calculated values are shown in Table 1. It is noticed that for η_e=0, F($\bar{E}$, T) and D ($\bar{E}$,η_e, T) provide the same values. This implies that Eq. (19) is the general representation of degenerately dopings and Eq. (15) is the special case of the former, with un-doped. Similarly, MB statistics with moderately dopings show different values using Eq. (21) as compared to Eq. (20) valid for un-doped case. Finally, we conclude that the positive values of $\bar{E}$ = (E- E_f) implies that E_f lies within forbidden band [4] for un-doped condition as expected from our earlier discussions.

Table 1. A comparative study of Fermi-Statistics(FS) and Maxwell- Boltzmann's(MB) statistics under (i) un-doped and (ii) Moderately doped system of semiconductors, for various values of $\bar{E}$ = (E- E_f) (eV) and η_e(eV) at T=300°K.

T=300°K	Fermi-Statistics (FS)				Maxwell-Boltzmann's Statistics(MB)		
	Un-doped	Moderately Doped			Un-doped	Moderately Doped	
$\bar{E}$ = (E- E_f) (ev), Eq.(7)	F($\bar{E}$,T), Eq.(15)	η_e(eV)	D ($\bar{E}$,η_e, T) Eq.(19)	Max. no. of Terms (M)	Exp $\left(-\frac{\bar{E}}{k_B T}\right)$ Eq.(20)	Exp[-$\left(\frac{\bar{E}}{k_B T}\right) + (\frac{\eta_e}{2k_B T})^2$] Eq.(21)	(M)
1.0×10^{-3}	0.490352422	0.0	0.4903211	250	0.962140143	0.962140143	1
		1.0×10^{-4}	0.490312576	,,		0.962143719	,,
		3.0×10^{-4}	0.49009341	,,		962172389	,,
		5.0×10^{-4}	0.479456216	,,		962229729	,,
1.0×10^{-2}	0.404692292	0.0	0.4046920564	33	0.67980361	0.67980361	1
		1.0×10^{-3}	0.404706746	,,		0.68005681	,,
		3.0×10^{-3}	0.40478453	,,		0.682085812	,,
		5.0×10^{-3}	0.372115791	,,		0.686162055	,,
5.0×10^{-2}	0.126777485	0.0	0.1267775	33	0.145183489	0.145183489	1
		1.0×10^{-3}	0.126808256	,,		0.145237565	,,
		3.0×10^{-3}	0.127054334	,,		0.145670906	,,
		5.0×10^{-3}	0.0.12754561	,,		0.146541446	,,
1.0×10^{-1}	0.020641244	0.0	0.0206431244	33	0.0210782439	0.0210782457	1
		1.0×10^{-3}	0.020650334	,,		0.0210860968	,,
		3.0×10^{-3}	0.0207081679	,,		0.0211490095	,,
		5.0×10^{-3}	0.0208242089	,,		0.0212753993	,,

4. Conclusions

Our results on Fermi-Statistics for degenerately dopings with impurities forming band-tail are worked out exactly and are general representations, with exponential and error functions having series summation solution. In the classical limiting cases, the conventional Fermi-statistics and the well-known Maxwell-Boltzman's distribution functions are obtained from our general results for non-degenerate and moderately doped semiconductors. These results might find more usefulness in the semiconductor device physics. Although the experimental verification of the basic content of this communication is not available in the literature to the best of our knowledge, the theoretical models as given here would be needful in analyzing the experimental data when they appear.

Acknowledgement:

The authors are grateful to the IACS, Kolkata, for providing library and computer facilities to complete the work.

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