Oscillatory Behavior of the Fermi-Integral and Density of States Functions in a Parabolic Band Semiconductor with Non-Degenerately Doped Impurities

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Abstract Exact quantum mechanical calculations of the Fermi-Integral (FI) associated with the density-of states (DOS) function for non-degenerately doped impurities in a parabolic band semiconductor were made. Unlike the results of previous approximate numerical calculations, present exact calculations showed novel oscillatory behavior of FI only for the positive values of the reduced Fermi-energies η (= E_f/k_BT), where E_f is the Fermi energy and k_B is the Boltzman constant and T is the absolute temperature. On the other hand, for the corresponding negative values, FI exhibited no oscillation. The observed non periodic oscillations were due to the Confluent Hypergeometric functional behavior of the presently derived expression of FI. Such oscillation might have massive effect on the dynamic behavior of quantum electronic properties of semiconductors as shown, for example, in case of Einstein relations (diffusivity-mobility ratio, DMR). Present finding also stimulate further investigation of DMR and similar other physical properties using the present exact expression of FI to explore the underlying new physics.

Keywords Fermi-Integral, Non-degenerately doped, Semiconductor, Density-of-state and Parabolic Band

1. Introduction

The Fermi-integral (FI) have been vastly used for the study of density of states (DOS) functions in semiconductors. It is well known that FI is involved with the integration of the product of DOS function and Fermi-Dirac (FD) distribution function for all possible values of the electron energy, E. The FI, generally defined by $F_i(\eta)$ [1-4], can be written as

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

where j is an integer or a fraction and $\eta = \frac{E_f}{k_B T}$ with E_f being the Fermi-energy. For the DOS function of a parabolic band, the value of j is $\frac{1}{2}$. Accordingly, the corresponding FI, $F_{1/2}(\eta)$ can be represented (using Eq(1) of [1-4]) in the form

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

 η is usually known as reduced Fermi-energy. Conventionally, $F_{1/2}(\eta)$ was evaluated numerically [1-6] for all practical purposes and the corresponding numerical

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Copyright © 2018 The Author(s). Published by Scientific & Academic Publishing This work is licensed under the Creative Commons Attribution International License (CC BY). http://creativecommons.org/licenses/by/4.0/ values were found to be comprised of only positive real values of the integrands. The numerical values are also available in a tabular form [1, 2] for both positive and negative values of η .

However, as the numerical integration is an approximate method, one cannot accurately find the exact values of reduced energy parameter, $\eta = \frac{E_f}{k_BT}$ related to many physical parameters of metals and semiconductors. Therefore, an exact solution of Eqs (1) and (2) are demanding to demonstrate the new electronic properties like Fermi-energy which in turn associated with the transport phenomena in doped semiconductors [6] as well as in nano-technology devices [5].

Therefore, an attempt has been made for an exact quantum mechanical calculation of the FIs $(\overline{F_j}(\eta) \text{ and } \overline{F_{\frac{1}{2}}}(\eta)$ applying a correct integration methods. Such calculations might reveal some interesting properties of $\overline{F_{\frac{1}{2}}}(\eta)$ which could not be visualized from the earlier numerical method of calculations discussed in this paper.

2. Theoretical Analysis

For an intrinsic semiconductor of parabolic band with lightly doped impurities, the band equation is given by:

$$E = \frac{\hbar^2 k^2}{2m_c}$$
(3)

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where \hbar is the reduced Planck's constant, \overline{k} is the wave vector, m_c is the un-perturbed conduction band edge effective electrons mass and E is the electron energy. The normal DOS function, N (E), can be written as

N (E)
$$=\frac{1}{2\pi^2} \cdot \left(\frac{2m_c}{\hbar^2}\right)^{\frac{3}{2}} \cdot E^{1/2}$$
 (4)

(energy range $E \rightarrow 0$ to $+\infty$).

For a non-degenerately doped semiconductor of carrier concentration, N_i , one can write the carrier statistical relation [4] as

$$N_{i} = \frac{1}{2\pi^{2}} \cdot \left(\frac{2m_{c}}{\hbar^{2}}\right)^{\frac{3}{2}} \int_{E=0}^{\infty} \frac{E^{\frac{1}{2}} dE}{1 + \exp \frac{E - E_{f}}{k_{B}T}}$$
(5)

 $= N_0 \times N_1$

where $N_0 = \frac{1}{2\pi^2} \cdot (\frac{2m_c}{\hbar^2})^{3/2}$ in Eq.5 and

$$N_D = \frac{N_i}{N_0} = \int_{E=0}^{\infty} \frac{E^{\frac{1}{2}} dE}{1 + \exp \frac{E - E_f}{k_B T}}$$
(6)

Eq. 6 can also be re-written as

$$\frac{N_D}{(k_B T)^{3/2}} = \frac{\sqrt{\pi}}{2} F_{1/2}(\eta) \tag{7}$$

where $x = \frac{E}{k_B T}$, $\eta = \frac{E_f}{k_B T}$ and

$$F_{1/2}(\eta) = \frac{2}{\sqrt{\pi}} \int_{x=0}^{\infty} \frac{x^{1/2} dx}{1 + \exp(x - \eta)}$$
(8)

Eq. (8) is identical with Eq. (2). The closed form of an exact solutions of $F_j(\eta)$ with special attention to j=1/2 for $F_{1/2}(\eta)$ can now be provided. We represent the exact solutions of Eq.(1) and Eq.(8) by $\overline{F_j}(\eta)$ and $\overline{F_{\frac{1}{2}}}(\eta)$, respectively. Performing some algebraic manipulations to the integrands in Eq.(1), an exactly form $\overline{F_j}(\eta)$ comes out to be

$$\overline{F}_{J}(\eta) = \frac{-\beta}{\Gamma\gamma} \int_{x=0}^{\infty} \frac{\exp(-x) \cdot x^{\gamma-1} \cdot dx}{1 - \beta \cdot \exp(-x)}$$
(9)

where $\beta = -\exp(\eta)$ and $\gamma = (j+1)$.

The new exact solution of Eq.(9) can be expressed [7] as

$$\overline{F}_{1}(\eta) = \exp(\eta) \cdot \Phi\{-\exp(\eta), (j+1); 1\} \text{ (for } j \ge 0.) \quad (10)$$

where the special function, $\Phi(a,b;z)$ is the Confluent Hypergeometric function with $a = -\exp(\eta)$, b=(j+1) and z=1 [7, 8]. For a given value of $\eta = \frac{E_f}{k_BT}$ and j, one can find the values of Φ (a,b; z) from the Table in [8]. However, for simple calculations for $\overline{F_j}(\eta)$, one can also use the series expansion of Φ (a,b; z) [7, 8]. For the series expansion of Φ (a,b; z) and the following relation [8]

$$\Phi (a,b; z) = 1 + \frac{a}{b} \cdot \frac{z}{1!} + \frac{(a)_2}{(b)_2} \cdot \frac{z^2}{2!} + \frac{(a)_3}{(b)_3} \cdot \frac{z^3}{3!} + \dots + \frac{(a)_n}{(b)n} \cdot \frac{z^n}{n!}$$
(11)

$$(a)_0 = 1$$
 and $(a)_n = a(a+1)(a+2)...(a+n-1)$ (12)

Substituting a=-exp (η); b= (j+1) and z=1, in Eqs.(11) and (12), the final exact solution of $\overline{F}_{j}(\eta)$ comes out to be

$$\overline{F}_{j}(\eta) = \exp(\eta). \left[1 - \frac{\exp(\eta)}{(j+1)} \cdot \frac{1}{1!} - \frac{\exp(\eta).((1 - \exp(\eta))}{(j+1)(j+2)} \cdot \frac{1^{2}}{2!} - \frac{\exp(\eta).((1 - \exp(\eta)).(2 - \exp(\eta))}{(j+1)(j+2)(j+3)} \cdot \frac{1^{3}}{3!} - .\text{to }\infty\right]$$
(13)

Eq. (13) represents the series solution to $\overline{F_j}(\eta)$ for any values of j and η . Thus, one can find the value of $\overline{F_j}(\eta)$ more accurately and conveniently than the conventional numerical approaches for $F_j(\eta)$ put forwarded earlier [1, 2]. For j=1/2, as a special case to the Fermi-integral, $\overline{F_j}(\eta)$, the series representation of the same can be given from Eq.(13) as

$$\overline{F}_{\frac{1}{2}}(\eta) = \exp(\eta) \cdot \left[1 - \frac{2}{3} \cdot \exp(\eta) - \frac{\exp(\eta) \cdot ((1 - \exp(\eta))}{3.5} \cdot \frac{2^2}{2!} - \frac{\exp(\eta) \cdot ((1 - \exp(\eta)) \cdot (2 - \exp(\eta))}{3.5.7} \cdot \frac{2^3}{3!} - \dots \cdot \cos \infty\right] (14a)$$

Now, for a given value of $\eta = \frac{E_f}{k_B T}$, we can compute $\overline{F}_{\frac{1}{2}}(\eta)$ from Eq.(14). $\overline{F}_{-1/2}(\eta)$ can also be easily computed from Eq.(13) with j=-1/2.

From Eq (14a) we find the exact form of the DOS, $S(\eta)$, as a function of reduced Fermi energy η as

$$S(\eta) = [\exp(-\eta). \bar{F}_{\frac{1}{2}}(\eta)] = \{1 - \frac{2}{3}, \exp(\eta) - \frac{\exp(\eta).((1 - \exp(\eta))}{3.5}, \frac{2^2}{2!} - \frac{\exp(\eta).((1 - \exp(\eta)).(2 - \exp(\eta))}{3.5.7}, \frac{2^3}{3!} - \dots + \cos \infty\} (14b)$$

The computed values of $\overline{F}_{\frac{1}{2}}(\eta)$ could be plotted as a function of η , for both positive and negative values which have been discussed below.

3. Results and Discussion

We demonstrate the variation of the calculated exact FI for the DOS as function of $\eta \ (=\frac{E_f}{k_BT})$ in the case of non-degenerately doped semiconductor. The values of FIs of half-integer order estimated by earlier classical calculation [1, 2] and those obtained from the present exact calculation are shown in Table 1 for comparison. The exact values of the function $\overline{F}_{\underline{1}}(\eta)$ calculated from the present series expansions of Eq. (14) is plotted in Figure 1. It is seen from the figure that the results of our present exact calculations for FI exhibits oscillations only for the positive values of η . On the other hand, for the negative values of η , no oscillation is exhibited. Earlier approximate numerical calculations of FI [1-6] did not, however, show any such oscillations. The nature of the said oscillations is not periodic like sinusoidal functions. That is, all the positive crest and the negative trough amplitudes are not uniform, rather successive amplitudes of the peaks and those of the valleys are decreasing in their magnitudes. Moreover, the distances (representing period of oscillation) between two successive peaks and valleys gradually decrease.

An attempt has been made to calculate the diffusivity-mobility ratio (DMR) also known as Einstein relation [4]. The DMR for various semiconductor device

performances [9-11] calculated from the conventional approach for FIs (i.e., the numerical integrations) comes out to be always positive (dotted line in Figure 2). Using the present exact calculations of the Fermi-Integrals $F_{\underline{1}}(\eta)$ and

 $F_{\frac{-1}{2}}(\eta)$, DMR can be defined as

DMR= (k_BT/e)[
$$\bar{F}_{\frac{1}{2}}(\eta) / \bar{F}_{-\frac{1}{2}}(\eta)$$
] (15)



Figure 1. Variations of the Fermi-Integral and DOS function, S (η) = [exp (- η). $\overline{F}_{\frac{1}{2}}(\eta)$] (Eq.14b) for non-degenerately doped semiconductor as a function of reduced Fermi energy η ($-\frac{E_f}{k_BT}$) using the data of Table 1



Figure 2. Comparison of room temperature (300K) DMR values obtained from the present exact calculation (Eq.15) and that obtained from the previous numerical calculation by Blackmore [2] (dotted curve)

Models of Computations of Fermi-Integrals of Half-Integer order								
	J. Mc Dougall and E.C. stoner & J.S. Blakemore				P.K. Chakraborty and B.N. Mondal			
η	$F_{\frac{-3}{2}}(\eta)$	$F_{\frac{-1}{2}}(\eta)$	$F_{\frac{1}{2}}(\eta)$	$F_{\frac{3}{2}}(\eta)$	$\overline{F}_{\frac{-3}{2}}(\eta)$	$\bar{F}_{\frac{-1}{2}}(\eta)$	$\bar{F}_{\frac{1}{2}}(\eta)$	$\overline{F}_{\frac{3}{2}}(\eta)$
-1.0	0.2367	0.29402	0.32780	0.34667	0.8921047	0.024995	0.2641784	0.30818663
-0.8	0.2667	0.34438	0.39154	0.41844	1.1763895	-0.0472093	0.2973627	0.3613927
-0.6	0.2971	0.40077	0.46595	0.50400	1.5371718	-0.1653153	0.3270025	0.4196298
-0.4	0.3268	0.46318	0.55224	0.60561	1.9777858	-0.3480116	0.3481471	0.4811916
-0.2	0.3548	0.53137	0.65161	0.72577	2.4830765	-0.6179825	0.3535775	0.5429851
0.0	0.3800	0.60490	0.76515	0.86720	3.0	-1.0	0.3333331	0.6000024
0.2	0.4019	0.68317	0.89388	1.0328	3.4060969	-1.5158827	0.2745165	0.6447316
0.4	0.4196	0.76510	1.0387	1.2258	3.4631249	-2.1741066	0.1617887	0.66668486
0.6	0.4328	0.85074	1.2003	1.4494	2.7585010	-2.951250	-0.0207513	0.6522183
0.8	0.4415	0.93826	1.3791	1.7071	0.6522377	-3.7627675	-0.2853131	0.5851824
1.0	0.4457	1.0271	1.5756	2.0023	-3.720068	-4.423456	-0.6325986	0.4490560
1.2	0.4459	1.1163	1.79	2.3385	-11.27854	-4.606463	-1.0395625	0.2314946
1.4	0.4427	1.2052	2.0221	2.7194	-22.47368	-3.8279712	-1.4434958	-0.0678440
1.6	0.4365	1.2931	2.272	3.1486	-36.16012	-1.5154806	-1.7272779	-0.4261199
1.8	0.4281	1.3796	2.5393	3.6294	-47.76406	2.7466371	-1.7183136	-0.7849614
2.0	0.4182	1.4643	2.8237	4.1654	-47.32019	8.6967182	-1.2241420	-1.0436269
2.2	0.4070	1.5468	3.1249	4.76	-19.72106	14.625242	-0.1337513	-1.07-7693
2.4	0.3954	1.6271	3.4423	5.4164	47.954132	16.776968	1.4043882	-0.0858741
2.6	0.3833	1.7049	3.7755	6.1380	145.86356	10.089621	2.7921123	-0.858741
2.8	0.3712	1.7804	4.1241	6.9277	211.07954	-7.9868693	2.9963998	0.7095146
3.0	0.3595	1.8535	4.4876	7.7886	122.67401	-30.27694	1.1221185	1.1689537
3.2	0.3481	1.9242	4.8653	8.7237	-197.715	-35.287853	-2.327161	0.8155246
3.4	0.3370	1.9927	5.2571	9.7357	-541.8664	-0.8510669	-4.4545397	-0.2982655
3.6	0.3267	2.0591	5.6623	10.827	-311.4929	54.739845	-1.7309298	-1.1786131
3.8	0.3167	2.1235	6.0806	12.001	702.63403	50.684658	4.3256855	-0.5953887
4.0	0.3075	2.1859	6.5115	13.260	-899.2412	3.3563582	6.254676	1.0597025

 Table 1. Comparison of FIs of Half Integer order estimated from the previous Classical Calculations [1, 2] with phase obtained from the Present exact quantum mechanical calculations (Eqn.13)

Figure 2 shows the variation of DMR with η (Eq. 15). The DMR values showing both positive and negative values (Figure 2) appearing due to the oscillations in FIs (Figure 1). This results contradicts the theoretical result obtained by Roichman and Tessler using the Monte Carlo simulation technique to calculate the inverse DMR which also did not exhibit oscillatory behavior [10] indicating that their calculations were also not exact where DMR showed only positive ones. This controversy arises due to the drawback of the previous approximate numerical calculations showing no oscillatory behavior of the FI. The present approach of exact calculation of FIs for the non-degenerately doped semiconductor is the most appropriate one as compared to the previous approximate ones [1-6, 10, 12]. Using the present exact theoretical model, new results, like DMR, are also expected from the calculations of all other physical parameters related to the Fermi energy.

4. Conclusions

We have, for the first time, made an exact quantum mechanical calculation for the FI for the non-degenerately doped impurities in parabolic band semiconductors and the results are compared with those of previous approximate calculations. Present calculation is superior compared to be the existing asymptotic expansions of the same FI generating new result as shown in the case of DMR. This is because of the presence of higher order terms of exp (η) in the present derived expression Eq. (14). Such exact analysis provided FI as a real function. A comparison of the FI of Half-integer order estimated from the previous classical calculation and those of on present quantum mechanical calculation have also been shown which might be useful for further studies of different physical parameters. As the FI is involved with DOS and Fermi-Dirac functions, the present new theoretical

results would provide more accurate explanations of quantum transport phenomena in semiconductors along with new applications in magnetic susceptibility, magnetoresistance and specific heat at low temperature.

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REFERENCES

- McDougall, J., Stoner, E.C., 1938, Roy, Soc. Philos. Trans. 237A, 67.
- [2] Blackmore, J.S., 1962, Semiconductor statistics, Pergamum Press, (London).
- [3] Seeger, K, 1973, Semiconductor Physics-An introduction 3rd Ed. (Springer Series in Solid State Physics Science, 40.

- [4] Nag, B.R., 1980, Electron Transport in Compound Semiconductor, (Springer Series in Solid State Sci.) 11, 74.
- [5] Kim, R., Lundstrom, M., 2011, Notes of Fermi-Dirac Integral, 3rd Ed., (Network for Computational Nanotechnology, Purdue Univ. 4, 1.
- [6] Natarajan, A., Mohan Kumar, N., 2001, Comput. Phys. Commun. 137, 361.
- [7] Gradshteyn, I.S., Ryzhik, I.M., 1980, Table of Integrals, Series and Products, Ed., Alan Jeffrey, 5th Edition, (Academic press), 371.
- [8] Abramowitz, M., Stegun, I.A., 1972, Handbook of Mathematical Functions, (Dover Publications, Inc., New York), 504.
- [9] Roichman, Y., Tessler, N., 2002, Appl. Phys. Lett. 80, 1948.
- [10] Roichman, Y., Tessler, N., 2001 Proc. Mater. Research Soc Symposium, San Francisco, 1-12.
- [11] Abd Elhamid, H., Ismail, Y., Deen, M. J. 2013, Opt. Quant. Electron, 45,885.
- [12] Garoni, T.M., Frankel, N.E., Glasser, M.L., 2001, J. Math. Phys., 42, 860.