COMPUTATION OF CHEMICAL POTENTIAL AND FERMI-DIRAC INTEGRALS APPLIED TO STUDY THE TRANSPORT PHENOMENA OF SEMICONDUCTORS

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In the given paper, two methods of calculating with high precision accuracy the chemical potential and the integrals of the type called the Fermi–Dirac of different indexes are presented. Our calculations are conclusive with already existing data. These data are essential not only in the study of the theory of solids but at the explanation of the experimental results of investigated transport phenomena in solids, namely, in semiconductors.

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Introduction

The physical laws of systems consisting of a huge number of particles are of a statistical nature. Statistical distribution determines the probability of having those or other defining states parameters of the particles of the system.[1] One example of systems of the huge number of particles that requires a statistical approach is the solid state, in particular, semiconductors. The distribution of electrons over energies, namely, the Fermi–Dirac distribution, is the most important. The Boltzmann distribution, which is valid for particles obeying classical mechanics, is the limiting case of the Fermi-Dirac distribution. In the state of statistical equilibrium, the ideal electrons gas in solid state obeys the Fermi–Dirac statistics.[2,3] Different physical phenomena are differently sensitive to the type of statistical distribution. When considering the transport properties in a solid state, we inevitably collide with integrals of the type called the Fermi–Dirac integrals.[2,3] These are certain integrals often encountered not only in the study of the theory of semiconductors but at the explanation of the experimental results of investigated transport phenomena in semiconductors.

In this case, we have to use not only the tables of values of the Fermi integral but also their approximate formulas.[4] However, the calculation of integrals according to approximate formulas and tables gives a sufficiently high value of error, especially for large and small values of the reduced Fermi level. The error can reach approximately 25%. Using approximations is inconvenient and inaccurate. Therefore, the goal of our paper is to find an appropriate method for calculation of the Fermi–Dirac integrals for application in the study of semiconductors properties with high accuracy <<1%. The presented paper allows also determining a normalization constant, included in the Fermi–Dirac statistics, - the chemical potential with high reasonable accuracy.

Methodology

Gauss–Legendre method integrals solution

Functional integral according to Gauss–Legendre method is presented as the sum of (*n-1*) coefficients:

$$I \approx C_0 f(x_0) + C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3) + \ldots + C_{n-1} f(x_{n-1}) \quad (1)$$

Let's say, at searching of integral we foresee only 2 coefficients, then it follows from (1):

$$I \approx C_0 f(x_0) + C_1 f(x_1) \quad (2)$$

This expression consists of 4 unknown coefficients (C_0, C_1, x_0, x_1) and, consequently, we need 4 boundary conditions:

$$f = const \quad f = x \quad f = x^2 \qquad f = x^3 \quad (3)$$

The value of integral may be taken at an arbitrary [*a*,*b*] boundary. In our case, we take [–1,1] interval and const=1. From (3), boundary conditions follow:

$$\begin{aligned} \int_{-1}^{1} 1dx &= C_0 f(x_0) + C_1 f(x_1) = 2 \\ \int_{-1}^{1} x dx &= C_0 f(x_0) + C_1 f(x_1) = 0 \\ \int_{-1}^{1} x^2 dx &= C_0 f(x_0) + C_1 f(x_1) = \frac{2}{3} \\ \int_{-1}^{1} x^3 dx &= C_0 f(x_0) + C_1 f(x_1) = 0 \end{aligned} \quad (4)$$

The solution of (4) equations gives the following values for C and x coefficients:

$$C_0 = 1 \quad x_0 = -\frac{1}{\sqrt{3}}$$
$$C_1 = 1 \quad x_1 = \frac{1}{\sqrt{3}} \tag{5}$$

Taking into account the value of two coefficients, the magnitude of integral is:

$$I = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) \tag{6}$$

Taking into account 4 coefficients, we have to add 4 boundary conditions: $f=x^4$, $f=x^5$, $f=x^6$, $f=x^7$. At these boundary conditions calculated coefficients are:

$$C_0 = \frac{18-\sqrt{30}}{36} \quad C_2 = \frac{18+\sqrt{30}}{36}$$
$$C_1 = \frac{18+\sqrt{30}}{36} \quad C_3 = \frac{18-\sqrt{30}}{36} \tag{7}$$
$$x_0 = -\frac{\sqrt{525+70\sqrt{30}}}{35} \quad x_2 = \frac{\sqrt{525-70\sqrt{30}}}{35}$$
$$x_1 = -\frac{\sqrt{525-70\sqrt{30}}}{35} \quad x_3 = \frac{\sqrt{525+70\sqrt{30}}}{35}$$

These coefficients are needed to be installed into (1) for calculation of the digital value of integral. If we take into account *n* coefficients, we will need 2*n* boundary conditions.

In general, our task is to solve integral

$$I = \int_a^b f(x)dx$$

in arbitrary boundaries. For calculation of integral, it is necessary to transfer the boundary [a,b] into [–1,1]. Let's say, the value of the new argument is given by:

$$x = a_1 + a_2 x_d \tag{8}$$

and we search the integral value in the form of

$$I = \int_{-1}^{1} f(x_d)dx_d$$

because integrals values are equal to each other:

$$I = \int_{-1}^{1} f(x_d)dx_d \quad = \quad I = \int_a^b f(x)dx$$

From this it follows new conditions:

$$a_1 + a_2 = b \qquad x = \frac{b+a}{2} + \frac{b-a}{2}x_d$$
$$a_1 - a_2 = a$$

$$dx = \frac{b-a}{2}dx_d$$

Finally, for integral solved with two coefficients we obtain formula:

$$\int_a^b f(x)dx = \int_{-1}^{1} \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}x_d\right)dx_d \tag{9}$$

The more terms we take into account in the formula (1), the more accurate value of integral will be. In general, taking into *n* coefficients:

$$\int_a^b f(x)dx = \sum_{i=1}^{n} C_i \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2}x_i\right) \tag{10}$$

where $f(x)$ is an arbitrary function, which is continuous in [a,b] interval and C_i and x_i are coefficients found from boundary conditions.

The second way to calculate C_i and x_i coefficients is to solve Legendre polynomial equitations:[5,6]

$$P_n(x_i) = 0 \tag{11}$$

$$C_i = \frac{2(1-x_i^2)}{[nP_{n-1}(x_i)^2]} \tag{12}$$

To obtain C_i and x_i coefficients, first, we have to generate Legendre polynomials and solve them. We can use MATLAB-s built-in functions to generate polynomials and solve them[7] (legendrePolynomials_1.m), or we can manually generate. Program (legendrePolynomials_2.m) uses polynomials properties:[5]

$$P_0(x) = 1$$
$$P_1(x) = x$$
$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$
$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

,

$$P_{(n+1)} = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x) \tag{13}$$

These values are uploaded on the repository (roots_2, weights_2).[7]

Method of undefined integrals solution

Let's say the integral is not given in limited [*a*,*b*] interval, but in [0,+∞] range. We can decompose integral into two parts:

$$\int_0^\infty f(x)dx = \int_0^1 f(x)dx + \int_1^\infty f(x)dx \tag{14}$$

In the second part of integral, we substitute the variable:

$$t = \frac{1}{x} \qquad dx = -\frac{1}{t^2}dt \qquad \begin{matrix} x = 1 & t = 1 \\ x = \infty & t \approx 0 \end{matrix}$$

Finally, we obtain formula (15) for approximate calculation of integral:

$$\int_0^{\infty} f(x)dx = \int_0^1 f(x)dx + \int_0^1 \frac{1}{t^2} f(\frac{1}{t})dt \qquad (15)$$

We can apply (10) formula to the two parts of this integral and solve any integral, which is defined in this range. Taking into account (14) and (15) formulas, we obtain:

$$\int_0^1 f(x)dx = \sum_{i=1}^{n} C_i 0.5 f(0.5 + 0.5x_i)$$
$$\int_0^1 \frac{1}{t} f(\frac{1}{t})dt = \sum_{i=0}^{n} C_i 0.5 \frac{1}{0.5 + 0.5x_i} f(\frac{1}{0.5 + 0.5x_i}) \qquad (16)$$

Calculation of integrals by (16) formulas and their summation give the final meaning of (14) integral.

Integral Fermi and its derivative

The general view of integrals of Fermi is given by the formula:

$$F_{(k)}(\xi) = \frac{1}{\Gamma(k+1)} \int_0^{\infty} \frac{x^k dx}{e^{x-\xi} + 1} \qquad (17)$$

where ξ is the chemical potential. Many authors do not take into account $\Gamma(k+1)$ member and introduce integral Fermi as:

$$F_{(k)}(\xi) = \int_0^{\infty} \frac{x^k dx}{e^{x-\xi} + 1} \qquad (18)$$

The formula for Fermi integrals derivative is given by:

$$\frac{dF_{(k)}(\xi)}{d\xi} = F_{(k-1)}(\xi) \qquad (19)$$

For gamma function, given in (17) formula, it can be written:

$$\Gamma(n) = (n-1)!$$

If *n* is a natural number,

$$\Gamma(n+1) = n\Gamma(n)$$

It is also known, that

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}$$

$$\Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2}$$

The graphics of integrand function in (18) formula for different values of *k* and ξ are given in Fig.1. It is clear from Fig.1 that these functions are decomposable and it is possible to integrate them in certain approximation.

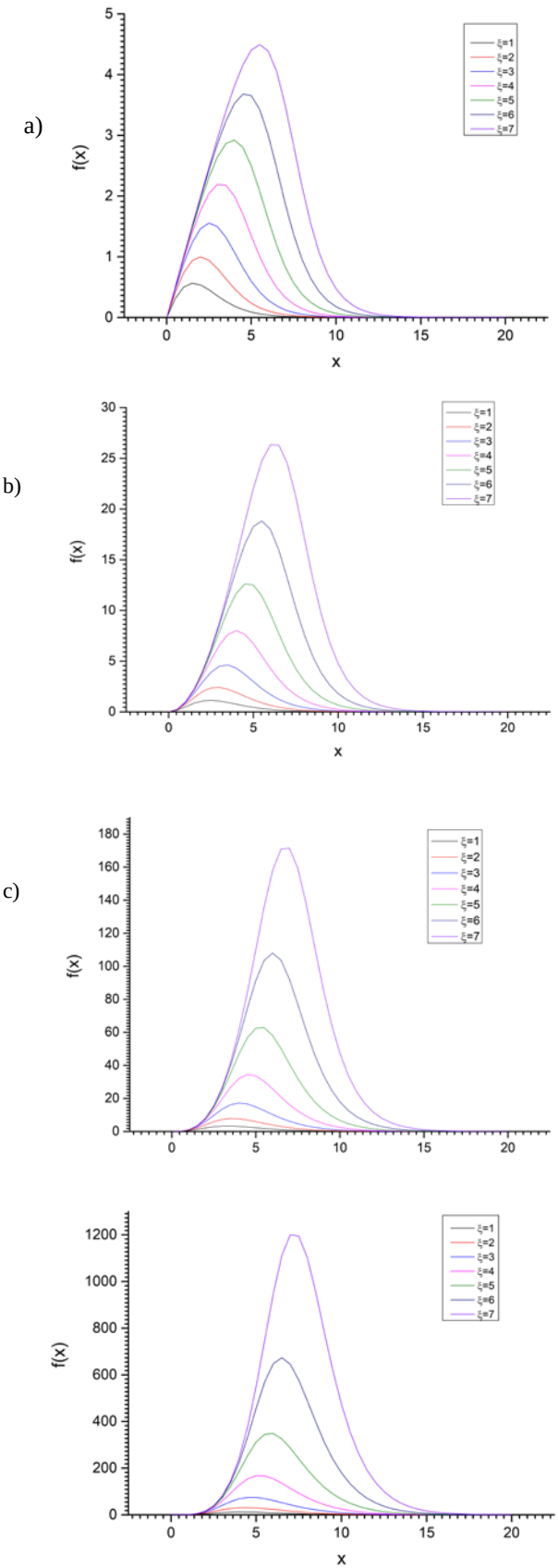

Figure 1. Dependence of integrand functions of Fermi integrals of different indexes (*k*) on *x* coefficient (parameter in Gauss–Legendre decomposition) for different values of chemical potential (ξ) according (18) formula.a) *k* = 1; b) *k* = 2; c) *k* = 3; d) *k* = 4

Table 1. Fermi integrals calculated using Gauss–Legendre numerical method for different *k* and ξ values.

ξ	$F_{(-0.5)}(\xi)$	$F_{(0)}(\xi)$	$F_{(0.5)}(\xi)$	$F_{(1)}(\xi)$	$F_{(1.5)}(\xi)$	$F_{(2)}(\xi)$	$F_{(2.5)}(\xi)$	$F_{(3)}(\xi)$	$F_{(3.5)}(\xi)$	$F_{(4)}(\xi)$
-10	0.000080	0.000045	0.000040	0.000045	0.000060	0.000091	0.000151	0.000272	0.000528	0.001090
-9.5	0.000132	0.000075	0.000066	0.000075	0.000100	0.000150	0.000249	0.000449	0.000871	0.001796
-9	0.000218	0.000123	0.000109	0.000123	0.000164	0.000247	0.000410	0.000740	0.001435	0.002962
-8.5	0.000359	0.000203	0.000180	0.000203	0.000270	0.000407	0.000676	0.001221	0.002367	0.004883
-8	0.000592	0.000335	0.000297	0.000335	0.000446	0.000671	0.001115	0.002013	0.003902	0.008051
-7.5	0.000975	0.000553	0.000490	0.000553	0.000735	0.001106	0.001838	0.003318	0.006433	0.013274
-7	0.001607	0.000911	0.000808	0.000912	0.001212	0.001824	0.003030	0.005471	0.010606	0.021884
-6.5	0.002649	0.001502	0.001332	0.001503	0.001998	0.003006	0.004996	0.009020	0.017486	0.036081
-6	0.004364	0.002476	0.002195	0.002477	0.003294	0.004956	0.008236	0.014870	0.028829	0.059485
-5.5	0.007188	0.004078	0.003617	0.004083	0.005429	0.008169	0.013577	0.024514	0.047527	0.098070
-5	0.011828	0.006715	0.005957	0.006727	0.008946	0.013465	0.022379	0.040410	0.078350	0.161676
-4.5	0.019442	0.011048	0.009807	0.011078	0.014739	0.022187	0.036883	0.066607	0.129153	0.266522
-4	0.031894	0.018150	0.016128	0.018232	0.024269	0.036548	0.060771	0.109768	0.212870	0.439322
-3.5	0.052154	0.029750	0.026480	0.029972	0.039930	0.060169	0.100090	0.180844	0.350780	0.724052
-3	0.084849	0.048587	0.043366	0.049180	0.065611	0.098963	0.164740	0.297801	0.577843	1.193037
-2.5	0.136919	0.078889	0.070724	0.080459	0.107580	0.162524	0.270855	0.490021	0.951367	1.965030
-2	0.218160	0.126927	0.114587	0.131012	0.175800	0.266264	0.444552	0.805316	1.564959	3.234531
-1.5	0.341047	0.201412	0.183801	0.211781	0.285771	0.434565	0.727643	1.320874	2.570653	5.318800
-1	0.518823	0.313260	0.290500	0.338646	0.460847	0.705127	1.185963	2.159830	4.213244	8.732095
-0.5	0.761071	0.474075	0.449791	0.533215	0.734656	1.134363	1.920729	3.515183	6.881824	14.300130
0	1.067828	0.693144	0.678091	0.822463	1.152798	1.803077	3.082572	5.682171	11.183664	23.330758
0.5	1.426306	0.974072	0.990205	1.236711	1.772785	2.820956	4.886692	9.098479	18.043955	37.857518
1	1.814084	1.313255	1.396369	1.806278	2.661670	4.328312	7.626501	14.389290	28.831181	60.969145
1.5	2.207291	1.701405	1.900824	2.558140	3.891958	6.494340	11.683107	22.412341	45.503037	97.230062
2	2.587770	2.126918	2.502446	3.513905	5.537229	9.512626	17.529341	34.298126	70.764217	153.186814
2.5	2.945461	2.578877	3.196584	4.689454	7.668770	13.595469	25.728853	51.482272	108.226761	237.947389
3	3.276968	3.048573	3.976967	6.095726	10.353670	18.968485	36.931900	75.729458	162.565639	363.816745
3.5	3.582928	3.529734	4.837044	7.739928	13.654142	25.866260	51.869575	109.149979	239.665390	546.972565
4	3.865848	4.018131	5.770701	9.626660	17.627625	34.529198	71.347717	154.210694	346.756231	808.168220
4.5	4.128776	4.511027	6.772544	11.758804	22.327231	45.201382	96.241199	213.742039	492.539785	1173.453445
5	4.374651	5.006692	7.837941	14.138143	27.802316	58.129185	127.488879	290.942425	687.305373	1674.906250
5.5	4.606044	5.504053	8.962954	16.765772	34.099026	73.560391	166.089248	389.380971	943.038083	2351.371837
6	4.825101	6.002447	10.144236	19.642358	41.260784	91.743648	213.096735	512.999179	1273.519828	3249.205875
6.5	5.033577	6.501470	11.378929	22.768310	49.328692	112.928137	269.618566	666.111973	1694.424439	4423.020466
7	5.232895	7.000876	12.664570	26.143874	58.341866	137.363360	336.812082	853.408342	2223.407698	5936.431785
7.5	5.424209	7.500513	13.999019	29.769204	68.337698	165.299026	415.882435	1079.951738	2880.192997	7862.808723
8	5.608459	8.000292	15.380397	33.644392	79.352082	196.984965	508.080574	1351.180315	3686.653190	10286.021973
8.5	5.786419	8.500157	16.807039	37.769497	91.419585	232.671085	614.701470	1672.907025	4666.888990	13301.193045
9	5.958728	9.000074	18.277454	42.144555	104.573587	272.607329	737.082509	2051.319588	5847.304234	17015.442795
9.5	6.125925	9.500023	19.790299	46.769583	118.846403	317.043638	876.602036	2492.980354	7256.678336	21548.639382
10	6.288463	9.999991	21.344352	51.644591	134.269371	366.229930	1034.678067	3004.826267	8926.236815	27034.147723
10.5	6.446730	10.499971	22.938496	56.769577	150.872948	420.416105	1212.767150	3594.168865	10889.719696	33619.578292
11	6.601061	10.999955	24.571701	62.144532	168.686770	479.852017	1412.363326	4268.694535	13183.449811	41467.545021
11.5	6.751748	11.499944	26.243030	67.769486	187.739872	544.787974	1634.998693	5036.469111	15846.411090	50756.452690
12	6.899048	11.999932	27.951588	73.644384	208.060299	615.473181	1882.237194	5905.919849	18920.251812	61681.049761
12.5	7.043184	12.499917	29.696558	79.769248	229.675833	692.158493	2155.684591	6885.876865	22449.502262	74453.755063
13	7.184368	12.999931	31.477293	86.144477	252.614812	775.098142	2456.990127	7985.568418	26481.571170	89305.014338
13.5	7.322766	13.499917	33.292849	92.769192	276.900355	864.529451	2787.775804	9214.382245	31066.001979	106481.391495
14	7.458527	13.999844	35.142482	99.643325	302.558861	960.706699	3149.769214	10582.385598	36256.535226	126253.971250
14.5	7.591864	14.499956	37.026477	106.770282	329.628301	1063.925362	3544.868194	12100.472868	42111.352067	148918.432812
15	7.722883	15.000121	38.943590	114.147113	358.120538	1174.378450	3974.595997	13778.315868	48685.456412	174767.250174
15.5	7.851551	15.499752	40.891069	121.765761	388.030742	1292.210038	4440.373101	15625.664267	56036.688211	204116.965869
16	7.978094	15.999386	42.870763	129.636690	419.428203	1417.862657	4944.839304	17657.354518	64244.638244	237379.517106
16.5	8.102938	16.500262	44.886890	137.777816	452.403877	1551.835529	5490.763439	19888.479776	73389.579386	274971.640142
17	8.225953	17.001340	46.934200	146.167673	486.885544	1693.957680	6078.195623	22323.282631	83509.382081	317148.914595
17.5	8.346576	17.499994	49.001676	154.764116	522.728902	1843.819144	6706.467018	24964.288331	94640.747025	364190.295690
18	8.465035	17.997093	51.093520	163.590796	560.072948	2002.228306	7380.152559	27836.647899	106918.386825	416801.505870
18.5	8.582563	18.497577	53.230315	172.736759	599.316143	2171.018229	8107.863355	30981.410198	120539.839988	475938.428659
19	8.699711	19.003177	55.417601	182.221026	640.533573	2350.541470	8891.492840	34409.422944	135568.153097	541963.950641
19.5	8.815135	19.507480	57.625903	191.912223	683.155636	2538.395308	9721.205939	38081.863815	151857.364686	614368.443194
20	8.927052	20.002597	59.821192	201.667330	726.598591	2732.281123	10588.381355	41968.724103	169316.409651	692959.229516
20.5	9.035835	20.490508	62.014455	211.548266	771.210166	2934.130082	11503.598132	46127.163845	188250.202101	779344.274730
21	9.144327	20.984056	64.264387	221.825881	818.251380	3149.859592	12494.815952	50690.082514	209293.696928	876570.581204
21.5	9.255096	21.494325	66.619219	232.712178	868.664160	3383.702824	13581.288777	55746.134990	232860.143722	986587.644347
22	9.367376	22.016786	69.054145	244.077558	921.793834	3632.438102	14747.505621	61222.093445	258610.281543	1107853.781600
22.5	9.477076	22.531761	71.475319	255.478027	975.555760	3886.350156	15948.528937	66911.728985	285605.661762	1236138.584063
23	9.580333	23.021253	73.799663	266.533674	1028.230269	4137.743722	17150.381409	72667.432314	313218.016810	1368839.633026
23.5	9.677238	23.486424	76.036815	277.313023	1080.265921	4389.406492	18369.776040	78586.789805	342005.732957	1509101.370114
24	9.772329	23.949657	78.297661	288.367539	1134.414867	4655.115422	19675.865035	85017.732716	373723.077942	1665785.362059
24.5	9.871685	24.440360	80.724949	300.392328	1194.072448	4951.506346	21150.402315	92363.210432	410361.858345	1848765.243487
25	9.978684	24.974206	83.391576	313.727459	1260.830453	5286.059615	22828.702401	100790.828387	452722.379407	2061888.667774
25.5	10.091017	25.538479	86.228622	328.004250	1332.737838	5648.543680	24657.529991	110025.528551	499392.470545	2297948.317296
26	10.201425	26.095944	89.045751	342.252668	1404.865112	6013.977515	26510.633196	119430.968104	547173.548812	2540911.531003
26.5	10.302280	26.608051	91.648688	355.496500	1472.321179	6357.929723	28266.366977	128403.557665	593081.912366	2776090.276727
27	10.390462	27.059599	93.964039	367.385216	1533.454004	6672.741724	29889.976731	136790.079311	636469.753387	3000921.095439
27.5	10.468938	27.466702	96.079651	378.399049	1590.894336	6972.848921	31460.775056	145026.735497	679737.892201	3228625.177457
28	10.545059	27.868165	98.200806	389.626352	1650.424856	7289.039459	33143.006230	153991.352743	727586.347713	3484409.762379
28.5	10.627588	28.310113	100.570847	402.353554	1718.859757	7657.477976	35128.967815	164708.313287	785481.846607	3797499.424296

29	10.723418	28.828660	103.379363	417.578079	1801.457447	8105.944774	37565.730293	177957.836926	857572.092172	4189989.132597
29.5	10.834220	29.431761	106.663945	435.476104	1899.035693	8638.191699	40470.262904	193815.317953	944184.493311	4663258.212882
30	10.954374	30.087872	110.248115	455.062998	2006.114497	9223.788410	43673.935454	211348.075056	1040169.670945	5188924.669727

Finally, the Fermi integrals values have been calculated by the Gauss–Legendre method, where C_i and x_i coefficients have been found from (11) and (12) formulas. The Program has been written in Matlab programming language (Fermi_integral_calculator_1.m) and it uses 100 points of Gauss–Legendre coefficients.[7] The values of calculated Fermi integrals for different parameters k and ξ are given in Table 1.

Simson's integral calculation method

Another way to calculate integrals of function $f(x)$, which are defined in $[a,b]$ range, is Simson's integration method, the general formula of which is given in (20):[7]

$$\int_a^b f(x)dx = \frac{\Delta x}{3}(f(a)+f(b)+4(f(x_1)+f(x_3)+.....$$

$$f(x_5)+f(x_{2n+1}))+2(f(x_2)+.....$$

$$f(x_4)+f(x_6)+...f(x_{2n})))$$

$$\Delta x = \frac{b-a}{n} \qquad (20)$$

$$\int_a^b f(x)dx = \frac{\Delta x}{3}(\text{First}+\text{Last}+4(\text{sum of odds})+2(\text{sum of evens}))$$

Results for Simson's rule are in good agreement with the Gauss–Legendre method.

Error estimation

Finally, we show the advantages of the method presented in the article by calculating the error of implemented calculations.

Gauss–Legendre method error estimation has been done by using (21) formula:

$$\text{Error} = Ef^{(2n)}(\theta) \qquad (21)$$

where

$$E = \frac{2^{(2n+1)}(n!)^4}{(2n+1)((2n)!)^3} \qquad (22)$$

and $a \le \theta \le b$.

The values of E parameter estimated by (22) formula are given for different n in Table 2.

Table 2. Values of E according to (22) formula for different n

n	*E*	*n*	*E*
2	0.00741	16	2.73804E-45
3	6.34921E-5	17	6.10607E-49
4	2.87946E-7	18	1.21246E-52
5	8.07929E-10	19	2.15736E-56
6	1.54087E-12	20	3.45947E-60
7	2.12743E-15	21	5.0253E-64
8	2.22477E-18	22	6.64363E-68
9	1.82325E-21	23	8.02751E-72
10	1.20251E-24	24	8.89959E-76
11	6.52056E-28	25	9.08485E-80
12	2.95829E-31	26	8.56732E-84
13	1.13949E-34	27	7.48625E-88
14	3.77297E-38	28	6.07844E-92
15	1.08539E-41	29	4.59789E-96
16	2.73804E-45	30	3.248E-100

It is clear that the increase of n-value decreases the value of E and error goes to nearly zero.

Conclusion

The chemical potential and Fermi–Dirac integrals are essential for a basic understanding of semiconductors properties. In this paper, there have been calculated Fermi–Dirac integrals by two different ways – Gauss–Legendre and Simson's methods. Both methods are in good agreement with each other. Our data let reduce the error of calculation of Fermi–Dirac integrals up to <<1%.

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References

[1]Lifshitz, E. M., and Pitaevskiĭ, L. P., *Statistical physics* / Part 2, *Theory of the condensed state*, Oxford; New Yor : Pergamon Press, **1980**.

[2]Blatt, F. J., *Theory of Mobility of Electrons in Solids*, Academic Press Inc., New York, **1957**.

[3]Anselm, A. I., *Introduction to the Theory of Semiconductors*, Nauka, Moscow, **1978**.

[4]Fistul, V. I., *Heavily doped semiconductors*, Phys.-Math. Lit. Press, Moscow, **1967**.

[5]Davis P. and Rabinowitz, P., Abscissas and Weights for Gaussian Quadratures of High Order, *J. Res. Natl. Bureau Standards*, **1956**, *56(1)*, 35-37. https://nvlpubs.nist.gov/nistpubs/jres/56/jresv56n1p35_A1b.pdf

[6]http://keisan.casio.com/exec/system/1280883022.

[7]https://github.com/scienceman001/Fermi-integrals.

[8]https://www.intmath.com/integration/6-simpsons-rule.php.

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