THE APPROXIMATION OF THE FERMI–DIRAC INTEGRAL $\mathcal{F}_{1/2}(\eta)$

D. BEDNARCZYK and J. BEDNARCZYK
Department of Solid State Physics, Pedagogical University, 42-201 Częstochowa, Poland

Received 25 October 1977

This paper presents the approximation of the Fermi–Dirac integral of order 1/2 with a relative error not exceeding 0.4% for any value of the position of the Fermi level.

The concentration of "free" electrons in the conduction band can be calculated from the formula [1, 2]:

$$n = 4\pi(2m_c^* kT)^{3/2} h^{-3} \int_0^\infty \frac{x^{1/2}\,\mathrm{d}x}{\exp(x-\eta)+1} = N_c\, 2\pi^{-1/2}\,\mathcal{F}_{1/2}(\eta), \tag{1}$$

where $N_c = 2(2\pi m_c^* kT)^{3/2} h^{-3}$ is the "effective density" of states in the conduction band, $m_c^* = (z^2 m_1^* m_2^* m_3^*)^{1/3}$ is the "density of states" effective mass in the conduction band, $m_{1,2,3}^*$ are the diagonal components of the effective-mass tensor, z is the number of energy minima in the conduction band, $x = E/kT$ is the energy in units of kT, $\eta = F/kT$ is the energy of the Fermi level in units of kT, $\mathcal{F}_{1/2}(\eta)$ is the Fermi–Dirac integral of order 1/2.

A similar dependence can be written for the concentration p of holes in the valence band.

It is generally known that the Fermi–Dirac $\mathcal{F}_{1/2}(\eta)$ integral cannot be integrated. It is only for the two extreme cases, i.e. for $\eta \ll -1$ and $\eta \gg +1$ that the integral can be expressed in the form of a rapidly converging series. For $\eta \ll -1$, i.e. for $\exp(\eta - x) \ll 1$:

$$\mathcal{F}_{1/2}(\eta) = \int_0^\infty \frac{x^{1/2}\exp(\eta-x)}{1+\exp(\eta-x)}\,\mathrm{d}x = \tfrac{1}{2}\sqrt{\pi}\exp\eta(1 - 2^{-3/2}\exp\eta + \ldots). \tag{2}$$

Taking into account one of the terms of the series (2) for $\eta \leqslant -4$ leads to the value $\mathcal{F}_{1/2}(\eta)$ with a relative error less than 0.65%, while two terms of the series give the value of the integral with an error less than 0.01%.

For $\eta \gg +1$ the Fermi–Dirac integral can be presented in the form of a series [3]:

$$\mathcal{F}_{1/2}(\eta) = \tfrac{2}{3}\eta^{3/2}[1 + \tfrac{1}{8}\pi^2\eta^{-2} + 0.267\,\eta^{-4} + \ldots]. \tag{3}$$

Taking into account one of the terms of the series (3) for $\eta \geqslant +10$ leads to an approximation of the Fermi–Dirac integral with a relative error less than 1.25%, whereas three terms of the series approximate the integral with an error less than 0.01%.

In the transitory interval $-4 < \eta < +10$ the Fermi–Dirac integral is determined from tables or numerically (e.g. using the Simpson method). In problems, where the Fermi–Dirac integral must be calculated repeatedly (e.g. refs. [4–7]) both using the tables and numerical calculation, are inconvenient and greatly increase the time of computing. Therefore it is convenient to use a function approximating the integral. Unfortunately, the approximation given in ref. [2] leads to over excessive error.

The function given below approximates the Fermi–Dirac integral of order 1/2 with a relative error not exceeding 0.4% for the value of η included in the range from $-\infty$ to $+\infty$. The approximation is expressed by the function:

$$\mathcal{F}_{1/2}(\eta) \approx \tfrac{1}{2}\sqrt{\pi}\,[\tfrac{3}{4}\sqrt{\pi}\,a^{-3/8}(\eta) + \exp(-\eta)]^{-1}, \tag{4}$$

where

$$a(\eta) = \eta^4 + 33.6\eta\{1 - 0.68\exp[-0.17(\eta+1)^2]\} + 50.$$

The relative error of the expression (4) in relation to the value of the Fermi–Dirac integral is presented in fig. 1. The data taken from the tables were assumed to be the "exact" value of $\mathcal{F}_{1/2}(\eta)$ in the range $-4 < \eta < +10$. For $\eta \leqslant -4$, the Fermi–Dirac integral was calculated from the series (2), and for $\eta \geqslant +10$ from the series (3). All the calculations have been made with

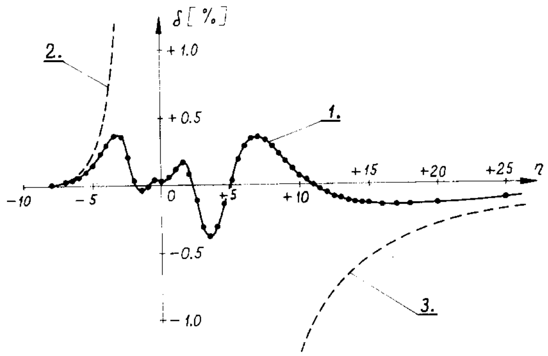

Fig. 1. Relative error of the function (4) approximating the Fermi–Dirac integral $\mathcal{F}_{1/2}(\eta)$ (curve 1). The calculated values are marked with points. For comparison, the relative errors of the two asymptotes were given (as approximations of $\mathcal{F}_{1/2}(\eta)$): $(\frac{1}{2}\sqrt{\pi})\exp\eta$ (curve 2) and $\frac{2}{3}\eta^{3/2}$ (curve 3).

the exactness exceeding 0.01%. It is easy to prove, that the formula (4) for $\eta \to -\infty$ leads to an asymptote $(\frac{1}{2}\sqrt{\pi})\exp\eta$, and for $\eta \to +\infty$ it leads to another asymptote $\frac{2}{3}\eta^{3/2}$. The errors of the asymptotes, as approximations of the Fermi–Dirac integral have been plotted in fig. 1 for comparison.

Expression (4) may be used as an approximation of the Fermi–Dirac integral for any value of the position of the Fermi η level with a relative error less than 0.4%.

References

[1] W. Brauer and H.W. Streitwolf, Theoretische Grundlagen der Halbleiterphysik (Akademie-Verlag, Berlin, 1973) (in German).

[2] P.S. Kiriejew, Fizyka półprzewodników (Państwowe Wydawnictwo Naukowe, Warszawa, 1971) (in Polish).

[3] L.A. Girifalco, Statistical physics of materials (Wiley–Interscience, New York, 1973).

[4] D. Bednarczyk, J. Bednarczyk and A. Węgrzyn, 3rd Intern. Conf. on Thin films, Budapest (1975); Thin Solid Films 36 (1976) 165.

[5] D. Bednarczyk, J. Bednarczyk and A. Węgrzyn, Sixth Czechoslovak Conf. on Electronics and vacuum physics, Bratislava (1976).

[6] D. Bednarczyk, J. Bednarczyk and A. Węgrzyn, Thin Solid Films 44 (1977) 137.

[7] D. Bednarczyk and J. Bednarczyk, Acta Phys. Polon. A51 (1977) 827.