### **REVIEW PAPER**

## APPROXIMATIONS FOR FERMI-DIRAC INTEGRALS, ESPECIALLY THE FUNCTION $\mathcal{F}_{1/2}(\eta)$ USED TO DESCRIBE ELECTRON DENSITY IN A SEMICONDUCTOR

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Abstract—The history of studies of the family of Fermi-Dirac integrals is briefly reviewed, and the relevance of these integrals to transport properties via the Boltzmann transport equation is noted. The role of the integral  $(2/\sqrt{\pi})F_{1/2}(\eta)\equiv \mathcal{F}_{1/2}(\eta)\equiv u$  in relating reduced Fermi energy  $\eta$  to electron density in a "parabolic" band makes it especially important that this member of the family be capable of expression in approximate forms of reasonable accuracy. High precision series forms, and published tabulations, for the various members of the family are noted, and the remainder of the paper deals with approximations that have been proposed for  $u(\eta)$  and for  $\eta(u)$ . The former permits deduction of carrier density from Fermi energy, and the latter permits the inverse. Successful expressions for each purpose are described, with graphs of the error so incurred.

#### NOTATION

D, electron diffusion coefficient

E electron energy

E<sub>c</sub> bottom of conduction band

 $E_F$  Fermi energy

Ei exponential integral

E, width of intrinsic gap

f(E) and  $f(\epsilon)$  Fermi-Dirac occupancy factor

 $\vec{F}_{j}(\eta)$  Sommerfeld notation for Fermi-Dirac integral, order j, argument  $\eta$ 

 $\mathcal{F}_j(\eta)$  Dingle notation for Fermi-Dirac integral, order j, argument n

g(E) density of band states with respect to energy

h Planck's constant

j order of Fermi-Dirac integral

k Boltzmann's constant

k electron wave vector

k. wave vector at base of conduction band

 $\tilde{m}_c$  density-of-states effective mass

 $m_{co}$  band edge effective mass in non-parabolic band

N<sub>c</sub> effective density of conduction states

 $n_0$  equilibrium electron density

T absolute (Kelvin scale) temperature

shorthand symbol for  $\mathscr{F}_{1/2}(\eta)$ 

α non-parabolicity parameter for conduction band

 $\Gamma(p)$  gamma function of order p

 $\epsilon$  dimensionless electron energy (in units of kT)

 $\eta$  dimensionless Fermi energy (in units of kT)

 $\mu_n$  electron mobility

 $\zeta(p)$  Riemann zeta function of order p

### 1. INTRODUCTION

The family of functions known as "Fermi-Dirac" integrals (hereafter referred to as F-D integrals) acquired that name in the 1920's, when Pauli[1] and Sommerfeld[2] used them in describing the degenerate electron gas of a metal. Sommerfeld developed asymptotic expansions for various orders of the F-D family, appropriate for the  $(E_F - E_c) \gg kT$  limit that is well satisfied by a normal metal with  $n_0 > 10^{22}$  cm<sup>-3</sup>.

A dimensionless energy scale is convenient for description of F-D integrals. Both n-type and p-type semiconductor situations can use the integrals, but the n-type terminology of the present paper shows the full scope of what needs to and can be done. With respect to the conduction band edge,  $\epsilon \equiv [(E-E_c)/kT]$  is a suitable dimensionless energy variable, while  $\eta \equiv \{(E_F-E_c)/kT\}$  is the reduced Fermi energy. Then  $f(\epsilon) = [1 + \exp(\epsilon - \eta)]^{-1}$  is the F-D occupancy probability for reduced energy  $\epsilon$ . In terms of  $\epsilon$  and  $\eta$ , Sommerfeld's definition for the F-D integral of order "j" was

$$F_{i}(\eta) = \int_{0}^{\infty} \frac{\epsilon^{i} d\epsilon}{1 + \exp(\epsilon - \eta)}$$
 (1)

Members of the  $F_j(\eta)$  family have been used widely in modeling the properties of semiconductors and metals, from the classical Boltzmann limit  $(n_0 \text{ small}, \eta \leq 0)$  to the Fermi-Dirac degenerate extreme  $(n_0 \text{ very large}, \eta \gg 0)$ . This has been accomplished despite the irksome fact that there are not analytic closed form expressions for any of the interesting  $j\neq 0$  members of the eqn (1) family.

Rather than dealing with the venerable  $F_i(\eta)$  themselves, this reviewer plans to follow a practice he has exercised elsewhere [3] in focusing attention instead on the related family of integrals

$$\mathscr{F}_{j}(\eta) = F_{j}(\eta)/\Gamma(j+1) = \frac{1}{\Gamma(j+1)} \int_{0}^{\infty} \frac{\epsilon^{j} d\epsilon}{1 + \exp(\epsilon - \eta)}.$$
(2)

Dingle [4] commented on several advantages of the functions  $\mathcal{F}_{j}(\eta)$ , in comparison with the  $F_{j}(\eta)$  family of eqn (1), as follows:-

(i) Unlike the  $F_i$ , the functions  $\mathscr{F}_i$  exist for negative integer orders. Indeed, the function  $\mathscr{F}_{-1}(\eta)$  is just  $(1 + e^{-\eta})^{-1}$ .

<sup>†</sup>The trivial case j = 0 has the simple solution  $F_0(\eta) = \ln(1 + e^{\eta})$ .

(ii) Interpolation between orders j, as well as between arguments  $\eta$ , is simplified when dealing with  $\mathcal{F}_i$  rather than  $F_j$ . The relation between a function and its derivative is also simplified. For,

$$\widetilde{\mathscr{F}}_{j}'(\eta) = \frac{\mathrm{d}}{\mathrm{d}\eta} \, \widetilde{\mathscr{F}}_{j}(\eta) = \widetilde{\mathscr{F}}_{j-1}(\eta) \tag{3}$$

(iii) In the non-degenerate  $\eta \le 0$  limit, all members of the  $\mathcal{F}_i(\eta)$  family reduce to  $\mathcal{F}(\eta) \to e^{\eta}$ , regardless of the order i.

The last of these three is a significant advantage for semiconductor work, where the non-degenerate limit is applicable for so many lightly doped situations. Accordingly, the  $\mathscr{F}_i(\eta)$  are discussed in what follows. Special emphasis is placed upon approximations for the function  $\mathscr{F}_{i/2}(\eta)$ , since this is so valuable for relating Fermi energy  $E_F$  to total electron density  $n_0$  in "normal parabolic" bands.

### 1.1 Fermi-Dirac integrals and electron transport

Several F-D integrals in addition to  $\mathcal{F}_{U2}(\eta)$  can become involved in describing electronic transport phenomena, from the Boltzmann transport equation approach. That approach was pioneered by Lorentz[5] for a Maxwell-Boltzmann "classical" electron gas, and by Sommerfeld[2] for the F-D limit. A transport integral

 $\int e^{B}(\partial f|\partial \epsilon) d\epsilon$  results in an F-D integral of order  $(\beta - 1)$ . Thus, Putley[6] showed that electrical conductivity involves an F-D integral of order  $(m + \frac{1}{2})$  if the relaxation time varies as  $e^{m}$ . For that situation, the Hall effect involves  $\mathcal{F}_{1/2}$ ,  $\mathcal{F}_{m+1/2}$ , and  $\mathcal{F}_{2m+1/2}$ .

Involvement of F-D integrals in transport expressions has been discussed extensively elsewhere, and various family members cataloged as to their involvement for electrical and thermal conductivities, thermoelectric effects, magnetotransport, etc. Comprehensive accounts for semiconductors include Putley [6], Madelung [7, 8], and Beer [9]. Seitz [10] and Wilson [11] emphasized metallic strong degeneracy. The reader who needs F-D integrals for modeling or analysis of transport effects is probably acquainted with some of the above [6-11], or with other accounts [e.g. 12-15] that draw upon the same information.

### 1.2 Relation between electron density and Fermi Energy

Any reader of this paper almost certainly already knows that  $\mathcal{F}_{1/2}(\eta) = (2/\sqrt{\pi})F_{1/2}(\eta)$  is the F-D family member used to relate electron density  $n_0$  and Fermi energy  $E_F$  for a parabolic conduction band. That is to say, a band for which  $(E-E_c) \propto |\mathbf{k} - \mathbf{k}_c|^2$  for every direction in  $\mathbf{k}$ -space away from a band minimum; without deviation from that square law behavior up to an energy at least several kT above  $E_c$ . The band may be anisotropic (i.e. the proportionality constant may depend on direction), but that, by itself, does not preclude a definition of a directionally-averaged density-of-states effective mass  $\bar{m}_c$ . The coexistence of several band minima at energy  $E_c$ , at symmetry-related Brillouin zone

locations, can also be incorporated into the numerical values of  $\bar{m}_{cc}$ 

In terms of  $\bar{m}_c$ , the density of conduction states (per unit volume) with respect to energy is

$$g(\epsilon) = 4\pi (2\bar{m}_c/h^2)^{3/2} (E - E_c)^{4/2}.$$
 (4)

Such states are filled to an extent that depends on their relation to  $E_E$ , through f(E). And so, the total electronic occupancy of such a band in thermal equilibrium is

$$n_0 = \int_0^\infty f(E)g(E) dE = N_c \widetilde{\mathcal{F}}_{1/2}(\eta). \tag{5}$$

Here the quantity

$$N_c = 2(2\pi \tilde{m}_c kT/h^2)^{3/2} \tag{6}$$

is usually called [3] the effective density of conduction band states for temperature T.  $N_c$  serves well in that capacity for a non-degenerate semiconductor ( $n_0$  small.  $\eta < 0$ ); for then  $\mathcal{F}_{1/2}(\eta) \rightarrow e^{\eta}$ , and  $n_0$  is the same as though the band were replaced by  $N_c$  states as a deltafunction distribution at energy  $E_c$ . That  $N_c$  varies as  $T^{3/2}$  is an inconvenience, which those who work with electron statistics learn to remember and accept.

It happens that  $\mathcal{F}_{1/2}(\eta) \approx 1$  when  $E_F$  is just slightly above  $E_c$  (for  $\eta \approx +0.35$ ). And so any situation for which  $n_0$  is clearly much smaller than  $N_c$  will automatically be a non-degenerate one ( $\eta \ll 0$ ). The strong degeneracy approximations for  $\eta \gg 0$  are correspondingly suitable whenever it is apparent that  $n_0 \gg N_c$ . Problems have been most apparent when  $n_0$  and  $N_c$  are comparable, and this has stimulated a variety of suggestions [3, 16] for approximate forms.

When the band is non-parabolic in the rise of energy with wave vector, then  $\mathcal{F}_{1/2}(\eta)$  and one or more additional orders in the F-D integral family are needed to relate  $n_0$  to  $E_F$ . For example, both  $\mathcal{F}_{1/2}(\eta)$  and  $\mathcal{F}_{3/2}(\eta)$  are needed to deal with  $n_0$  for the conduction band minimum at the center of the zone for a III-V compound such as InSb or GaAs. Vrehen[17] showed that the simple  $\mathbf{k} \cdot \mathbf{p}$  model of Kane[18] for this imperfectly parabolic band minimum leads to an approximation valid near the bottom of the band of

$$E \approx E_c + (\hbar^2 k^2 / 2m_{co})[1 - (\alpha / E_i)(\hbar^2 k^2 / 2m_{co})],$$

$$(E - E_c) \ll E_c. \tag{7}$$

Here  $m_{co}$  is the effective mass of the band-edge curvature, the slight anisotropy of the band is neglected, and  $\alpha$  is a numerical parameter determined by the ratio of spin-orbit splitting to bandgap  $E_{ir}$  (As one example,  $\alpha \approx 0.83$  for GaAs.) With that same limitation of energy to the lowest portion of the band,

$$g(E) \approx 4\pi (2m_{co}/h^2)^{3/2} (E - E_c)^{1/2} [1 + (5\alpha/2E_t)(E - E_c)]$$
(8)

as the density of states with respect to energy. The integration procedure of eqn (5), to express  $n_c$  for a

given  $E_F$ , then yields

$$\underline{n_o} \approx N_{co} \left[ \mathcal{F}_{1/2}(\eta) + (15\alpha kT/4E_i) \mathcal{F}_{3/2}(\eta) \right]$$
 (9)

where  $N_{co}$  denotes  $2(2\pi m_{co}kT/h^2)^{3/2}$ , in terms of  $m_{co}$  and T. It will be seen that the influence of the term involving  $\mathcal{F}_{3/2}(\eta)$  increases with temperature, to an extent that depends on whether the reduced Fermi energy  $\eta$  is negative or positive.

Fog a given temperature, the  $\mathcal{F}_{3/2}(\eta)$  term contributes a larger fraction of the total on the right of eqn (9) if the situation is degenerate  $(n_o \gg N_{co}, \eta \gg 0)$ , since then  $\mathcal{F}_{3/2}(\eta)$  is several times larger than  $\mathcal{F}_{1/2}(\eta)$ . However, the effect of the  $\mathcal{F}_{3/2}(\eta)$  term at any finite temperature does not go away no matter how small the electron density is.

Thus in the non-degenerate limit of  $n_o 
leq N_{co}$ ,  $\eta 
leq 0$ , we have that  $\mathcal{F}_{1/2}(\eta) = \mathcal{F}_{3/2}(\eta) = e^{\eta}$ . Then  $n_o$  exceeds  $N_{co}$   $e^{\eta}$  that a parabolic band would have accommodated, by a factor  $[1 + (15\alpha kT/4E_i)]$ . This factor is about 1.057 for GaAs at room temperature; a matter to be taken into account in weakly n-type, and semi-insulating or near-intrinsic, gallium arsenide [19].

Since both  $\mathcal{F}_{1/2}(\eta)$  and  $\mathcal{F}_{3/2}(\eta)$  are needed for n-type III-V semiconductors (especially when  $n_o$  is large, and degeneracy is encountered), the recent description in this journal by Aymerich-Humet et al.[20] of analytical approximations for both of these F-D integrals has been interesting and welcome. While most of the ensuing sections of this review do concentrate on  $\mathcal{F}_{1/2}(\eta)$ ; on the grounds that this is needed most often for "well-behaved" situations, and in view of the preponderance of expressions developed for that member, the work of Aymerich-Humet et al. is reviewed in Section 4.3.

### 2. MOTIVATIONS FOR PUBLISHED WORK ON F-D INTEGRALS

The past 50 yr have seen numerous published studies, and several tabulations, for various  $F_i(\eta)$  or  $\mathcal{F}_i(\eta)$ , with a variety of motivations. A common factor has been the lack of exact analytic expressions. Those varied motivations are classified in this section.

### 2.1 Modeling of electron transport and other measurable properties

The relevance of F-D integrals to solutions of the Boltzmann transport equation was noted in Section 1.2 and some literature using these integrals for that purpose noted [6-15]. Early work of Nordheim [21] and Stoner [22] was directed towards treatment of the electronic specific heat for a degenerate metal.

A number of studies [23-26] have been inspired by the added complexity in the Einstein relation between diffusion coefficient and mobility for a degenerate electron gas.<sup>‡</sup> That complexity must be invoked whenever drift and diffusion components of current density must

be compared in a device structure that includes strongly doped regions.

### 2,2 Mathematical considerations

Several investigations have been made into the mathematical properties of  $F_i(\eta)$  and/or  $\mathcal{F}_i(\eta)$ , and of their relationships to other mathematical functions. Sommerfeld [2] examined the  $F_i(\eta)$  for strongly degenerate conditions and was concerned with asymptotic mathematical forms that would be suitable for the electron gas of a normal metal. That emphasis continued in the work of Nordheim [21], Stoner [22] and Gilham [27].

These contributed to the basis for a massive 1938 paper containing an analysis (and tabulation) of  $F_{-1/2}(\eta)$ ,  $F_{1/2}(\eta)$  and  $F_{3/2}(\eta)$ , by McDougall and Stoner [28]. The McDougall and Stoner work tackled the much more difficult region *between* non-degenerate and strongly degenerate conditions. Their tabulation in noted again in Section 2.4.

Among other things, McDougall and Stoner [28] produced and displayed the differentiation condition between  $F'_{j}$  and  $F_{j-1}$ . This has been reproduced here, as eqn (3), in the rather simpler relation between  $\mathscr{F}_{j}$  and  $\mathscr{F}_{j-1}$ . The inverse of that relation,

$$\mathscr{F}_{j}(\eta) = \mathscr{F}_{j}(0) + \int_{0}^{\eta} \mathscr{F}_{j-1}(\eta') \,\mathrm{d}\,\eta' \tag{10}$$

has been used in several subsequent studies, as in the work of Rhodes [29] concerning the relation between  $F_i(\eta)$  and  $F_i(-\eta)$ , when j is an integer.

Dingle [4, 30] made extensive studies of the various mathematical properties of the  $\mathcal{F}_j(\eta)$  family. His investigations included the relation between  $\mathcal{F}_j(\eta)$  and  $\mathcal{F}_j(-\eta)$  when j is not an integer: this involves the generalized Riemann zeta function. Dingle also explored the relationships of the  $\mathcal{F}_j(\eta)$  to the  $\mathcal{U}$  and Ei integerals [31, 32], and the representations of the  $\mathcal{F}_j(\eta)$  possible through Mellin transform inversion.

The mathematical foundation laid by Sommerfeld [2], McDougall and Stoner [28], Rhodes [29] and Dingle [4, 30], has underlain various subsequent treatments of expressing the  $F_i(\eta)$  or  $\mathcal{F}_i(\eta)$  to an appropriate number of significant figures. Work with a focus on numerical precision is noted next.

### 2.3 High precision series expansions

Any F-D integral can—in principle—be expressed to any desired degree of precision: regardless of the order j and (more importantly), regardless of where the argument  $\eta$  lies on the range from  $-\infty$  to  $+\infty$ . The necessary proviso in that statement is that mathematical complexity, and the number of terms retained in a possibly cumbersome series expansion, be not considered an impediment.

Thus, Sommerfeld[2] asserted that  $F_j(\eta)$  for the domain  $\eta > 0$  could be represented by a leading term varying as  $\eta^{j+1}$ , with a remainder series in increasing powers of  $\eta^{-2}$ . Deficiencies of this were demonstrated by Rhodes for integer values of j and the more com-

<sup>†</sup>Except for  $F_0(\eta) = \mathcal{F}_0(\eta) = \ln{(1 + e^{\eta})}$ , and  $\mathcal{F}_{-1}(\eta) = (1 + e^{\eta})^{-1}$ . †The Einstein relation is just  $eD_n = kT\mu_n$  for non-degenerate conditions, and becomes  $(eD_n/kT\mu_n) = \mathcal{F}_{1/2}(\eta)/\mathcal{F}_{-1/2}(\eta)]$  when degeneracy enforces a difference between  $\mathcal{F}_{1/2}(\eta)$  and  $\mathcal{F}_{-1/2}(\eta)$ . See Spenke [14], for example.

plicated form of that deficiency when j is *not* an integer was brought out by Dingle [4]. Despite that, for any positive value of  $\eta$ , a combination of any  $\mathcal{F}_j(\eta)$  and its corresponding  $\mathcal{F}_j(-\eta)$  can be expressed as nominally converging infinite series for non-integer j and a polynomial for integer j. As discussed elsewhere [3],

$$\widetilde{\mathscr{F}}_{j}(\eta) - \cos(j\pi)\widetilde{\mathscr{F}}_{j}(-\eta) = \frac{\eta^{j+1}}{\Gamma(j+2)} + \sum_{r=1}^{j} \frac{\alpha_{r}\eta^{j+1-2r}}{\Gamma(j+1-2r)}, \eta > 0.$$
(11)

Here, each of the coefficients  $\alpha_r$  is itself an infinite series,

$$\alpha_r = \sum_{\mu=-1}^{r} 2(-1)^{\mu+1} \mu^{-2r}$$
 (12)

and all  $\alpha_r$  for r > 4 are numerically very close to 2. This is by no means a panacea, because of problems that arise with the summation of eqn (11) when j is not an integer, and  $\eta$  is not large enough to neglect terms of  $r > (j + \frac{1}{2})$ . However, there are ways around these problems [3, 4].

Similarly, it has been known and used since the work of McDougall and Stoner[28] that any F-D integral can be expressed in a series form for  $n \le 0$ .

$$\mathscr{F}_{j}(\eta) = \sum_{r=1}^{\infty} (-1)^{r+1} \exp(r\eta) r^{-j-1}, \, \eta \le 0.$$
 (13)

As one would expect, very few terms of that summation suffice to give any desired numerical accuracy when  $\eta \ll 0$ . It is the situations of  $\eta$  small and negative that make eqn (13) arduous in terms of the number of terms necessary. At least for the limit of applicability for eqn (13), at  $\eta = 0$ , the series does join forces with another well-known mathematical function:

$$\mathscr{F}_{j}(0) = \sum_{r=1}^{5} (-1)^{r+1} r^{-j-1} = [1-2^{-j}] \zeta(j+1)$$
 (14)

where  $\zeta(j+1)$  is the ordinary Riemann zeta function. The property demonstrated by eqn (14) has proved useful in connection with use of Eqn (10)—e.g. in the work of Rhodes [29].

The series of eqns (11) and (13) have encouraged several polynomial forms for F-D integrals. Some have resulted in tables (Section 2.4) and others in itemized recommended formats and coefficients for use with a computer. Among the latter, Werner and Raymann[33] suggested a fifth degree polynomial, for representation of  $F_{1/2}(\eta) = \pm 0.05\%$ . Arpigny[34] gave coefficients for polynomials describing  $F_{3/2}$ ,  $F_{1/2}$  and  $F'_{1/2}$  to an accuracy of 10 °. Similar accuracy was claimed by Battocletti[35]

with an eighth degree polynomial for  $\mathcal{F}_{1/2}(\eta)$  over the range  $-1 < \eta < +12$ . Jones [36] estimated deviations of 10 ° or less with his polynomials for j=0, (1/2), 1, (3/2) and 2; these used Pade approximants in powers of e", based on eqn (13), which satisfied the Chebyshev criterion [37] for deviation minimization. Rational Chebyshev approximations for j=(-1/2), (1/2) and (3/2) were also proposed by Cody and Thacher [38], with accuracy expected to 10 ° or better.

The last paragraph's proposals were all attuned to the availability of substantial computational facilities, true now as never before. Cody and Thacher used a CDC 3600, with 25 decimal floating point arithmetic—a far cry from the "Brunsviga calculating machine" used 28 yr earlier by McDougall and Stoner[28] to generate their tables (Section 2.4), to an accuracy between 5 and 7 significant figures. Many users of F-D integral information can easily have various sets of coefficients stored to generate any  $\mathcal{F}_t(\eta)$  at will, to any imaginable numerical precision.

Many other research workers need F-D integral data of respectable accuracy, but do not have—or do not choose to use—a large computer capability for that purpose. For these workers, tabulations of  $F_i(\eta)$  and  $\mathcal{F}_i(\eta)$  have been published at various times, as itemized in Section 2.4, with interpolation recommended between published values. Numerous analytic approximations have also been proposed, with varying degrees of precision and varying ranges of applicability. The latter give this paper its main purpose, and they are examined in Sections 4 and 5.

The work of Joyce and Dixon[39, 40], referred to again in Section 5.1, has the words "analytic approximations" in the titles; though is in practice a polynomial approach. In contrast to the polynomial forms noted above. Joyce and Dixon expressed  $\eta$  by means of a polynomial in powers of  $\mathcal{F}_{1/2}$ , as a contribution to the interesting 1970s literature on expressing  $E_F$  as a function of  $n_o$ , rather than the other way about.

### 2.4 Published tabulations of F-D integrals

McDougall and Stoner[28] undertook the first major tabulation of  $F_i(\eta)$ , for j=(1/2) and (3/2) to six-figure accuracy; and with lesser precision (by successive differentiations) for j=(-1/2) and (-3/2). Their tabulation is the first entry in Table 1, followed by tabulations and compilations of later years.

Of these, short tables by Wright[12] and by Johnson and Shipley[13], each with a large interval  $\Delta \eta = 1$ , were included in Madelung's tabulation [8] for a large number of j values. The smaller-interval ( $\Delta \eta = 0.1$ ) tabulation by Rhodes[29] for integer j values and  $\eta < 0$  ( to six figure accuracy) was complemented by Dingle's table [4] for  $\eta > 0$  with those same j values.

Tabulations by Beer *et al.*[41] included reprinting the McDougall and Stoner entries for J=-1/2, 1/2 and 3/2 and then extension of the tabulation order for half-integer values as far as j=11/2, using an Euler-Maclaurin numerical integration. Tables of  $\mathcal{F}_j(\eta)$  provided elsewhere by the present writer[3] were based on McDougall and Stoner[28] and Beer *et al.*[41] for half-

 $<sup>^{\</sup>dagger}$ Note that values of 2j, not of j itself, are listed in the last column of Table 1. This was done to avoid having to write fractions for the various half-integer j values that have been tabulated.

<sup>‡</sup>Dingle[4] also provided tables for  $\mathcal{F}_1(\eta)$  and  $\mathcal{F}_0(\eta)$ . Since these particular functions can be expressed analytically, their tabulation was unnecessary.

Table 1. Published tabulations of Fermi-Dirac integrals

Author(s)	Reference		Range of η, and Interval Δη	Values for 2j in This Tabulation †
McDougall and Stoner (1938)	[28]	Fj	-4 (0.1) +20	-1, 1, 3
Rhodes (1950)	[29]	F <sub>j</sub>	-4 (0.1) 0	2, 4, 6, 8
Wright (1951)	[12]	Fj	-4 (1) +20	2, 4
Johnson and Shipley (1953)	[13]	<sup>F</sup> j	-4 (1) +20	4, 6, 7, 9
Beer, Chase & Choquard (1955		Fj	-4 (0.1) +20	-1, 1, 3, 5, 7, 9, 11
Madelung (1957	) [8]	F <sub>j</sub>	-4 (1) +20	-2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14
Dingle (1957)	[4]	<b>F</b> j and	-4 (0.1) +10 d 0 (0.1) +10	-2, 0 2, 4, 6, 8
Blakemore (1962, 1982)	[3]	<b>*</b> j	-4 (0.1) +4 +4 (0.2) +10	-3, -2, -1, 0, 1, 2, 3, 4, 5, 6, 7, 8

<sup>\*</sup>Note that the column at the right of this table lists values for 2j, not for j itself. This is done to avoid printing a fraction for every half-integer value of the order j.

integer j values, and on Rhodes [29] and Dingle [4] for integer j values.

The existence of these tables has not curbed attempts at providing analytic approximations of usable accuracy, especially for  $F_{1/2}(\eta)$  or  $\mathcal{F}_{1/2}(\eta)$ . Since that function is used so often in connection with the  $n_o \rightleftharpoons E_F$  relation for a "standard parabolic" band, attempts at modeling that relation take up most of Sections 4 and 5.

# 2.5 Analytic approximation of $\mathcal{F}_{1/2}(\eta)\equiv u$ , and its inverse A shorthand terminology for $\mathcal{F}_{1/2}(\eta)$ is useful when this function is to be quoted many times. In what follows, the terminology $\mathcal{F}_{1/2}(\eta)\equiv u$ suggested by Nilsson[26] is followed.

Literature from 1928 to 1970 for this function was always concerned with description of u as a function of  $\eta$ ; the thrust from a knowledge of  $E_F$  towards a description of  $(n_o/N_c)$  for a parabolic band. Some more recent work [20, 42] has continued towards analytic representation of  $u(\eta)$ , and Section 4 reviews the essence of what is available on the subject. The various analytic approximations for  $u(\eta)$  provide accuracies of from  $\pm 2\%$  to  $\pm 0.2\%$ , commensurate with the precision of typical experimental data for dopant and carrier densities in semiconductor bulk material and device structures. For the minority of real-life situations which mandate precision to many significant figures, a computer-based polynomial approach [35–38] is advisable.

It is common for carrier density  $n_o$  to be known, with

a desire then to evaluate  $E_F$ . That is best done with an expression for  $\eta(u)$  rather than of  $u(\eta)$ , and Nilsson[26, 43] and Joyce and Dixon[39, 40] have both described simulation of  $\eta(u)$ . This is reviewed in Section 5.

### 3. THE MEANING OF ACCURACY IN APPROXIMATIONS FOR $\eta(U)$ and $\mathrm{U}(\eta)$

The implications of "accuracy" depend on whether  $E_F$  is being used to describe  $n_o$  through  $u(\eta)$ , or the other way about. For as  $\eta$  changes from negative to positive values with increasing  $n_o$ , the form of u changes from  $e^{\eta}$  to  $\eta^{3/2}$  behavior. That alters the balance between the sensitivity of u to an error  $\Delta \eta$ , and of  $\eta$  to a fractional error  $(\Delta u/u)$ , as illustrated by Fig. 1.

The abscissa scales of Fig. 1 cover a range from tolerably non-degenerate conditions at the left  $(\eta = -2, u \approx 0.13)$  to fairly degenerate conditions at the right  $(\eta = +10, u \approx 24)$ . Now an error  $\Delta \eta \equiv (\eta_{\rm calc} - \eta)$ , and the corresponding fractional error  $(\Delta u/u)$  are numerically the same for a non-degenerate situation. That results from the  $\mathcal{F}_i(\eta) \rightarrow e^{\eta}$  asymptotic behavior for  $\eta \ll 0$ , and the description

$$e = \lim_{n \to \infty} (1 + 1/n)^n$$
 (15)

for the base of Naperian logarithms.

The relative error sensitivity is quite different for

degenerate situations. Just as far as the right edge of Fig. 1,  $\Delta \eta$  can be seen to be seven times larger than  $(\Delta u/u)$ . For *strong* degeneracy, when any  $\mathcal{F}_j(\eta)$  is given by the first term on the right of eqn (11), so that inversion provides  $\eta \rightarrow (3\sqrt{(\pi)}u/4)^{2/3}$ , then

$$\Delta \eta \rightarrow (2\eta/3)(\Delta u/u), \ \eta \geqslant 0.$$
 (16)

That makes it easier to construct an expression modeling  $u(\eta)$  for strong degeneracy, as needed to progress from  $E_F$  data towards carrier density. By the same token, it is especially difficult to hold down the errors in devising an expression to model  $\eta(u)$  for strong degeneracy, as needed to evaluate  $E_F$  corresponding to a known (large)  $n_o$ . That difficult task motivated Nilsson in proposing four analytical expressions [26, 43], and also led Joyce and Dixon[39, 40] to evaluate series approximations—as reported in Section 5.

### 4. USEFUL APPROXIMATIONS FOR $\mathbf{u} \equiv \hat{\mathcal{F}}_{1/2}(\eta)$

### 4.1 Starting from the degenerate extreme

Equation (11) has often been used as a starting point in attempts to model  $u(\eta)$  when  $\eta$  is positive but not necessarily very large. An obliging feature of the half-integer values of j is that the term in  $\mathscr{F}_j(-\eta)$  has a coefficient  $\cos(j\pi) = 0$ . Equation (11) for j = 1/2 thus comes down to

$$u = (4/3 \sqrt{\pi}) \eta^{3/2} [1 + (\pi^2/8 \eta^2) - (7\pi^4/640 \eta^4) + \dots].$$
(17)

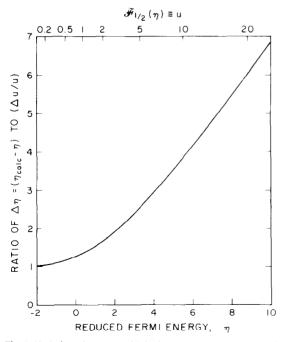


Fig. 1. Variation of error sensitivity in computing reduced Fermi energy  $\eta$  as compared with computing  $\mathcal{F}_{1/2}(\eta) = u$ , as one progresses from non-degeneracy into the degenerate domain. For  $\eta \leq 0$ , the quantities  $\Delta \eta = (\eta_{\text{calc}} - \eta)$  and  $(\Delta u/u)$  are the same; whereas  $\Delta \eta \approx (2\eta \Delta u/3u)$  for  $\eta \geq 0$ .

Some crude approximations have been tried of the type

$$u \approx (4/3 \nabla \pi) \eta^{3/2} (1 + A/\eta^2)$$
 (18)

with  $A \approx \pi^2/8$  as the starting point. An alternative, of

$$u \approx (4/3\sqrt{\pi})(n^2 + B)^{3/4}$$
 (19)

has also been proposed [16], with  $B \approx \pi^2/6$ , but this is unable to do very much about increasing the range of  $\eta$  downwards at an acceptable accuracy. Attempts at adding further terms to eqns (18 or (19) have been unrewarding. Expressions that *start* correctly from the non-degenerate end provide a better basis for describing  $u(\eta)$  when  $\eta \approx 0$ , and these are noted next.

### 4.2 Starting from the non-degenerate end

Equation (13) gave  $\mathcal{F}_j(\eta)$  in series form for  $\eta \le 0$ . The terms of the series for  $j = \frac{1}{2}$  are

$$u = e^{\eta} - (e^{2\eta}/\sqrt{8}) + (e^{3\eta}/\sqrt{27}) - (e^{4\eta}/8) + \dots$$
 (20)

This converges rapidly when  $\eta \ll 0$ , but much less efficiently as  $\eta$  approaches zero. Proposals were made [16, 44–46] in the 1950s to simulate  $u(\eta)$  up to modest degeneracy by a form

$$u \approx (e^{-u} + \xi)^{-1} \tag{21}$$

with  $\xi$  a constant parameter. Thus one can hold the fractional error  $|\Delta u/u| < 0.03$  for the range  $-\infty \le \eta \le +1.3$  (i.e.  $u \le 2$ ) by use of the value  $\xi \approx 0.27$  [16]. In conjunction with eqn (19) using  $B \approx \pi^2/6$ , it is thus possible to cover the entire range with modest accuracy. Fortunately, work reported in recent years has made this procedure, with a switch in equations about  $\eta \approx +1$ , quite unnecessary.

For two groups of investigators have recently described analytical formulae that cover  $u(\eta)$  continuously for  $-\infty \le \eta \le +\infty$  with a single (necessarily rather complicated) expression. These two formulae are now described in Section 4.3. Each is an outgrowth of eqn (21), but with  $\xi$  made a function of  $\eta$ .

### 4.3 Expressions for $u(\eta)$ valid for all values of $\eta$

Suppose, as indicated in the last sentence, that eqn (21) be elaborated to

$$u(\eta) = [e^{-\eta} + \xi(\eta)]^{-1}. \tag{22}$$

What attributes must  $\xi(\eta)$  have, in order to cover the complete range from non-degeneracy to total degeneracy? Three needed attributes are: (i) For non-degenerate conditions  $(\eta < 0)$ , one needs  $\xi(\eta) < e^{-\eta}$ . (ii) When  $\eta$  is negative but small,  $\xi(\eta)$  must increase, to retard the growth rate of  $u(\eta)$ . [That was the reasoning behind proposals of a finite  $\xi$  in eqn (21).] (iii) The term  $e^{-\eta}$  soon ceases to be a controlling influence when  $\eta$  becomes positive.  $\xi(\eta)$  must then assume complete control. It must thus be asymptotic to  $(3\sqrt{\pi}/4\eta^{3/2})$  for  $\eta > 0$ , in order to provide the leading term of eqn (17).

Bednarczyk and Bednarczyk[42] proposed the use of eqn (22) with

$$\xi = 3\sqrt{(\pi)/4\nu^{3/8}}.$$
 (23)

Here,  $\nu(\eta)$  signifies the function

$$\nu(\eta) = \eta^4 + 50 + 33.6 \ \eta \{1 - 0.68 \exp \left[ -0.17(\eta + 1)^2 \right] \}. \tag{24}$$

This may look a little ungainly, but it does work. Equations (23) and (24) are constructed so that  $\xi(\eta)$  is trivially small for  $\eta \le 0$ , rises to a maximum  $\xi_{\text{max}} = 0.34$  for  $\eta = -1.5$ , and then decreases again when  $\eta$  becomes positive, decreasing in a fashion which is asymptotically correct to endow  $u(\eta)$  with the properties of eqn (17) for strong degeneracy.

Figure 2 shows the fractional error  $(\Delta u/u)$  associated with the use of eqns (22)–(24). The abscissa of the figure covers the range  $-10 \le \eta \le +25$ , a range in which u increases from  $\sim 10^{-4}$  to nearly 100. It can be seen that  $|\Delta u/u| < 0.004$  throughout that range. This is accurate enough for the vast majority of applications involving carrier density in a semiconductor sample, or through the various parts of a device structure.

One might well have thought that the accuracy provided by the single procedure of eqns (22)–(24) would have tended to discourage further attempts at modeling  $u(\eta)$ , at least for a time. However, a different approach at modeling  $\xi(\eta)$  of eqn (22) was proposed only 3 yr after the work of Bednarczyk and Bednarczyk, in a paper in this journal, by Aymerich-Humet et al.[20]. These workers had two objectives in mind: (i) A less complicated formulation for  $\xi(\eta)$ , without excessive sacrifice of accuracy; and with, naturally, retention of proper asymptotic behavior. (ii) A means of describing a common algebraic form for  $\xi_i(\eta)$  to serve for both j=1/2 and j=3/2, with—of course—the opportunity to make some of the numerical parameters specific to the order. Three such parameters were individually set.

Thus Avmerich-Humet et al. used a fit of the form

 $\xi_j(\eta) = 2^{j+1} \Gamma(j+2) [(\eta+b) + (|\eta-b|^c + a)^{1/c}]^{-j}$ 

$$\mathcal{F}_i(\eta) = \left[ e^{-\eta} + \xi_i(\eta) \right]^{-1} \tag{25}$$

where

Fig. 2. The fractional error  $(\Delta u/u)$  involved in the representation of  $u(\eta)$  by eqns (22) through (24), as proposed by Bednarczyk and Bednarczyk [42].

For order j = 1/2 (i.e. for the function u), the recommended values for the parameters a, b and c, were:-

$$\begin{array}{l}
 a = 9.60 \\
 b = 2.13 \\
 c = 2.40
 \end{array}
 \text{ for } j = +1/2 \tag{27}$$

so that

$$\xi_{1/2}(\eta) = 3\sqrt{(\pi/2)[(\eta + 2.13) + (|\eta - 2.13|^{2.4} + 9.6)^{5/12}]^{-3/2}}.$$
(28)

The curve in Fig. 3 labelled j = +1/2 indicates the fractional error  $(\Delta u/u)$  associated with the use of eqns (25) and (28) in modeling the behavior of  $u = \mathcal{F}_{1/2}(\eta)$ .

Aymerich-Humet *et al.* recommended, for j = +3/2, parameter values

$$\begin{cases}
 a = 14.9 \\
 b = 2.64 \\
 c = 2.25
 \end{cases}
 \text{ for } j = +3/2$$
(29)

so that

$$\xi_{3/2}(\eta) = 15\sqrt{(\pi/2)[(\eta + 2.64) + (|\eta - 2.64|^{2.25} + 14.9)^{4/9}]^{-5/2}}.$$
 (30)

The fractional error  $(\Delta \mathcal{F}/\mathcal{F})$  associated with the use of eqn (30) in eqn (25) is shown as the j = +3/2 error curve in Fig. 3.

For both of the orders represented by Fig. 3, the error oscillates in sign several times. As Aymerich-Humet *et al.* had pointed out [20], the maximum error excursions for  $\mathcal{F}_{1/2}(\eta)$  slightly exceed  $\pm 0.5\%$ . Thus the function is not constrained within limits *quite* as close as is possible using eqns (22)–(24). The difference in error limits is probably not the major factor in a decision as to whether one or other of these approaches is a good one for one's specific needs. Either one is easy to program for even a microcomputer. However eqn (28) is simpler for a pocket-type calculator. One gratifying feature of the j=+1/2 curve in Fig. 3 is that this does show a decisive approach to the strongly degenerate asymptotic requirements.

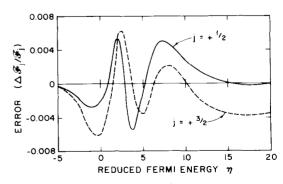


Fig. 3. The fractional errors involved in representation of  $\mathcal{F}_j(\eta)$  for the two values j = +1/2 and j = +3/2 in the manner proposed by Aymerich-Humet *et al.*[20]. Equation (28) describes the function  $\xi_{1/2}(\eta)$  to be used in eqn (25) for order j = +1/2; while  $\xi_{3/2}(\eta)$  from eqn (30) is used in the case of j = +3/2.

In that last regard, the parameters of eqn (29), for  $j=\pm 3/2$ , do not appear to work quite so well. There is less precision when  $\eta \sim 0$ , while an error near -0.4% seems to continue persistently as strong degeneracy is attained. Nevertheless, it is decidedly useful to have this expression available for  $\mathcal{F}_{3/2}(\eta)$ . It can be expected that this will be of assistance both in connection with electronic transport in moderately degenerate semiconductor situations and for description of the relation between total electron density and Fermi energy for non-parabolic bands—as happens in GaAs [19] and other semiconductors. For that purpose, characterization of  $\mathcal{F}_{3/2}(\eta)$  within  $\pm 1\%$  limits is amply good enough in normal circumstances.

### 5. APPROXIMATIONS FOR REDUCED FERMI ENERGY AS FUNCTION OF $u = \tilde{x_1}, s(\eta)$

Expressions such as those of eqns (21) and (22) are intended for obtaining u (and hence  $n_o$ ) from data concerning  $\eta$  (i.e. a known  $E_F$ ). What if the free carrier density is known, and the Fermi energy is to be found—a very common circumstance. Suitable expressions were not proposed until comparatively recently, in the work of Nilsson[26, 43], and of Joyce and Dixon[39, 40].

Now as a first and over-simplified procedure, eqn (21) can be inverted to be written

$$\eta = -\ln[(1/u) - \xi]$$
 (31)

This can provide a modest improvement over  $\eta = \ln(u)$ , valid only for completely non-degenerate conditions. With a constant value for  $\xi$  in eqn (31) [such as the value  $\xi = 0.27$  noted in connection with eqn (21)], one may hope to progress as far as  $E_F = (E_c + kT)$ , but not much further. There is thus ample room for improvement, and such improvements have materialized.

### 5.1 Joyce and Dixon's series approach

That limitation on the utility of eqn (31) with a fixed value for  $\xi$  led Joyce and Dixon[39] to examine series solutions for n, with  $\ln(u)$  as the first term:-

$$\eta = \ln(u) + A_1 u + A_2 u^2 + A_3 u^3 + A_4 u^4 + \dots$$
 (32)

They arrived at appropriate values for the coefficients  $A_1$ ,  $A_2$ , etc., from the inversion properties of eqn (13). That procedure yielded a set of numbers of which the first four are

$$A_{1} = +3.5355 \times 10^{-1} = \sqrt{1/8}$$

$$A_{2} = -4.9501 \times 10^{-3} = \left[ (3/16 - \sqrt{1/27}) \right]$$

$$A_{3} = +1.4839 \times 10^{-4} = \left[ \frac{1}{8} + \frac{5}{24\sqrt{2}} - \frac{\sqrt{6}}{9} \right]$$

$$A_{4} = -4.4256 \times 10^{-6} = \left[ \frac{1585}{6912} + \frac{5}{16\sqrt{2}} - \frac{5}{8\sqrt{3}} - \frac{1}{\sqrt{125}} \right]$$
(33)

When eqn (32) is used with the four coefficients from eqn (33), the resulting error  $\Delta \eta \equiv (\eta_{\rm cale} - \eta_{\rm true})$  in rendering  $\eta$  from information about electron density is shown as curve (A) in Fig. 4.

Curve (A) shows that the error  $\Delta \eta$  increases monotonically, in the negative direction. It reaches  $\Delta \eta \simeq -0.01$  by the time  $\eta \simeq +5.5$ , corresponding to  $u \simeq 10$ . As can be verified from the curve in Fig. 1, an imperfection in one's knowledge of carrier density of some 0.25% would also produce an error  $|\Delta \eta| \simeq 0.01$ , for a situation of  $\eta \simeq +5$ .

Since the coefficients of eqn (33) make the magnitude of  $\Delta \eta$  rise monotonically, one could envisage a slightly modified set of coefficients that might do a little better. It might be preferable to let  $\Delta \eta$  alternate in sign, while  $|\Delta \eta|$  stayed within desired bounds up to a larger  $u_{\rm max}$ .

Getting further than  $u_{\max} \approx 10$  was not the primary concern of Joyce and Dixon[39]. Their main interest was deduction of  $E_F$  for the doping strengths used in diode lasers. Joyce [40] subsequently looked at shorter polynomia, for when the range of  $\eta$  requiring coverage does not go far above zero. Thus one may verify that, with  $A_1$  and  $A_2$  slightly modified, and all  $A_m$  set at zero for m > 2, then the simple expression

$$\eta = \ln(u) + 0.36u - 0.005u^2 \tag{34}$$

is a viable possibility. This provides an error  $\Delta \eta$  which is at first positive, and changes to negative as the degeneracy increases, but with  $|\Delta \eta| < 0.03$  up to the condition  $\eta = +5$ , u = 9.

### 5.2 Nilsson's "Square Root" approach

In 1973, Nilsson [26] proposed two expressions for  $\eta(u)$ . Each was designed to model  $\eta(u)$  for the entire range, from the non-degenerate conditions of  $u \le 1$ ,  $\eta \le 0$ , to strong degeneracy situations of  $u \ge 1$ ,  $\eta \ge 0$ . It was thus essential that each of these expressions be constructed so as to become asymptotically correct for both extremes. Nilsson's proposals for fulfilling those requirements are described in Section 5.3.

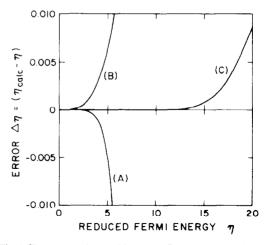


Fig. 4. The error  $\Delta\eta$  incurred in three different representations of  $\eta(u)$ , all intended to work from complete non-degeneracy *into* the degenerate region—but none designed to work when  $u \to \infty$ . (A) The approach of Joyce and Dixon[39], using eqn (32) with the coefficients of eqn (33). (B) Equation (35), as proposed by Nilsson[43]. (C) The more complicated expression of eqn (36) that Nilsson proposed.

It is useful first to examine two rather simpler expressions that Nilsson proposed some 5 yr later [43]. These are asymptotically correct for  $u \le 1$ , but not for the opposite extreme. From comments made by Nilsson in this later paper, it would appear that his renewed activity was prompted by the work of Joyce and Dixon.

A constraint adopted by Nilsson in his 1978 equations was that successive square root operations be employed, since that capability is to be found on almost any pocket calculator. Nilsson could well have been more demanding, since advances in solid-state electronics provide more complicated keystroke capabilities for calculators with each passing year. At any rate, one of the two 1978 proposals of Nilsson [43] was

$$\eta = \ln(u) + u(64 + 3.6u)^{-1/4}. \tag{35}$$

Curve (B) of Fig. 4 shows the error  $\Delta \eta$  resulting from the use of eqn (35). Note that the error is opposite in sign from curve (A) [which had used eqn (32), with the eqn (33) coefficient set]. For either curve (A) or (B), it can be seen that  $\eta_{\text{max}} = +5.5$ ,  $u_{\text{max}} = 10$ , if it is desired that  $|\Delta \eta| \leq 0.01$ .

A second, and more complicated, expression proposed by Nilsson in that 1978 paper was

$$\eta = \ln(u) + u[64 + 0.05524u(64 + \sqrt{u})]^{-1/4}.$$
 (36)

As with eqn (35) and as with eqn (32) of Joyce and Dixon's work, this has an unadorned ln(u) for its first term. The error  $\Delta \eta$  resulting from use of eqn (36) is shown as curve (C) of Fig. 4. Quite clearly apparent from Fig. 4 is that eqn (36) does a great deal better than either of the other expressions represented in that figure, up to a very large electron density.

Equation (36) does in fact generate an error  $\Delta \eta$  with several alternations of sign in the range  $0 < \eta < 12$ , but with peak excursions  $|\Delta \eta_{\rm max}| < 10^{-4}$  that are imperceptible on the scale of Fig. 4. For  $\eta > 12$ , the error does rise monotonically, but has reached only  $\Delta \eta \approx 0.01$  for  $\eta \approx +20$  ( $u \approx 67$ ) as the figure shows. Even for  $\eta \approx +25$  ( $u \approx 95$ ), the error still has the very modest value  $\Delta \eta \approx 0.03$ .

From a pedantic point of view, one may note that neither of eqs (35) or (36) could be asymptotically correct for  $u \to \infty$ . For to be asymptotically proper for maximum degeneracy, it is required that  $\eta$  vary as  $u^{2/3}$ , in view of eqn (11). In contrast, the strong degeneracy limit for the right side of eqn (35) is  $u^{3/4}$ , while that of eqn (36) is  $u^{5/8}$ .

The restriction noted in the last paragraph is certainly significant from a mathematical standpoint. The practical consequences are unlikely to be severe, however, for discussing the relation between  $n_o$  and  $E_F$  in a doped semiconductor, except for a situation of a non-zero but

modest  $n_o$  as  $T \rightarrow 0$ . That assertion is made since very heaving doping, as necessary to make  $n_o$  exceed (say)  $50N_c$  for a more "ordinary" temperature (from the liquid nitrogen range upwards) will usually cause enough impurity banding and band tailing to modify g(E) significantly from its "pure semiconductor" form. Thus even if eqn (4) is valid in the weakly doped forms of the semiconductor, eqns (4) and (5) become invalid with heavy doping, to an extent that depends specifically on the semiconductor host and on the impurity species [47, 48], as well as upon  $N_d$ .

What about using a form of  $\eta(u)$  that is to be valid up to  $u \gg 1$  in order to describe the quasi Fermi levels for a highly excited non-equilibrium condition? These are of considerable significance in various kinds of active device. One should not, however, pretend excessive accuracy for many of these situations in which the large carrier population is imperfectly thermalized over the band states.

Thus situations of large  $n_o$ , or of large non-thermal n and p, need to be handled with appropriate caution. Even so, it is useful that expressions for  $\eta(u)$  were suggested in 1973 by Nilsson[26] that did track the entire range of u and  $\eta$ .

### 5.3 Nilsson's full range proposals for $\eta(u)$

Each of the two expressions proposed by Nilsson[26] for  $\eta(u)$  was asymptotic to  $\ln(u)$  for  $u \le 1$ , and to  $(3\sqrt{(\pi)u/4})^{2/3}$  for  $u \ge 1$ . Of the two, one required more fitting parameters than the other, and accordingly enjoyed smaller excursions of  $\Delta \eta$ . The simpler of these two can be written

$$\eta = \frac{\ln(u)}{1-u} + (3\sqrt{(\pi)}u/4)^{2/3} + \frac{8\sqrt{(\pi)}u}{3(4+\sqrt{(\pi)}u)^2}.$$
 (37)

It can readily be seen that the first term on the right controls  $\eta$  for small u, and the second for very large u. The final term is empirically constructed to perform the "bridging" function. Curve (A) of Fig. 5 shows the error  $\Delta \eta = (\eta_{\text{calc}} - \eta_{\text{true}})$  that results from the use of eqn (37).

When eqn (37) is employed, the error, oscillatory in sign, has  $|\Delta\eta| > 0.01$  for  $\eta \approx +2$ , and again for  $\eta \approx -1$ . The latter of these is equivalent to about a 1% error in  $(\Delta u/u)$ . The further lobe of error with a maximum for  $\eta \approx -5$  is slightly smaller in terms of  $\Delta\eta_{\rm max}$ , and in terms of its connotation for an equivalent  $(\Delta u/u)$ . Thus if one is able to deduce the electron or hole density in a semiconductor to a 1% accuracy (a quite typical situation), eqn (37) is quite good enough for deduction of the corresponding  $E_F$  behavior.

The second, and more elaborate, expression that Nilsson[26] suggested for full range coverage can be written

$$\eta = \frac{\ln(u)}{1 - u^2} + \frac{(3\sqrt{(\pi)u/4})^{2/3}}{1 + [0.24 + 1.08(3\sqrt{(\pi)u/4})^{2/3}]^{-2}}.$$
 (38)

The error curve of  $\Delta \eta$  resulting from use of eqn (38) is shown as curve (B) in Fig. 5. The numbers 0.24 and 1.08 in eqn (38) were chosen empirically to minimize the error

<sup>&</sup>lt;sup>†</sup>Equation (36) is obviously inappropriate for a metal, where the quantized free electron model gives  $E_{F0} = (h^2/8 m_o)(3 n_o f \pi)^{2/3}$  as the low temperature form. With  $m_c$  substituted from  $m_0$ , that is also proper when weak impurity banding keeps  $n_o$  finite down to the lowest temperatures.

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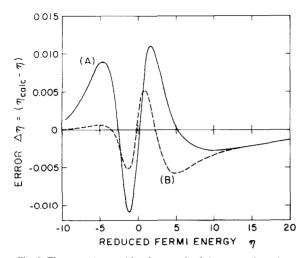


Fig. 5. The error  $\Delta \eta$  resulting from each of the expressions that Nilsson[26] proposed to represent  $\eta(u)$  for any value of  $\eta$ , negative or positive; i.e. from  $u \le 1$  to  $u \ge 1$ . (A) With  $\eta(u)$  simulated by eqn (37). (B) Using eqn (38) to represent  $\eta(u)$ .

in the middle part of the range. A comparison of curves (A) and (B) in Fig. 5 shows that  $|\Delta \eta_{\rm max}|$  excursions for the latter are only about one-half as large as in the former case.

For fairly strong degeneracy (u > 25,  $\eta > +10$ ), the two error curves in Fig. 5 are very similar. That is *not* the case for a non-degenerate semiconductor (u < 0.02,  $\eta < -4$ ), where curve (B) shows that eqn (38) does very well, while eqn (37) as portrayed by curve (A) is noticeably less satisfactory. That is, in practice, a significant distinction only if electron concentration data are reliably known to a small fraction of a percent.

Thus, by means of eqns (37) or (38) as considered necessary and/or convenient,  $E_F$  can be deduced when both temperature and the equilibrium carrier density are known. This is much more convenient than having to deduce  $\eta$  by interpolation among entries in a table of  $u(\eta)$ . And so, simple and useful approximations of respectably high accuracy are now available for deduction of either  $\eta(u)$  or  $u(\eta)$ , as desired.

### 6. CONCLUDING COMMENTS

The situation for  $u(\eta)$  and for its inverse,  $\eta(u)$ , is thus rather satisfactory now. However this does not mean to say that other suggestions that accomplish the work of eqns. (23) and (24), or of eqn (28), in characterizing  $\xi_{1/2}(\eta)$  for the purposes of  $u(\eta)$ , will not be forthcoming. Alternatives to eqns (36)–(38) for describing  $\eta(u)$  may well be proposed also, possibly using functional forms that Nilsson eschewed and which are now readily available as pocket calculator keystroke operations.

For Fermi-Dirac integrals of order other than j = +(1/2), the proposal in eqn (30) for j = 3/2 has been the only evidence of any recent interest. There are certainly opportunities here for the quiet investigator, though

with a prospective reader and user audience of modest

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