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Numerical method for calculation of the Fermi integrals

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Abstract. A general numerical method for calculation of the Fermi integrals based on the approximation of a dilogarithm by a series of Chebyshev polynomials is developed. The accuracy of the method proposed is analysed in detail. As an example, the Fermi integral of the model electron density for iron at the Curie temperature is considered.

1. Introduction

The calculation of many quantities in solid state physics, and in particular the electron density and total energy, local magnetic moments and susceptibilities, is reduced to the computation of the so-called Fermi integrals

$$I = \int_{-\infty}^{\infty} g(\varepsilon) f(\varepsilon)\, \mathrm{d}\varepsilon \tag{1.1}$$

where $g(\varepsilon)$ is an arbitrary function, vanishing at $\varepsilon \to -\infty$ and increasing not faster than any power of ε at $\varepsilon \to +\infty$, and $f(\varepsilon) = [\exp((\varepsilon - \mu)/T) + 1]^{-1}$ is the Fermi function. (Henceforth the temperature is expressed in energy units.)

In the general case the calculation of integrals (1.1) is a very complicated problem, but in two important particular cases this problem is essentially simplified: for metals in the free-electron model and for non-degenerate semiconductors with $g(\varepsilon)$ in the form of a power function.

First we consider the situation in metals ($\mu/T \gg 1$). Integrating (1.1) by parts we have

$$I = \int_{-\infty}^{\infty} \phi(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \mathrm{d}\varepsilon \tag{1.2}$$

where

$$\phi(\varepsilon) = \int_{-\infty}^{\varepsilon} g(\varepsilon')\, \mathrm{d}\varepsilon'. \tag{1.3}$$

Because of the delta-shaped character of the function $-\partial f/\partial \varepsilon$, only the values of ε close to μ contribute to the integral (1.2). Therefore, assuming that the function $g(\varepsilon)$ is sufficiently smooth in the neighbourhood of $\varepsilon = \mu$, it is natural to use the Taylor series expansion of $\phi(\varepsilon)$ in powers of $\varepsilon - \mu$ and by simple calculations (see, e.g., [1]) we obtain

$$I^T = \int_{-\infty}^{\mu} g(\varepsilon)\, \mathrm{d}\varepsilon + \frac{\pi^2}{6} T^2 g'(\mu) + \frac{7\pi^4}{360} T^4 g'''(\mu). \tag{1.4}$$

In the free-electron approximation, usually the first two terms are retained in (1.4). However, beyond the free-electron approximation it is difficult to use equation (1.4). Firstly, in real

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calculations the function $g(\varepsilon)$ as a rule is not analytic but tabular, and computing the derivatives $g^{(n)}(\mu)$ represents an independent (ill-posed!) problem. Secondly, and above all, in the majority of metals the function $g(\varepsilon)$ is not sufficiently smooth in the neighbourhood of μ, even in the simplest case, when it represents the electron density of states (see, e.g., [2]).

In [3], it has been shown that singularities of the density of states $\nu(\varepsilon)$ can have a substantial and sometimes even decisive influence on the temperature dependence of the physical quantities. For example, a sharp break in $\nu(\varepsilon)$ at some point ε_0 chose to μ results in the appearance of a contribution different from T^2 in the temperature dependence of the unenhanced magnetic susceptibility. Similar results should be expected also for other physical quantities expressed in terms of the Fermi integrals.

Now we consider the situation in semiconductors. In the case of non-degenerate semiconductors ($-\mu/T \gg 1$) the Fermi function is simplified to $f(\varepsilon) \simeq A\exp(-\varepsilon/T)$, i.e. it transfers to the Maxwell–Boltzmann distribution with the normalization constant $A = \exp(\mu/T)$ and, when $g(\varepsilon)$ is the power function, the integral (1.1) can be calculated analytically. For degenerate semiconductors the integrals (1.1) cannot be calculated analytically for any $g(\varepsilon)$ but the constant. In this case, Fermi integrals with $g(\varepsilon) \sim \varepsilon^j$ arise, where j is an integer or a half-integer value. All previous research is devoted to approximations for precisely such integrals (see, e.g., [4, 5] and references therein).

However, at present it is necessary to compute repeatedly various Fermi integrals for tabular functions $g(\varepsilon)$ (see, e.g., [6]). In this connection in the present paper we suggest a simple numerical method for calculation of the integrals (1.1). Its accuracy is analysed in detail. As an example, the Fermi integrals involving the model density of states of iron are calculated.

2. Method

First let us linearly interpolate the tabular function $g(\varepsilon)$ by the formula

$$g(\varepsilon) = \sum_{i=1}^{N} \Delta g_i'(\varepsilon - \varepsilon_i)\theta(\varepsilon - \varepsilon_i) \tag{2.1}$$

where N is the number of sites and $\theta(x)$ is a step function equal to zero at $x < 0$ and unity at $x \geqslant 0$;

$$\begin{aligned} &\Delta g_1' = g_1' \qquad \Delta g_i' = g_i' - g_{i-1}' \qquad i = 2, 3, \ldots, N-1 \qquad \Delta g_N' = -g_{N-1}' \\ &g_i' = (g_{i+1} - g_i)/(\varepsilon_{i+1} - \varepsilon_i) \qquad g_i \equiv g(\varepsilon_i) \qquad i = 1, 2, \ldots, N-1. \end{aligned} \tag{2.2}$$

Substitution of (2.1) into (1.1) gives

$$I = \sum_{i=1}^{N} \Delta g_i' \int_0^\infty f(\varepsilon, \xi_i, T)\varepsilon \,\mathrm{d}\varepsilon = -\tfrac{1}{2}\sum_{i=1}^{N} \Delta g_i' \int_0^\infty \varepsilon^2 \frac{\partial f(\varepsilon, \xi_i, T)}{\partial \varepsilon}\,\mathrm{d}\varepsilon \tag{2.3}$$

where $\xi_i = \mu - \varepsilon_i$.

Next let us consider an integral of more general form than the integral in (2.3):

$$J_n(\xi, T) = \int_0^\infty \varepsilon^{n+1} \frac{\partial f(\varepsilon, \xi, T)}{\partial \varepsilon}\,\mathrm{d}\varepsilon \qquad n = 0, 1, 2, \ldots. \tag{2.4}$$

Integrating by parts we obtain

$$J_n(\xi, T) = -(n+1)\int_0^\infty f(\varepsilon, \xi, T)\varepsilon^n \,\mathrm{d}\varepsilon$$

$$= (n+1)T\int_0^\infty \varepsilon^n \,\mathrm{d}\left\{\ln\left[1+\exp\left(-\frac{\varepsilon-\xi}{T}\right)\right]\right\}. \tag{2.5}$$

At $n = 0$ this integral is calculated analytically:

$$J_0(\xi, T) = -T F_0(-\xi/T) \tag{2.6}$$

$$F_0(x) = \ln[1+\exp(-x)]. \tag{2.7}$$

At $n = 1, 2, \ldots$, it is reduced to the iterated integral

$$J_n(\xi, T) = -(n+1)!T^{n+1}F_n(-\xi/T) \tag{2.8}$$

$$F_n(x) = \int_x^\infty \mathrm{d}x_n \int_{x_n}^\infty \mathrm{d}x_{n-1}\ldots\int_{x_2}^\infty \ln[1+\exp(-x_1)]\,\mathrm{d}x_1. \tag{2.9}$$

It is easy to prove that for $F_n(x)$ the following recursion relations are valid:

$$F_n(-|x|) = D_n(|x|) + F_n(0) \tag{2.10}$$

$$D_n(|x|) = \int_0^{|x|} D_{n-1}(t)\,\mathrm{d}t + |x|F_{n-1}(0) \tag{2.11}$$

$$D_0(|x|) = \ln[1+\exp(|x|)] - F_0(0). \tag{2.12}$$

These relations can be used to calculate $F_n(x)$ at $x < 0$. Equations (2.8)–(2.11) have been given in [3], but without their proofs. Brief proofs of all equations (2.8)–(2.12) are given in appendices 1 and 2.

We dwell on the calculation of $F_n(x)$ at $x \geqslant 0$. The integrals (2.9) cannot be analytically calculated. Substituting the power series of $\ln[1+\exp(-x)]$ into (2.9) and integrating term by term, which is valid because of uniform convergence of the series at $x \geqslant 0$, we obtain

$$F_n(x) = \sum_{k=1}^\infty (-1)^{k+1}\frac{\exp(-kx)}{k^{n+1}}. \tag{2.13}$$

Hence, at $x \to \infty$ the function $F_n(x)$ decreases as $\exp(-x)$, and at zero it has the value

$$F_n(0) = (1-2^{-n})\zeta(n+1) \tag{2.14}$$

where $\zeta(m)$ is the Riemann zeta function. Taking into account the asymptotic value at infinity, the following simple approximate formula [3] can be used for calculation of $F_n(x)$:

$$F_n(x) \simeq F_n^R(x) = [\exp(x) + q_n]^{-1} \tag{2.15}$$

where the parameter q_n is chosen so that $F_n(x)$ and $F_n^R(x)$ coincide at $x = 0$. Taking into account (2.14), we obtain

$$q_n = [F_n(0)]^{-1} - 1 = [(1-2^{-n})\zeta(n+1)]^{-1} - 1. \tag{2.16}$$

As the numerical calculations show, the error $\Delta F_n^R(x) = |F_n(x) - F_n^R(x)|$ for calculation of $F_n(x)$ by (2.15) within the whole interval $[0, \infty)$ does not exceed 0.31×10^{-2} for $n = 1$ and slightly decreases with increase in n (table 1). For many model problems using the Fermi integrals, this accuracy of the $F_n(x)$ calculation is quite sufficient. For exact values of $F_n(x)$ we used partial sums of the expansion (2.13) by which $F_n(x)$ can be computed to any required accuracy. Since the series (2.13) is alternating and its elements monotonically decrease in absolute value, then the remainder in absolute value is less than its first term. Clearly, for practical calculation of $F_n(x)$ at small x the series (2.13) is unsuitable; for calculation of $F_1(0)$, say with the accuracy 10^{-8}, it is necessary to add 10^4 terms together.

Table 1. Maximum errors in the calculation of iterated integrals $F_n(x)$ by the approximate formula $F_n^R(x) = [\exp(x) + q_n]^{-1}$ and using the Chebyshev approximation.

	Value for the following n				
	1	2	3	4	5
$\max_{x\geqslant 0} \Delta F_n^R(x)$	0.31×10^{-2}	0.17×10^{-2}	0.77×10^{-3}	0.32×10^{-3}	0.13×10^{-3}
$\max_{x\geqslant 0} \Delta F_{n7}^C(x)$	0.45×10^{-7}	0.25×10^{-6}	0.78×10^{-6}	0.16×10^{-5}	0.25×10^{-5}

The following method is suitable for effective and practically exact calculation of the integrals $F_n(x)$. By substituting $t = \exp(-x_1)$ the integral $F_1(x)$ is reduced to a dilogarithm:

$$F_1(x) = L[\exp(-x)] \qquad x \geqslant 0$$
$$L(y) = \int_0^y \frac{\ln(1+t)}{t}\,\mathrm{d}t \qquad 0 \leqslant y \leqslant 1.$$

Using the expansion of a dilogarithm in the series of Chebyshev polynomials

$$L(y) = \sum_{k=0}^{\infty} a_k T_k^*(y) \qquad 0 \leqslant y \leqslant 1$$

where a_k are the Chebyshev coefficients, and

$$T_k^*(y) = \sum_{j=0}^{k} b_{kj} y^{k-j}$$

are shifted Chebyshev polynomials of the first kind, we obtain

$$F_1(x) = \sum_{k=0}^{\infty} a_k T_k^*[\exp(-x)] = \sum_{k=0}^{\infty} a_k \sum_{j=0}^{k} b_{kj} \exp[-(k-j)x] \qquad x \geqslant 0. \tag{2.17}$$

Since these series converge very rapidly and the coefficients a_k and b_{kj} are known up to large k-values (see, e.g., [7], pp. 74 and 494), the integral $F_1(x)$ can be calculated with a high accuracy from (2.17). As table 2 shows, the maximum error of approximation of the integral $F_1(x)$ by the m partial sum of the series of Chebyshev polynomials given by

$$F_{1m}^C(x) = \sum_{k=0}^{m} a_k \sum_{j=0}^{k} b_{kj} \exp[-(k-j)x] \qquad x \geqslant 0 \tag{2.18}$$

decreases very quickly with increase in m and at $m = 7$ becomes equal to 0.45×10^{-7}, i.e. five orders smaller than in approximation by (2.15) (see table 1). However, unlike $\Delta F_1^R(x)$ that vanishes on increase in x, the error $\Delta F_{1m}^C(x)$ for large values of x remains small but finite:

$$F_{1m}^C(\infty) = \lim_{x\to\infty} F_{1m}^C(x) = \sum_{k=0}^{m} a_k b_{kk}.$$

In this connection in the calculation of the iterated integral $F_n(x)$ at $n > 1$ the function $F_{1m}^C(x)$ is substituted by the function

$$\tilde{F}_{1m}^C(x) \equiv F_{1m}^C(x) - F_{1m}^C(\infty) = \sum_{k=1}^{m} a_k \sum_{j=0}^{k-1} b_{kj} \exp[-(k-j)x] \tag{2.18a}$$

which has correct asymptotic behaviour at infinity. The substitution of (2.18*a*) into (2.9) gives

$$F_{nm}^{C}(x) = \sum_{k=1}^{m} a_k \sum_{j=0}^{k-1} b_{kj} \frac{\exp[-(k-j)x]}{(k-j)^{n-1}} \qquad n > 1. \tag{2.19}$$

Maximum errors in the calculation of the integrals $F_n(x)$ by (2.19) increase slightly with increase in n but, as one can see from table 1, even at small m they remain several orders smaller than in the calculation by the approximate formula (2.15).

Table 2. Maximum error in the approximation of integral $F_1(x)$ by the m partial sum of the series of Chebyshev polynomials.

	Value for the following m				
	3	4	5	6	7
$\max_{x\geqslant 0} \Delta F_{1m}^{C}(x)$	0.15×10^{-3}	0.16×10^{-4}	0.20×10^{-5}	0.26×10^{-6}	0.45×10^{-7}

Now let us return to the integral (2.3). Taking into account (2.4) and (2.8), the integral can be written in the form

$$I(T) = T^2 \sum_{i=1}^{N} \Delta g_i' \, F_1(-\xi_i/T) \tag{2.20}$$

where according to (2.10)–(2.12)

$$F_1(-|x|) = \frac{x^2}{2} + 2F_1(0) - F_1(|x|) \qquad x < 0. \tag{2.21}$$

Dividing the sum with respect to i into two sums $x_i \equiv -\xi_i/T = -(\mu - \varepsilon_i)/T < 0$ and $x_i \geqslant 0$, and taking into account (2.14), we have

$$I(T) = T^2 \left\{ \sum_{x_i<0} \Delta g_i' \left[\frac{x_i^2}{2} + \zeta(2) - F_1(|x_i|) \right] + \sum_{x_i\geqslant 0} \Delta g_i' F_1(x_i) \right\}. \tag{2.22}$$

At $T = 0$ in (2.22), indeterminacy appears. Removing the parentheses, we obtain

$$I(0) = \tfrac{1}{2} \sum_{\xi_i>0} \Delta g_i' \xi_i^2. \tag{2.23}$$

Thus, the problem of calculation of the Fermi integrals by using the linear interpolation (2.1) is reduced to the problem of the calculation of the integral $F_1(x)$ only at $x \geqslant 0$. The integral $F_1(x)$ and the errors in its approximation by (2.15) and the third partial sum of series of Chebyshev polynomials are represented in figure 1. As seen from the figure, the function $F_1(x)$ monotonically decreases (at $x \to \infty$ it decreases exponentially). As for the error $\Delta F_1^R(x)$, it monotonically increases initially, achieving a maximum near $x = 0.5$, and then monotonically decreases (to zero at $x \to \infty$). The error $\Delta F_{1m}^{C}(x)$ has an oscillating character, its oscillations being condensed to the origin. The number of zeros of the function $\Delta F_{1m}^{C}(x)$ is equal to the order m of the corresponding partial sum. At $x \to \infty$ the function $\Delta F_{1m}^{C}(x)$ increases, asymptotically approaching the value $F_{1m}^{C}(\infty)$. This value even at $m = 3$ is a twentieth of the maximum error in $F_1(x)$ calculated by (2.15).

The subroutine for calculation of the Fermi integrals $I(T)$, named FINT and based on the method outlined, is given in [8]. The subroutine allows us to calculate $I(T)$ using both the simple approximate formula (2.15) and the Chebyshev approximation. By FINT the

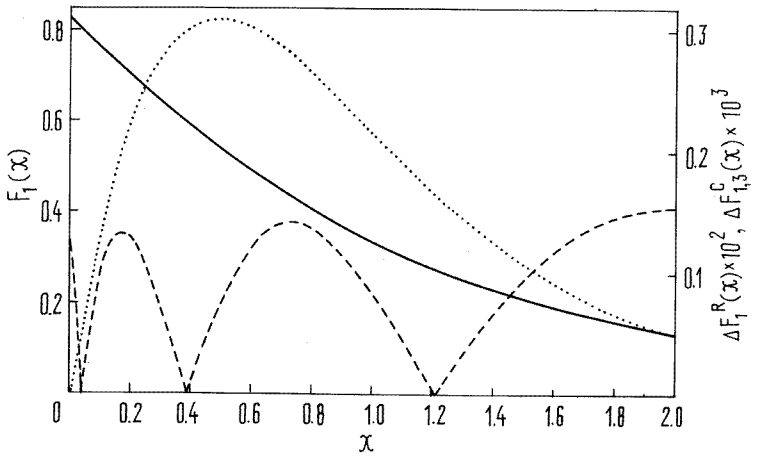

Figure 1. Integral $F_1(x)$ (——) and errors in its approximation by the function $[\exp(x)+q_n]^{-1}$ (· · · · · ·) and the third partial sum of the series of Chebyshev polynomials (- - - -).

Fermi integral can be calculated, if necessary, also to any required accuracy. The subroutine FINT is written in FORTRAN and is included in the illustrating program that realizes the test given below.

3. Test and results

We used the model electron density of states $\nu(\varepsilon)$ of iron represented in figure 2 as a test function $g(\varepsilon)$ for calculation of the Fermi integral (1.1). It mainly reflects the behaviour of the actual density of states of iron obtained in self-consistent calculations (see, e.g., [2]) and it is often used, for example, in the numerical calculations of the itinerant-electron magnetism theory (see, e.g., [9] and references therein). In figure 2 the integrated density of states $N(\varepsilon)$ is also represented, which gives the number of electron states below ε. The Fermi level determined from the relation $N(\varepsilon_F) = 8$ (the total number of 3d and 4s electrons in iron) is equal to 5.87 eV. The Fermi integral (1.1) with $g(\varepsilon) = \nu(\varepsilon)$ is the electron density.

The test calculation of Fermi integral $I(T)$ by (2.22) has been carried out at the Curie temperature ($T_C = 1044/11\,604.5$ eV) and at two values of the chemical potential $\mu = 5.90$ and 5.99 eV, approaching the energy $\varepsilon_0 = 6.0$ eV corresponding to the peak of density of states. Strictly speaking, the chemical potential μ in figure 2 must shift downwards slightly along a slope of the peak with increasing temperature, but in the test calculation the opposite situation is of greater interest. The results of the Fermi integral calculation using the approximate values for $F_1(x)$ obtained by (2.15) and (2.18) at $m = 5$, and exact values obtained by (2.13), are given in table 3. In the same table the value of the Fermi integral I^T obtained by (1.4) is given for comparison. The errors in the Fermi integral calculation by the three methods considered are given in table 4. As seen from table 4, the error ΔI^T, in the calculation using the Taylor series is equal to approximately 10^{-2} and increases as the chemical potential μ approaches the energy ε_0 corresponding to the peak of density of states. The error in the calculation by using the simple formula (2.15) is two orders smaller than ΔI^T, and by using the Chebyshev approximation, at $m = 5$, it is almost equal to zero ($< 10^{-7}$); in both cases it does not depend on the position of μ relative to ε_0.

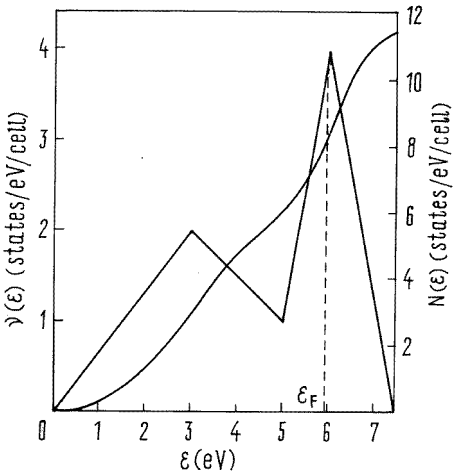

Figure 2. Model density and number of states of iron. The vertical broken line indicates the Fermi level.

Table 3. Fermi integral I of the model electron density for iron and its approximations using the Taylor series (I^T), equation (2.15) (I^R) and the Chebyshev approximation (I^C).

μ (eV)	I^T	I^R	I_5^C	I
5.90	8.154 934 9	8.140 843 4	8.140 930 3	8.140 930 3
5.99	8.500 085 8	8.465 689 8	8.465 758 6	8.465 758 5

Table 4. Errors in the calculation of the Fermi integral of the model electron density for iron using the Taylor series (ΔI^T), equation (2.15) (ΔI^R) and the Chebyshev approximation (ΔI^C).

μ (eV)	ΔI^T	ΔI^R	ΔI_5^C
5.90	0.14×10^{-1}	0.87×10^{-4}	0.40×10^{-7}
5.99	0.34×10^{-1}	0.69×10^{-4}	0.52×10^{-7}

4. Conclusion

The proposed numerical method of calculation of the Fermi integrals is universal, simple and practically exact. The universality of the method is obvious. The simplicity and exactness are justified by the fact that, for a dilogarithm, to the calculation of which the problem is reduced, the expansion in the series of Chebyshev polynomials already exists with rather high accuracy. As our realization, described in [8] in detail, showed, the method is highly efficient as well; even the fifth partial sum of the series gives the possibility of calculating the Fermi integral of the model electron density which has an error $< 10^{-7}$.

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Appendix 1. Reduction of the integral $J_n(\xi, T)$ to the iterated integral

From (2.5) it follows that

$$J_n(\xi,T) = (n+1)T\left\{\varepsilon^n \ln\left[1+\exp\left(-\frac{\varepsilon-\xi}{T}\right)\right]\Bigg|_0^\infty - n\int_0^\infty \varepsilon^{n-1}\ln\left[1+\exp\left(-\frac{\varepsilon-\xi}{T}\right)\right]\mathrm{d}\varepsilon\right\}.$$

The first term is equal to zero since the function $\ln(1+\exp(-(\varepsilon-\xi)/T))$ decreases exponentially at $\varepsilon \to \infty$. Substituting $(\varepsilon-\xi)/T = x_n$, $\varepsilon = Tx_n + \xi$, $\mathrm{d}\varepsilon = T\,\mathrm{d}x_n$ in the second term, we have

$$J_n(\xi,T) = -(n+1)nT^2\int_{-\xi/T}^\infty (Tx_n+\xi)^{n-1}\ln[1+\exp(-x_n)]\,\mathrm{d}x_n.$$

Now, writing $(Tx_n+\xi)^{n-1}$ in the form $(Tx_n+\xi)^{n-2}(Tx_n+\xi)$, we obtain

$$J_n(\xi,T) = -(n+1)nT^2\left[T\int_{-\xi/T}^\infty (Tx_n+\xi)^{n-2}x_n\ln[1+\exp(-x_n)]\,\mathrm{d}x_n + \xi\int_{-\xi/T}^\infty (Tx_n+\xi)^{n-2}\ln[1+\exp(-x_n)]\,\mathrm{d}x_n\right]. \tag{A1.1}$$

Integration by parts gives for the first integral from (A1.1)

$$\begin{aligned}\int_{-\xi/T}^\infty (Tx_n+\xi)^{n-2}x_n\ln[1+\exp(-x_n)]\,\mathrm{d}x_n &= -\int_{-\xi/T}^\infty x_n\,\mathrm{d}\left(\int_{x_n}^\infty (Tx_{n-1}+\xi)^{n-2}\ln[1+\exp(-x_{n-1})]\,\mathrm{d}x_{n-1}\right)\\ &= -\frac{\xi}{T}\int_{-\xi/T}^\infty (Tx_{n-1}+\xi)^{n-2}\ln[1+\exp(-x_{n-1})]\,\mathrm{d}x_{n-1}\\ &\quad +\int_{-\xi/T}^\infty \mathrm{d}x_n\int_{x_n}^\infty (Tx_{n-1}+\xi)^{n-2}\ln[1+\exp(-x_{n-1})]\,\mathrm{d}x_{n-1}.\end{aligned} \tag{A1.2}$$

Substituting (A1.2) into (A1.1), we obtain

$$J_n(\xi,T) = -(n+1)nT^3\int_{-\xi/T}^\infty \mathrm{d}x_n\int_{x_n}^\infty (Tx_{n-1}+\xi)^{n-2}\ln[1+\exp(-x_{n-1})]\,\mathrm{d}x_{n-1}.$$

Then, writing $(Tx_{n-1}+\xi)^{n-2}$ in the form $(Tx_{n-1}+\xi)^{n-3}(Tx_{n-1}+\xi)$ and operating as above, we have

$$J_n(\xi,T) = -(n+1)n(n-1)T^4\int_{-\xi/T}^\infty \mathrm{d}x_n\int_{x_n}^\infty \mathrm{d}x_{n-1} \times\int_{x_{n-1}}^\infty (Tx_{n-2}+\xi)^{n-3}\ln[1+\exp(-x_{n-2})]\,\mathrm{d}x_{n-2}.$$

Continuing the reduction of degree of the factor $(Tx_{n-2}+\xi)^{n-3}$, finally we obtain (2.8) and (2.9).

Appendix 2. Recursion relations for the integrals $F_n(x)$

By definition

$$F_n(-|x|) = \int_{-|x|}^{\infty}\int_{x_n}^{\infty}\dots\int_{x_2}^{\infty}\ln[1+\exp(-x_1)]\,\mathrm{d}x_1\dots\mathrm{d}x_n = \int_{-|x|}^{\infty} f(x_n)\,\mathrm{d}x_n \tag{A2.1}$$

where

$$f(x_n) = \int_{x_n}^{\infty}\int_{x_{n-1}}^{\infty}\dots\int_{x_2}^{\infty}\ln[1+\exp(-x_1)]\,\mathrm{d}x_1\dots\mathrm{d}x_{n-1}. \tag{A2.2}$$

Let us represent the integral (A2.1) as a sum of two integrals:

$$F_n(-|x|) = \int_{-|x|}^{0} f(x_n)\,\mathrm{d}x_n + \int_0^{\infty} f(x_n)\,\mathrm{d}x_n = D_n(|x|) + F_n(0) \tag{A2.3}$$

where

$$D_n(|x|) = \int_{-|x|}^{0} f(x_n)\,\mathrm{d}x_n = \int_0^{|x|} f(-t)\,\mathrm{d}t. \tag{A2.4}$$

Consider $f(-t)$ in more detail:

$$\begin{aligned} f(-t) = {} & \int_{-t}^{0}\int_{x_{n-1}}^{\infty}\dots\int_{x_2}^{\infty}\ln[1+\exp(-x_1)]\,\mathrm{d}x_1\dots\mathrm{d}x_{n-1} \\ & + \int_0^{\infty}\int_{x_{n-1}}^{\infty}\dots\int_{x_2}^{\infty}\ln[1+\exp(-x_1)]\,\mathrm{d}x_1\dots\mathrm{d}x_{n-1} \\ = {} & D_{n-1}(t) + F_{n-1}(0). \end{aligned} \tag{A2.5}$$

Substituting (A2.5) into (A2.4) we obtain

$$D_n(|x|) = \int_0^{|x|} D_{n-1}(t)\,\mathrm{d}t + |x|F_{n-1}(0) \qquad n = 1, 2, \dots. \tag{A2.6}$$

Let us find the explicit form of $D_0(|x|)$. According to (A2.4) and (A2.2),

$$D_1(|x|) = \int_0^{|x|}\ln[1+\exp(t)]\,\mathrm{d}t.$$

On the other hand, according to (A2.6), it should be

$$D_1(|x|) = \int_0^{|x|} D_0(t)\,\mathrm{d}t + |x|F_0(0).$$

Setting the right-hand sides of the two last expressions equal, we have

$$\int_0^{|x|}\ln[1+\exp(t)]\,\mathrm{d}t = \int_0^{|x|} D_0(t)\,\mathrm{d}t + |x|F_0(0).$$

Whence, differentiating with respect to $|x|$, we obtain

$$D_0(|x|) = \ln[1+\exp(|x|)] - F_0(0). \tag{A2.7}$$

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