

# The Fermi-Dirac Distribution Function

①

From Modular Series Volume VI  
Advanced Semiconductor Fundamentals  
P. F. Pierret pp 100-105

## 4.2 FERMION FUNCTION

### Introduction

The Fermi function,  $f(E)$ , is a probability density function that tells one the ratio of filled to total allowed states at a given energy  $E$ . As we will see, statistical arguments are employed to establish the general form of the function. Basically, the electrons are viewed as indistinguishable "balls" which are being placed in allowed-state "boxes." Each box is assumed to accommodate a single ball. The boxes themselves are grouped into rows, the number of boxes per row corresponding to the allowed electronic states at a given energy. The numerical occurrence of all possible arrangements of balls per row yielding the same over-all system energy is determined statistically, and the most likely arrangement identified. Finally, the Fermi function is equated to the most likely arrangement of balls (electrons) per row (energy). The cited arrangement, it turns out, occurs more often than all other arrangements combined. Moreover, the distribution of arrangements is highly peaked about the most probable arrangement. Thus it is reasonable to use the Fermi function—the most probable arrangement—to describe the filling of allowed states in actual electronic systems.

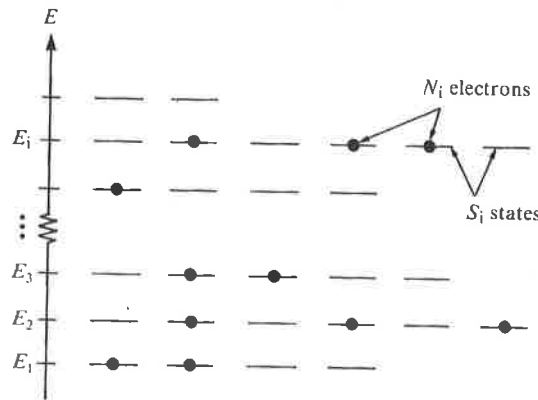
**Table 4.1** Density of States Effective Masses for Ge, Si, and GaAs.

Effective Mass		Ge	Si	GaAs
$m_n^*/m_0$	T = 4 °K	0.553	1.062	0.067
	T = 300 °K	.....	1.182	0.0655 <sup>†</sup>
$m_p^*/m_0$	T = 4 °K	0.357	0.590	0.532
	T = 300 °K	.....	0.81	0.524

<sup>†</sup>The band edge effective mass ratio is 0.0632. The value quoted here takes into account the non-parabolic nature of the GaAs conduction band and yields the correct nondegenerate carrier concentrations when employed in computational expressions developed later in this chapter.

**Problem Specification**

We consider the placement of  $N$  electrons into a multi-level energy system. The assumed system is totally arbitrary: our considerations are not restricted to a specific material or set of materials. The system, as pictured in Fig. 4.5, contains  $S_i$  available states at an allowed energy  $E_i$  ( $i = 1, 2, 3, \dots$ ).  $N_i$  is taken to be the number of electrons with energy  $E_i$ . The electrons are assumed to be indistinguishable: the interchange of any two electrons would leave the electronic configuration unperturbed. Also, the likelihood of filling an individual state is taken to be energy independent.



**Fig. 4.5** Envisioned multi-level energy system of a totally arbitrary nature which contains  $S_i$  states and  $N_i$  electrons at an energy  $E_i$  ( $i = 1, 2, 3, \dots$ ).

**102 EQUILIBRIUM CARRIER STATISTICS**

The placement of electrons in the various allowed states is subject, however, to the following restrictions:

- (1) Each allowed state can accommodate one and only one electron.<sup>†</sup>
- (2)  $N = \sum N_i = \text{constant}$ ; the total number of electrons in the system is fixed.
- (3)  $E_{\text{TOT}} = \sum E_i N_i = \text{constant}$ ; the total energy of the system is fixed.

As outlined previously, and subject to the cited constraints, the task at hand is to determine the most likely arrangement of the  $N$  electrons in the  $E_1, E_2, E_3, \dots$  energy-level system. The  $N_i$  values thereby determined can then be divided by  $S_i$  and equated to the value of the Fermi function at  $E_i$ —that is,  $f(E_i) = N_i(\text{most probable})/S_i$ .

**Derivation Proper**

Consider first the number of different ways ( $W_i$ ) in which the  $N_i$  indistinguishable electrons in the  $i^{\text{th}}$  level can be placed into the available  $S_i$  states. By direct computation, or preferably by reference to a “probability and statistics” textbook, one finds

$$W_i = \frac{S_i!}{(S_i - N_i)! N_i!} \tag{4.28}$$

If more than one level is considered, the number of different arrangements increases as the product of the individual  $W_i$ -values. Since eq. (4.28) holds for any  $E_i$  level, the total number of different ways ( $W$ ) in which the  $N$  electrons can be arranged in the multi-level system is therefore concluded to be

$$W = \prod_i W_i = \prod_i \frac{S_i!}{(S_i - N_i)! N_i!} \tag{4.29}$$

It should be pointed out that the above  $W$  expression is valid for any set of  $N_i$  values meeting the  $\sum N_i = N$  and  $\sum E_i N_i = E_{\text{TOT}}$  restrictions. We seek the set of  $N_i$  values for which  $W$  is at its maximum. This can be obtained in the usual fashion by setting the total differential of  $W$  equal to zero and solving for  $W_{\text{MAX}}$ . The maximization procedure is drastically simplified, however, if  $d(\ln W) = 0$  replaces  $dW = 0$  as the maximization criteria. As deduced from eq. (4.29),

$$\ln W = \sum_i [\ln S_i! - \ln(S_i - N_i)! - \ln N_i!] \tag{4.30}$$

Since  $d(\ln W) = dW/W$  and  $W_{\text{MAX}} \neq 0$ ,  $d(\ln W) = 0$  when  $dW = 0$  and the two maximization criteria are clearly equivalent.

<sup>†</sup>The *Pauli Exclusion Principle* from quantum mechanics dictates that no two electrons in a system can be characterized by the same set of quantum numbers.

Before proceeding it is important to note that the number of available states,  $S_i$ , and the number of electrons populating those states,  $N_i$ , are typically quite large for  $E_i$  values of interest in real systems. (This is certainly true for the near-band-edge portion of the conduction and valence bands in semiconductors.) We can therefore justify invoking Stirling's approximation to simplify the factorial terms in eq. (4.30). Specifically noting

$$\ln x! \approx x \ln x - x \quad \dots \text{Stirling's approximation} \quad (4.31)$$

( $x$  large)

one can write

$$\ln W \approx \sum_i [S_i \ln S_i - S_i - (S_i - N_i) \ln(S_i - N_i) + (S_i - N_i) - N_i \ln N_i + N_i] \quad (4.32a)$$

$$= \sum_i [S_i \ln S_i - (S_i - N_i) \ln(S_i - N_i) - N_i \ln N_i] \quad (4.32b)$$

We are finally in a position to perform the actual maximization. Recognizing that  $dS_i = 0$  (the  $S_i$  are system constants), one obtains

$$d(\ln W) = \sum_i \frac{\partial \ln W}{\partial N_i} dN_i \quad (4.33a)$$

$$= \sum_i [\ln(S_i - N_i) + 1 - \ln N_i - 1] dN_i \quad (4.33b)$$

$$= \sum_i \ln(S_i/N_i - 1) dN_i \quad (4.33c)$$

Setting  $d(\ln W) = 0$  then yields

$$\sum_i \ln(S_i/N_i - 1) dN_i = 0 \quad (4.34)$$

The solution of eq. (4.34) for the most probable  $N_i$  value set is of course subject to the  $\sum N_i = N$  and  $\sum E_i N_i = E_{TOT}$  restrictions. These solution constraints can be recast into the equivalent differential form

$$\sum_i dN_i = 0 \quad (4.35a)$$

and

$$\sum_i E_i dN_i = 0 \tag{4.35b}$$

To solve eq. (4.34) subject to the eq. (4.35) constraints, we employ the method of Lagrange multipliers.<sup>†</sup> This method consists of multiplying each constraint equation by an as yet unspecified constant. (Let the undetermined multipliers be  $-\alpha$  and  $-\beta$ , respectively.) The resulting equations are then added to eq. (4.34), giving

$$\sum_i [\ln(S_i/N_i - 1) - \alpha - \beta E_i] dN_i = 0 \tag{4.36}$$

In principle,  $\alpha$  and  $\beta$  can always be chosen such that two of the bracketed  $dN_i$  coefficients vanish, thereby eliminating two of the  $dN_i$  from eq. (4.36). We assume this to be the case. With two of the  $dN_i$  eliminated, all of the remaining  $dN_i$  in eq. (4.36) can be varied independently, and the summation will vanish for all choices of the independent differentials only if

$$\ln(S_i/N_i - 1) - \alpha - \beta E_i = 0 \quad \dots \text{all } i \tag{4.37}$$

Eq. (4.37) is the sought-after relationship for the most probable  $N_i$ . Solving eq. (4.37) for  $N_i/S_i$  we therefore conclude

$$f(E_i) = \frac{N_i}{S_i} = \frac{1}{1 + e^{\alpha + \beta E_i}} \tag{4.38}$$

For closely spaced levels, as encountered in the conduction and valence bands of semiconductors,  $E_i$  may be replaced by the continuous variable  $E$  and

$$f(E_i) \rightarrow f(E) = \frac{1}{1 + e^{\alpha + \beta E}} \tag{4.39}$$

### Concluding Discussion

To complete the derivation of the Fermi function it is necessary to evaluate the solution constants,  $\alpha$  and  $\beta$ . This is usually accomplished by performing supplemental theoretical analyses or by comparing the general form of the result with experimental data. Thermodynamic arguments and the analysis of real systems using statistical mechanics

<sup>†</sup>For an excellent discussion of the Lagrange multiplier method (also referred to as the method of undetermined multipliers), see L. P. Smith, *Mathematical Methods for Scientists and Engineers*, Dover Publications, Inc., New York, 1953, pp. 39-42.

6

or the kinetic theory of gases, for example, lead to the conclusion that

$$\alpha = -\frac{E_F}{kT}$$

and

$$\beta = \frac{1}{kT}$$

where  $E_F$  is the electrochemical potential or Fermi energy of the electrons in the solid,  $k = 8.614 \times 10^{-5}$  eV/°K is Boltzmann's constant<sup>†</sup>, and  $T$  is the system temperature. Thus we arrive at the final form of the Fermi function

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}} \tag{4.40}$$

A sample plot of the Fermi function versus  $E - E_F$  for a select number of temperatures is displayed in Fig. 4.6.

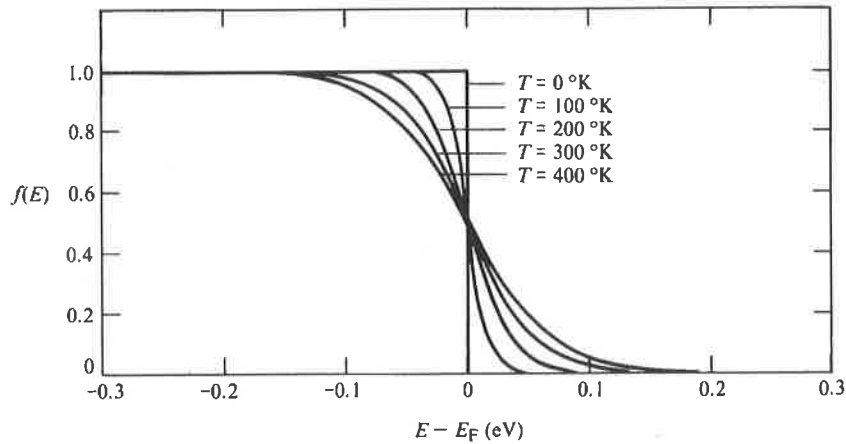


Fig. 4.6 Value of the Fermi function versus energy with the system temperature as a parameter.

<sup>†</sup>  $k$  is widely employed as the symbol of choice for both the wavenumber and Boltzmann's constant. The correct interpretation of the symbol can invariably be determined from the context of an analysis.

# The Lagrange Multiplier

From: *Mathematical Methods for Physicists*  
Second Edition, Arfken (Academic Press).

In this section the concept of a constraint is introduced. To simplify the treatment, the constraint appears as a simple function and not as an integral. In this section we are not concerned with the calculus of variations, but in Section 17.7 the constraints, with our newly developed Lagrangian multipliers, are incorporated into the calculus of variations.

Consider a function of three independent variables,  $f(x, y, z)$ . For the function  $f$  to be a maximum (or extreme)<sup>1</sup>

$$df = 0. \quad (17.88)$$

The necessary and sufficient condition for this is

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = \frac{\partial f}{\partial z} = 0, \quad (17.89)$$

in which

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz. \quad (17.90)$$

Often in physical problems the variables  $x, y, z$  are subjected to constraints so that they are no longer all independent. It is possible, at least in principle, to use each constraint to eliminate one variable and to proceed with a new and smaller set of independent variables.

The use of Lagrangian multipliers is an alternate technique that may be applied when this elimination of variables is inconvenient or undesirable. Let our equation of constraint be

$$\varphi(x, y, z) = 0, \quad (17.91)$$

from which

$$d\varphi = \frac{\partial \varphi}{\partial x} dx + \frac{\partial \varphi}{\partial y} dy + \frac{\partial \varphi}{\partial z} dz = 0. \quad (17.92)$$

Returning to Eq. 17.88, we see that Eq. 17.89 no longer follows because there are now only two independent variables. If we take  $x$  and  $y$  as these independent variables,  $dz$  is no longer arbitrary. However, we may add Eq. 17.90 and a multiple of Eq. 17.92 to obtain

$$df + \lambda d\varphi = \left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} \right) dy + \left( \frac{\partial f}{\partial z} + \lambda \frac{\partial \varphi}{\partial z} \right) dz = 0. \quad (17.93)$$

Our Lagrangian multiplier  $\lambda$  is chosen so that

$$\frac{\partial f}{\partial z} + \lambda \frac{\partial \varphi}{\partial z} = 0, \quad (17.94)$$

assuming that  $\partial \varphi / \partial z \neq 0$ . Equation 17.93 now becomes

$$\left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} \right) dy = 0. \quad (17.95)$$

<sup>1</sup> Including a four-dimensional saddle point.

However,  $dx$  and  $dy$  are arbitrary and the quantities in parentheses must vanish,

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial \varphi}{\partial x} = 0, \quad (17.96)$$

$$\frac{\partial f}{\partial y} + \lambda \frac{\partial \varphi}{\partial y} = 0.$$

When Eqs. 17.94 and 17.96 are satisfied,  $df = 0$  and  $f$  is an extremum. Notice that there are now four unknowns:  $x$ ,  $y$ ,  $z$ , and  $\lambda$ . The fourth equation is, of course, the constraint (17.91). Actually, we want only  $x$ ,  $y$ , and  $z$ ;  $\lambda$  need not be determined. For this reason  $\lambda$  is sometimes called Lagrange's undetermined multiplier. This method will fail if all the coefficients of  $\lambda$  vanish at the extremum,  $\partial\varphi/\partial x$ ,  $\partial\varphi/\partial y$ ,  $\partial\varphi/\partial z = 0$ . It is then impossible to solve for  $\lambda$ .

#### EXAMPLE 17.6.1. PARTICLE IN A BOX

As an example of the use of Lagrangian multipliers, consider the quantum mechanical problem of a particle (mass  $m$ ) in a box. The box is a rectangular parallelepiped with sides  $a$ ,  $b$ , and  $c$ . The ground state energy of the particle is given by

$$E = \frac{h^2}{8m} \left( \frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right). \quad (17.97)$$

We seek the shape of the box that will minimize the energy  $E$ , subject to the constraint that the volume is constant,

$$V(a, b, c) = abc = k. \quad (17.98)$$

With  $f(a, b, c) = E(a, b, c)$  and  $\varphi(a, b, c) = abc - k = 0$ , we obtain

$$\frac{\partial E}{\partial a} + \lambda \frac{\partial V}{\partial a} = -\frac{h^2}{4ma^3} + \lambda bc = 0. \quad (17.99)$$

Also

$$-\frac{h^2}{4mb^3} + \lambda ac = 0,$$

$$-\frac{h^2}{4mc^3} + \lambda ab = 0.$$

Multiplying the first of these expressions by  $a$ , the second by  $b$ , and the third by  $c$ , we have

$$\lambda abc = \frac{h^2}{4ma^2} = \frac{h^2}{4mb^2} = \frac{h^2}{4mc^2}. \quad (17.100)$$

Therefore, our solution is

$$a = b = c, \quad \text{a cube.} \quad (17.101)$$

Notice that  $\lambda$  has not been determined. It remains an undetermined multiplier.



EXAMPLE 17.6.2. CYLINDRICAL NUCLEAR REACTOR

A further example is provided by the nuclear reactor theory. Suppose a (thermal) nuclear reactor is to have the shape of a right circular cylinder of radius  $R$ , height  $H$ . Neutron diffusion theory supplies a constraint:

$$\varphi(R, H) = \left(\frac{2.4048}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2 = \text{constant.}^1 \quad (17.102)$$

We wish to minimize the volume of the reactor

$$f(R, H) = \pi R^2 H. \quad (17.103)$$

Application of Eq. 17.96 leads to

$$\begin{aligned} \frac{\partial f}{\partial R} + \lambda \frac{\partial \varphi}{\partial R} &= 2\pi R H - 2\lambda \frac{(2.4048)^2}{R^3} = 0, \\ \frac{\partial f}{\partial H} + \lambda \frac{\partial \varphi}{\partial H} &= \pi R^2 - 2\lambda \frac{\pi^2}{H^3} = 0. \end{aligned} \quad (17.104)$$

By multiplying the first of these equations by  $R/2$  and the second by  $H$  we obtain

$$\pi R^2 H = \lambda \frac{(2.4048)^2}{R^2} = \lambda \frac{2\pi^2}{H^2} \quad (17.105)$$

or

$$H = \frac{\sqrt{2\pi R}}{2.4048} = 1.847R. \quad (17.106)$$

for the minimum volume right-circular cylindrical reactor.

Strictly speaking, we have found only an extremum. Its identification as a minimum follows from a consideration of the original equations.

## EXERCISES

The following problems are to be solved by using Lagrangian multipliers.

**17.6.1** The ground state energy of a particle in a pillbox (right-circular cylinder) is given by

$$E = \frac{\hbar^2}{2m} \left( \frac{(2.4048)^2}{R^2} + \frac{\pi^2}{H^2} \right),$$

in which  $R$  is the radius and  $H$ , the height of the pillbox. Find the ratio of  $R$  to  $H$  that will minimize the energy for a fixed volume.

$$\text{Ans. } \frac{R}{H} = 0.5413.$$

<sup>1</sup> 2.4048 ... is the lowest root of Bessel function  $J_0(R)$  (cf. Section 11.1).

17.6.2 Find the ratio of  $R$ (radius) to  $H$ (height) that will minimize the total surface area of a right-circular cylinder of fixed volume.

17.6.3 A thermal nuclear reactor is subject to the constraint

$$\varphi(a, b, c) = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2 = B^2, \text{ a constant.}$$

Find the ratios of the sides of the rectangular parallelepiped reactor of minimum volume.  
*Ans.  $a = b = c$ , cube.*

17.6.4 For a simple lens of focal length  $f$  the object distance  $p$  and the image distance  $q$  are related by  $1/p + 1/q = 1/f$ . Find the minimum object-image distance ( $p + q$ ) for fixed  $f$ . Assume real object and image ( $p$  and  $q$  both positive).

17.6.5 A rectangular parallelepiped is inscribed in an ellipsoid of semiaxes  $a, b$ , and  $c$ . Maximize the volume of the inscribed rectangular parallelepiped. Show that the ratio of the maximum volume to the volume of the ellipsoid is  $2/\pi\sqrt{3} \approx 0.367$ .

17.6.6 A deformed sphere has a radius given by  $r = r_0\{\alpha_0 + \alpha_2 P_2(\cos \theta)\}$  where  $\alpha_0 \approx 1$  and  $\alpha_2 \approx 0$ . From Exercise 12.5.14 the area and volume are

$$A = 4\pi r_0^2 \alpha_0^2 \left\{ 1 + \frac{4}{5} \left( \frac{\alpha_2}{\alpha_0} \right)^2 \right\}$$

$$V = \frac{4\pi r_0^3}{3} \alpha_0^3 \left\{ 1 + \frac{3}{5} \left( \frac{\alpha_2}{\alpha_0} \right)^2 \right\}.$$

Terms of order  $\alpha_2^3$  have been neglected.

- (a) With the constraint that the enclosed volume be held constant, i.e.,  $V = 4\pi r_0^3/3$ , show that bounding surface of minimum area is a sphere, ( $\alpha_0 = 1, \alpha_2 = 0$ ).
- (b) With the constraint that the area of the bounding surface be held constant, i.e.,  $A = 4\pi r_0^2$ , show that the enclosed volume is a maximum when the surface is a sphere.

Note concerning the following exercises:

In a quantum-mechanical system there are  $g_i$  distinct quantum states between energy  $E_i$  and  $E_i + dE_i$ . The problem is to describe how  $n_i$  particles are distributed among these states subject to two constraints:

(a) Fixed number of particles:

$$\sum_i n_i = n.$$

(b) Fixed total energy:

$$\sum_i n_i E_i = E.$$

17.6.7 For identical particles obeying the Pauli exclusion principle the probability of a given arrangement is

$$W_{FD} = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!}.$$

Show that maximizing  $W_{FD}$  subject to a fixed number of particles and fixed total energy leads to

$$n_i = \frac{g_i}{e^{\lambda_1 + \lambda_2 E_i} + 1}.$$

With  $\lambda_1 = -E_0/kT$  and  $\lambda_2 = 1/kT$ , this yields Fermi-Dirac statistics. *Hint.* Try working with  $\ln W$  and using Stirling's formula. The justification for *differentiation* is that we are dealing here with a large number of particles,  $\Delta n_i/n_i \ll 1$ .

From C. Kittel & H. Kroemer  
Thermal Physics - 2nd Edition  
(Freeman)

## Appendix A Some Integrals Containing Exponentials

439

### THE GAUSS INTEGRAL

Let

$$I_0 = \int_{-\infty}^{+\infty} \exp(-x^2) dx = 2 \int_0^{\infty} \exp(-x^2) dx. \quad (1)$$

The following trick is used to evaluate  $I_0$ . Write (1) in terms of a different integration variable:

$$I_0 = \int_{-\infty}^{+\infty} \exp(-y^2) dy. \quad (2)$$

Multiply (1) and (2) and convert the result to a double integral:

$$I_0^2 = \int_{-\infty}^{+\infty} \exp(-x^2) dx \int_{-\infty}^{+\infty} \exp(-y^2) dy = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp-(x^2 + y^2) dx dy. \quad (3)$$

This is an integral over the entire  $x$ - $y$  plane. Convert to polar coordinates  $r$  and  $\varphi$ , as shown in Figure A.1. Then,  $x^2 + y^2 = r^2$ , and the area element  $dA = dx dy$  becomes  $dA = r dr d\varphi$ :

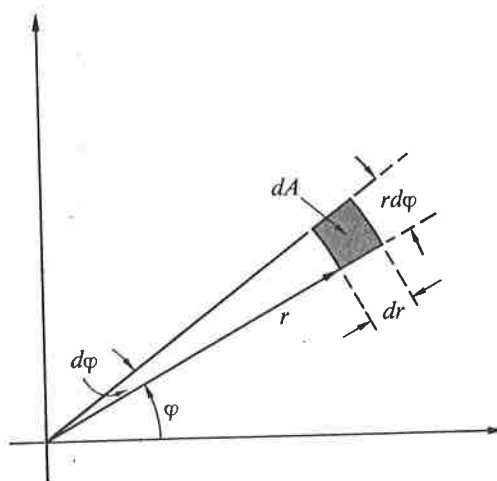
$$I_0^2 = \int_0^{2\pi} \left[ \int_0^{\infty} \exp(-r^2) r dr \right] d\varphi = 2\pi \int_0^{\infty} \exp(-r^2) r dr.$$

Because of  $d[\exp(-r^2)] = -2 \exp(-r^2) r dr$ , the integral over  $r$  is elementary:

$$I_0^2 = -\pi \int d[\exp(-r^2)] = -\left[ \pi \exp(-r^2) \right]_{r=0}^{r=\infty} = \pi.$$

Thus

$$I_0 = \int_{-\infty}^{+\infty} \exp(-x^2) dx = 2 \int_0^{\infty} \exp(-x^2) dx = \pi^{1/2}. \quad (4)$$

Figure A.1 The area element  $dA = r dr d\varphi$ .

### GENERALIZED GAUSS INTEGRALS, AND GAMMA FUNCTION INTEGRALS

Integrals of the form

$$I_m = 2 \int_0^{\infty} x^m \exp(-x^2) dx, \quad (m > -1), \quad (5)$$

where  $m$  need not be an integer, may be reduced to the widely tabulated gamma function  $\Gamma(z)$ , by the substitutions  $x^2 = y$ ,  $2dx = y^{-\frac{1}{2}} dy$ :

$$I_m = \int_0^{\infty} y^n e^{-y} dy = \Gamma(n + 1), \quad n = (m - 1)/2. \quad (6)$$

The integral in (6) may be viewed as the definition of  $\Gamma(z)$  for noninteger positive values of  $z$ .

The gamma function satisfies the recursion relation

$$\Gamma(n + 1) = n\Gamma(n). \quad (7)$$

It is easily obtained for  $n > 0$  from (6) by integration by parts, and it is used to extend the definition (6) of  $\Gamma(z)$  to negative values of  $z$ . By using (7) repeatedly it is always possible to reduce  $\Gamma(z)$  for arbitrary argument to a value in the interval  $0 < z \leq 1$ .

For  $m = 0, n = -\frac{1}{2}$ ; from (4):

$$I_0 = \int_0^\infty y^{-\frac{1}{2}} e^{-y} dy = \Gamma\left(\frac{1}{2}\right) = \pi^{1/2}. \quad (8)$$

If  $m$  is an even integer,  $m = 2l > 0$ ,  $n$  is a half-integer, and  $n = l - \frac{1}{2}$ , then we find by repeated application of (7), with the aid of (8), that

$$\begin{aligned} I_{2l} &= 2 \int_0^\infty x^{2l} \exp(-x^2) dx = \int_0^\infty y^{l-\frac{1}{2}} e^{-y} dy \\ &= \Gamma\left(l + \frac{1}{2}\right) = \left(l - \frac{1}{2}\right) \times \left(l - \frac{3}{2}\right) \times \cdots \times \frac{3}{2} \times \frac{1}{2} \times \pi^{1/2}. \end{aligned} \quad (9)$$

For  $m = 1, n = 0$ :

$$I_1 = 2 \int_0^\infty x \exp(-x^2) dx = \int_0^\infty e^{-y} dy = \Gamma(1) = 1. \quad (10)$$

If  $m$  is an odd integer,  $m = 2l + 1 \geq 1$ ,  $n$  is an integer,  $n = l \geq 0$ , and we find similarly, with the aid of (10),

$$\begin{aligned} I_{2l+1} &= 2 \int_0^\infty x^{2l+1} \exp(-x^2) dx = \int_0^\infty y^l e^{-y} dy \\ &= \Gamma(l + 1) = l \times (l - 1) \times \cdots \times 2 \times 1 = l! \end{aligned} \quad (11)$$

The gamma function for positive integer argument is simply the factorial of the integer preceding the argument.

## THE STIRLING APPROXIMATION

For large values of  $n$ ,  $n!$  can be approximated by

$$n! \simeq (2\pi n)^{1/2} n^n \exp\left[-n + \frac{1}{12n} + O\left(\frac{1}{n^2}\right)\right] \quad (12a)$$

or

$$\log n! \simeq \frac{1}{2} \log 2\pi + (n + \frac{1}{2}) \log n - n + \frac{1}{12n} + O\left(\frac{1}{n^2}\right). \quad (12b)$$

Here the term  $1/12n$  is the first term of an expansion by powers of  $1/n$ , and  $O(1/n^2)$  stands for omitted higher order terms in this expansion, of order  $1/n^2$

or higher. In practice, even the term  $1/12n$  is usually omitted. Its principal role is to check on the accuracy of the approximation. If the effect of the  $1/12n$ -correction introduces only a change below the desired accuracy, the entire expression has the desired accuracy.

To derive (12) we write, in accordance with (11),

$$n! = \int_0^{\infty} x^n e^{-x} dx = \int_0^{\infty} \exp[f(x)] dx, \quad (13)$$

where

$$f(x) = n \log x - x. \quad (14)$$

We make the substitution

$$x = n + yn^{\frac{1}{2}} = n(1 + yn^{-\frac{1}{2}}), \quad dx = n^{\frac{1}{2}} dy. \quad (15)$$

Then

$$f(x) = n \log n - n + g(y), \quad (16)$$

where

$$g(y) = n[\log(1 + yn^{-\frac{1}{2}}) - yn^{-\frac{1}{2}}]. \quad (17)$$

With these,

$$\exp[f(x)] = n^n e^{-n} \exp[g(y)], \quad (18)$$

$$n! = n^{1/2} n^n e^{-n} \int_{-n^{1/2}}^{\infty} \exp[g(y)] dy. \quad (19)$$

The function  $g(y)$  has its maximum at  $y = 0$ :  $g(0) = 0$ . Using the Taylor expansion of the logarithm,

$$\log(1 + s) = s - \frac{1}{2}s^2 + \frac{1}{3}s^3 - \frac{1}{4}s^4 + \dots, \quad (20)$$

with  $s = (y^2/n)^{1/2}$ , we expand  $g(y)$ :

$$\begin{aligned} g(y) &= n \left[ -\frac{1}{2} \frac{y^2}{n} + \frac{1}{3} \left( \frac{y^2}{n} \right)^{3/2} - \dots \right] \\ &= -\frac{1}{2} y^2 + 0(s^3). \end{aligned} \quad (21)$$

In the limit  $n \rightarrow \infty$ ,  $s \rightarrow 0$ , and all but the first term in (21) vanish, and the integral in (19) becomes

$$\int_{-n^{1/2}}^{\infty} \exp[g(y)] dy = \int_{-\infty}^{+\infty} \exp(-y^2/2) dy = (2\pi)^{1/2}, \quad (22)$$

with the aid of (4). If (22) is inserted into (19) the result is identical to (12a) except for the correction term  $1/12n$ . Its derivation is a bit tedious. We work with  $\log n!$  and write

$$\log n! = \frac{1}{2} \log 2\pi + (n + \frac{1}{2}) \log n - n + \frac{A}{n} + o\left(\frac{1}{n^2}\right). \quad (23a)$$

If we replace  $n$  by  $n - 1$ ,

$$\begin{aligned} \log(n-1)! &= \frac{1}{2} \log 2\pi + (n - \frac{1}{2}) \log(n-1) - (n-1) \\ &\quad + \frac{A}{n-1} + o\left(\frac{1}{n^2}\right). \end{aligned} \quad (23b)$$

We subtract (23b) from (23a):

$$\begin{aligned} \log n! - \log(n-1)! &= \log \frac{n!}{(n-1)!} = \log n \\ &= (n + \frac{1}{2}) \log n - (n - \frac{1}{2}) \log(n-1) - 1 \\ &\quad + \frac{A}{n} - \frac{A}{n-1} + o\left(\frac{1}{n^3}\right), \end{aligned} \quad (24)$$

where all omitted terms are now at least of order  $1/n^3$ . The two terms in  $A$  can be combined:

$$\frac{A}{n} - \frac{A}{n-1} = -\frac{A}{n(n-1)} = -\frac{A}{n^2} + o\left(\frac{1}{n^3}\right). \quad (25)$$

If this is inserted into (24), we find

$$\frac{A}{n^2} = (n - \frac{1}{2}) \log \frac{n}{n-1} - 1 + o\left(\frac{1}{n^3}\right). \quad (26)$$

For large  $n$  the logarithm may be expanded according to (20), with  $s = -1/n$ :

$$\log \frac{n}{n-1} = -\log\left(1 - \frac{1}{n}\right) = \frac{1}{n} + \frac{1}{2n^2} + \frac{1}{3n^3} + o\left(\frac{1}{n^4}\right) \quad (27)$$

$$\begin{aligned} (n - \tfrac{1}{2}) \log \frac{n}{n-1} &= 1 + \frac{1}{2n} - \frac{1}{2n} + \frac{1}{3n^2} - \frac{1}{4n^2} + o\left(\frac{1}{n^3}\right) \\ &= 1 + \frac{1}{12n^2} + o\left(\frac{1}{n^3}\right). \end{aligned} \quad (28)$$

If this is inserted in (26) we see that  $A = 1/12$ .

We are often interested not in  $n!$  but only in  $\log n!$ , and only to an accuracy such that the relative error between an approximate value of  $\log n!$  and the true value decreases with increasing  $n$ . Such an approximation is obtained by neglecting all terms in (12b) that increase less rapidly than linearly with  $n$ :

$$\log n! \simeq n \log n - n. \quad (29)$$