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FOR A DIFFUSE FERMI GAS

J. TÖKE, GSI

W.J. ŚWIĄTECKI, GSI AND NUCL. SCI. DIV., LBL

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Gesellschaft für Schwerionenforschung mbH
Planckstr. 1 · Postfach 110541 · D-6100 Darmstadt 11 · Germany

SURFACE-LAYER CORRECTIONS TO THE LEVEL-DENSITY FORMULA
FOR A DIFFUSE FERMI GAS.

J. Töke *

Gesellschaft für Schwerionenforschung
6100 Darmstadt, W. Germany

W. J. Świątecki

Gesellschaft für Schwerionenforschung
6100 Darmstadt, W. Germany

and

Nuclear Science Division, Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720, U.S.A.

Abstract: Using the Thomas-Fermi treatment and the leptodermous expansion in powers of $A^{-1/3}$, we derive a formula for the level-density parameter a , which corrects the conventional expression for the presence of the diffuse surface region. This appears to remove the discrepancy (of about a factor of 1.7) between the empirical values of a/A and those that would follow from considering the nucleus to be a simple Fermi gas at constant (bulk) density.

* Permanent address: Institute of Experimental Physics,
University of Warsaw, 00681 Warsaw, Poland

1. Introduction

An expression for the level density $\rho(A, E)$ of a Fermi gas of A (nearly) independent particles at an excitation energy E , is a useful starting point for the discussion of the thermodynamic properties of different systems. In the context of nuclear physics this approach is described, for example, in ref.¹⁾.

At temperatures low compared to the Fermi energy ϵ of the Fermi gas, the key quantity entering the expression for ρ is the density g of single-particle levels near the Fermi energy. For example, in the case of a nucleus with A nucleons, the dominant term in the logarithm of the level density may be written as [ref.¹⁾, eq.(2-117)]:

$$\ln \rho \approx 2\sqrt{aE} \quad , \quad (1)$$

where

$$a = \frac{\pi^2}{6} g = \frac{\pi^2 A}{4\epsilon} \quad , \quad (2)$$

with

$$g = \frac{3A}{2\epsilon} \quad . \quad (3)$$

Equation (3) for the single-particle level density g is valid for a homogeneous Fermi gas with a volume sufficiently large for effects associated with the diffuse surface region to be negligible. Corrections to eq.(3) due to the diffuseness of the nuclear density distribution have been considered in the past [see, for example, ref.¹⁾, eq.(2-125a) and ref.^{2,3)] and appear to be substantial. This is to be expected, since the surface diffuseness, even for the heaviest nuclei, is not very small compared to the radius. In the quite analogous case of nuclear binding energies, the surface energy, even though smaller than the volume energy, is far from being negligible.}

Recently an attempt was made in ref.⁴⁾ to derive theoretically surface and curvature corrections to eq.(2), and to discuss such corrections in the light of experimental information. In the present paper we shall make a similar expansion in powers of the ratio (proportional to $A^{-1/3}$) between the surface diffuseness and the size of the system,

using the standard Thomas-Fermi approach to nuclear properties and the canonical leptodermous expansion technique [refs.^{5,6,7)].}

2. The Thomas-Fermi Method

The Thomas-Fermi method is based on the circumstance that in phase space the density of quantum states is one per h^3 . (Here h is Planck's constant.) According to this method, the particle density $n(r)$ at a point where the local Fermi momentum is $p(r)$ is given by the standard expression

$$\begin{aligned} n &= \frac{(\text{number of particles in a volume element})}{(\text{volume element})} \\ &= \frac{(\text{volume in phase space})(\text{level degeneracy})/h^3}{(\text{volume element})} \\ &= (\text{volume in momentum space})(\text{degeneracy})/h^3 \\ &= \frac{4}{3} \pi p^3 (4/h^3) \quad . \end{aligned} \quad (4)$$

(The degeneracy 4 is appropriate for standard nuclear matter.)

The local Fermi momentum p is related to the potential $V(r)$ in which the particles move and to the Fermi energy ϵ of the whole system by

$$\frac{p^2}{2m} = \epsilon - V \quad , \quad (5)$$

where m is the average nucleon mass. (The zero of the energy scale will be taken at the bottom of the potential well, so that $V=0$ in the bulk of the nucleus.) It follows that

$$n = \frac{16\pi(2m)^{3/2}}{3h^3} (\epsilon - V)^{3/2} \quad , \quad (6)$$

or

$$\frac{n}{n_0} = \left(\frac{\epsilon - V}{\epsilon} \right)^{3/2}, \quad (7)$$

where n_0 denotes the value of n in the bulk. Note that by comparing eqs. (6) and (7) we may write

$$\frac{n_0}{\epsilon^{3/2}} = \frac{16\pi(2m)^{3/2}}{3\hbar^3} \quad (8)$$

The total number of particles is given by

$$A = \iiint_{\text{ndt}} = \frac{16\pi(2m)^{3/2}}{3\hbar^3} \iiint (\epsilon - V)^{3/2} dt,$$

where the integration extends over the inside of the volume enclosed by the surface defined by the vanishing of $\epsilon - V$.

The number of single-particle states, ΔA , per unit interval of energy, $\Delta\epsilon$, is found by taking the derivative

$$\begin{aligned} g &\equiv \frac{dA}{d\epsilon} = \frac{16\pi(2m)^{3/2}}{3\hbar^3} \frac{3}{2} \iiint (\epsilon - V)^{1/2} dt \\ &= \frac{3n_0}{2\epsilon} \iiint \left(\frac{\epsilon - V}{\epsilon} \right)^{1/2} dt \\ &= \frac{3n_0}{2\epsilon} \iiint \left(\frac{n}{n_0} \right)^{1/3} dt \end{aligned} \quad (9)$$

(It may be verified that the dependence of the volume of integration on the Fermi energy ϵ does not contribute to the derivative $dA/d\epsilon$.)

In the case of a not too small nucleus, the dimensionless function $(n/n_0)^{1/3}$ is approximately constant and equal to unity in the bulk, falling off to zero in a relatively thin, diffuse region around a surface $\mathcal{L}$ defining the nuclear shape. In the idealization where (n/n_0) is assumed exactly one inside and zero outside such an effective sharp surface (defined so that the volume it encloses times the bulk density n_0 is the total number of particles) eq. (9) evidently reduces to the standard result, eq. (3), according to which g is proportional to A .

3. The Leptodermous Expansion

In any problem where a volume integral is to be carried out over an integrand that is essentially constant in the bulk and falls off to zero in a surface region, whose (essentially constant) thickness is small compared to the size of the system, a standard expansion technique may be used to approximate the integral by a power series in the small parameter of the problem, proportional to the diffuseness divided by the size of the system. This method is most familiar in the context of nuclear binding energies [ref. 5)], but it is quite general and has, in fact, been applied recently to the discussion of the nuclear "one-body" dissipation function [refs. 6, 7)]. In what follows we shall apply it to the evaluation of the integral appearing in eq. (9).

We begin by adding and subtracting from eq. (9) its limiting form, valid when the surface has negligible diffuseness, i.e. eq. (3):

$$\begin{aligned} g &= \frac{3}{2\epsilon} A - \frac{3}{2\epsilon} \iiint_{\text{ndt}} + \frac{3n_0}{2\epsilon} \iiint \left(\frac{n}{n_0} \right)^{1/3} dt \\ &= \frac{3}{2\epsilon} A + \frac{3n_0}{2\epsilon} \iiint \left[\left(\frac{n}{n_0} \right)^{1/3} - \left(\frac{n}{n_0} \right) \right] dt \\ &= \frac{3}{2\epsilon} A + \frac{3n_0}{2\epsilon} \oint_{\mathcal{L}} \int_{\mathcal{L}} dz \frac{d\phi(z)}{d\sigma} \end{aligned} \quad (10)$$

In the last line we have split up the volume integral into a surface integral over $\mathcal{L}$ and an integration along normals z set up on $\mathcal{L}$. This is useful because the integrand $[(n/n_0)^{1/3} - (n/n_0)]$, denoted for brevity by ϕ , is confined to the vicinity of the surface $\mathcal{L}$. (The two terms in ϕ cancel in the bulk and tend to zero separately on the outside.) In the normal integration along a "normal tube", intercepting the surface $\mathcal{L}$ in a surface element $d\sigma$, the factor $d\phi(z)/d\sigma$ allows for the fact that (when $\mathcal{L}$ is curved) the tube cross-section varies with the distance z . From elementary geometry the following relation is known:

$$d\phi(z) = (1 + Kz + \text{higher powers of } z) d\sigma,$$

where κ is the total curvature ($\kappa = R_1^{-1} + R_2^{-1}$), where R_1 , R_2 are the two principal radii of curvature at the point in question). The following equations follow elementarily:

$$g = \frac{3}{2\varepsilon} A + \frac{3n_0}{2\varepsilon} \oint_{\Sigma} d\sigma \int dz (1 + \kappa z + \dots)^{\frac{1}{2}} \\ = \frac{3}{2\varepsilon} A + \frac{3n_0 b}{2\varepsilon} \oint_{\Sigma} (dz \zeta^{\frac{1}{2}}) \oint_{\Sigma} d\sigma + \frac{3n_0 b^2}{2\varepsilon} \oint_{\Sigma} (dz \zeta^{\frac{1}{2}}) \oint_{\Sigma} d\sigma \kappa + \dots$$

and, if we write n_0 as $A/(\frac{4}{3}\pi R^3)$,

$$a = \frac{\pi^2}{4\varepsilon} A [1 + 3(b/R) \nu_0 F_2 + 6(b/R)^2 \nu_1 F_3 + \dots] \quad (11)$$

In the above, we have introduced the Süssmann surface width b [ref. 8)] as unit of length in the integrations over z , and have used the symbols ν_0 , ν_1 for the zeroth and first moments of $\zeta^{\frac{1}{2}}$, viz.:

$$\nu_0 = \int d\zeta \zeta^{\frac{1}{2}}$$

and

$$\nu_1 = \int d\zeta \zeta^{\frac{3}{2}},$$

where $\zeta = z/b$. (Recall that z is the outward normal distance from the effective sharp surface.)

The quantities F_2 , F_3 are the surface area and the integrated curvature of the surface Σ , in units of their values for the spherical shape, viz.

$$F_2 = \oint_{\Sigma} d\sigma / (4\pi R^2),$$

and

$$F_3 = \oint_{\Sigma} d\sigma \kappa / (8\pi R).$$

A generalization of eq. (11) to the case of a nucleus with N neutrons and Z protons may be obtained by considering the single-particle density of levels to be the sum of two contributions:

$$g = g_N + g_Z,$$

i.e.

$$a = a_N + a_Z, \quad (12)$$

where

$$a_N = \frac{\pi^2}{4\varepsilon_N} N [1 + 3(b_N/R_N) \nu_0 F_2 + 6(b_N/R_N)^2 \nu_1 F_3 + \dots], \quad (13)$$

$$a_Z = \frac{\pi^2}{4\varepsilon_Z} Z [1 + 3(b_Z/R_Z) \nu_0 F_2 + 6(b_Z/R_Z)^2 \nu_1 F_3 + \dots]. \quad (14)$$

Here ε_N , ε_Z are the Fermi energies of the neutrons and protons, R_N and R_Z are the effective sharp radii of the neutron and proton distributions, and b_N , b_Z are the two relevant surface widths. Using eq. (8) we may readily verify that

$$\varepsilon_N = K \frac{(2N)^{2/3}}{R_N^2}, \quad \varepsilon_Z = K \frac{(2Z)^{2/3}}{R_Z^2}, \quad \varepsilon = K \frac{A^{2/3}}{R^2},$$

where

$$K = \left(\frac{9\pi^2}{8} \right)^{2/3} \frac{\hbar^2}{2m}.$$

The radii R_N , R_Z , R may, in general, be slightly different. Drop-let Model formulae for R_N , R_Z , R may be found in refs. 9, 10). The difference $R_N - R_Z$ is the "neutron skin". If the neutron skin is disregarded and we write $R_N = R_Z = R = r_0 A^{1/3}$ and $b_N = b_Z = b$, then eq. (12) may be written as

$$a = \frac{\pi^2}{4\varepsilon} A [1 + 3(b/R) \nu_0 F_2 + 6(b/R)^2 \nu_1 F_3 + \dots] \left[1 - \frac{1}{9} \left(\frac{N-Z}{A} \right)^2 + \dots \right] \\ = \frac{\pi^2}{4\varepsilon} A [1 + 3(b/r_0) \nu_0 F_2 A^{-1/3} + 6(b/r_0)^2 \nu_1 F_3 A^{-2/3} + \dots] \left[1 - \frac{1}{9} \left(\frac{N-Z}{A} \right)^2 + \dots \right] \quad (15)$$

The last term in eq. (15) is the correction to $\underline{a}$ due to the neutron excess, analogous to the symmetry energy correction in the nuclear binding-energy formula.

Equation (15) is the leptodermous expansion for the level density

parameter $\bar{a}$, carried out to order $A^{1/3}$. We may note that the next term, of order A^0 , consists of two contributions, proportional to $(b/r_0)^3 F_4$ and $(b/r_0)^3 F_4'$, where F_4 is the integrated Gaussian curvature and F_4' is the integrated squared curvature of the surface Σ . [See ref.⁵].]

7. Estimates of Coefficients

In illustrating eq.(11) we shall use $r_0 = 1.16$ fm as a representative value describing the bulk matter density of finite nuclei. [See Fig.(12) in ref.⁹.] This leads to $\epsilon = 36.05$ MeV for the Fermi energy. With b taken as about 1 fm [ref.⁹], this leaves only the pure numbers v_0 and v_1 to be estimated from an assumed density fall-off profile (n/n_0) . In the Appendix we present a study of the dependences of v_0 and v_1 on the profile function. A choice that appears to us reasonable in view of this study is the "standard profile", proportional to the error function complement, i.e.

$$\frac{n}{n_0} = f(\xi) = \frac{1}{2\pi\tau} \int_{\xi}^{\infty} e^{-t^2/2} dt = \frac{1}{2} (1 - \operatorname{erf} \frac{\xi}{\sqrt{2}}) \quad (16)$$

This profile is qualitatively like a Woods-Saxon profile, but approaches more rapidly its asymptotic values at $\pm\infty$. It is "standard" in the sense that its (negative) derivative is a standard Gaussian distribution, with zero mean and skewness.

With this choice of (n/n_0) a numerical integration yields

$$\begin{aligned} v_0 &= 1.2042 \\ v_1 &= 1.2619 \end{aligned}$$

This leads to

$$a = \frac{\bar{A}}{14.61 \text{ MeV}} (1 + 3.114A^{-1/3} F_2 + 5.626A^{-2/3} F_3 + \dots), \quad (17)$$

if the slight dependence on the neutron excess is disregarded.

5. Discussion

For a heavy spherical nucleus ($A=216$, $F_2=F_3=1$) eq.(13) gives

$$a = \frac{\bar{A}}{14.61 \text{ MeV}} (1 + 0.5190 + 0.1563) = \frac{\bar{A}}{8.721 \text{ MeV}} = 24.77 \text{ MeV}^{-1},$$

to be compared with the empirical rule

$$a \approx \frac{\bar{A}}{8.5 \text{ MeV}} \approx 25.41 \text{ MeV}^{-1}.$$

For a lighter nucleus, $A=64$,

$$a = \frac{\bar{A}}{14.61 \text{ MeV}} (1 + 0.7785 + 0.3516) = \frac{\bar{A}}{6.859 \text{ MeV}} = 9.33 \text{ MeV}^{-1}.$$

For a very light nucleus, $A=27$, where the convergence of the leptodermous expansion is questionable,

$$a = \frac{\bar{A}}{14.61 \text{ MeV}} (1 + 1.0380 + 0.6251) = \frac{\bar{A}}{5.486 \text{ MeV}} = 4.92 \text{ MeV}^{-1}.$$

Comparing the trend of these numbers with the trend deduced from experiments [allowing for shell effects that reduce the values of a_{exp} near magic numbers - see Fig.(2-12) in ref.¹] there seems to be no evidence for major discrepancies, such as would be present if only the volume term, $a \sim \bar{A}/14.61$ MeV, were retained. (The ratio of 14.61 MeV to the empirical 8.5 MeV is 1.72.) This agreement is, perhaps, somewhat fortuitous, since other non-negligible corrections to the level density are anticipated. [See the discussion following eq.(2-117) in ref.¹] and the discussion of the curvature correction in the Appendix.] However, even with this reservation, eq.(17) should be more useful than the usual empirical relation $a \sim \bar{A}/8.5$ MeV, since it at least makes allowances for an obvious geometrical effect that must be present: the availability of an effective volume (for particles near the Fermi energy) greater than would be estimated by assuming all nucleons to reside at the bulk density. Since this effect is associated with the surface region,

eq. (17) also assigns, through the functions F_2, F_3 , the approximately correct shape dependence to the correction. [Tables of F_2 and F_3 for fission saddle-point shapes are provided in ref. ¹¹.]

Appendix

For a surface profile ("profile L") defined by an arbitrary power, m , of a linear function of z viz.:

$$f_L \equiv \frac{n}{n_0} = \begin{cases} \left(\frac{z_2 - z}{z_2 - z_1} \right)^m & \text{for } z < z_1 \\ 1 & \text{for } z_1 < z < z_2 \\ 0 & \text{for } z > z_2 \end{cases}$$

we find for the location of the effective sharp surface z_0 the formula

$$z_0 = z_2 - (z_2 - z_1) \frac{m}{m+1} \quad (A1)$$

and for the Süssmann width b the formula

$$b = (z_2 - z_1) \left[\frac{m}{(m+2)(m+1)} z \right]^{1/2} \quad (A2)$$

For the zeroth and first dimensionless moments of Φ ($\equiv f^1, f$) we then find

$$v_0 = \frac{2\sqrt{m(m+2)}}{m+3} \quad (A3)$$

and

$$v_1 = \frac{2(3m^2 + 5m - 3)}{(m+3)(m+6)} \quad (A4)$$

For a surface profile ("profile Q") defined by a power (equal to $3m/2$, where m is a positive integer) of a quadratic function of z viz.:

$$f_Q \equiv \frac{n}{n_0} = \begin{cases} 1 - \left(\frac{z - z_1}{z_2 - z_1} \right)^{2m/2} & \text{for } z < z_1 \\ 0 & \text{for } z_1 < z < z_2 \\ 0 & \text{for } z > z_2 \end{cases}$$

we find

$$z_0 = z_1 + (z_2 - z_1) \frac{(3m)!}{(3m+1)!} p, \quad (A5)$$

where $p=1$ if m is even and $p=\pi/2$ if m is odd. We also find

$$b = (z_2 - z_1) \left\{ \frac{2}{3m+2} - \left[\frac{(3m)!}{(3m+1)!} \right]^{1/2} \right\}, \quad (A6)$$

$$v_0 = \left[\frac{m!}{(m+1)!} - \frac{(3m)!}{(3m+1)!} p \left\{ \frac{2}{3m+2} - \left[\frac{(3m)!}{(3m+1)!} \right]^{1/2} \right\} \right]^{-1/2}, \quad (A7)$$

$$v_1 = \left\{ \frac{2m}{(m+2)(3m+2)} - \frac{(3m)!}{(3m+1)!} \left[\frac{m!}{(m+1)!} - \frac{(3m)!}{(3m+1)!} \right] \right\} \cdot \left\{ \frac{2}{3m+2} - \left[\frac{(3m)!}{(3m+1)!} \right]^{1/2} \right\}^{-1} \quad (A8)$$

The following table illustrates these results

m	PROFILE L	PROFILE Q
	v_0	v_0
1	0.866	0.357
2	1.131	0.950
3	1.291	1.444
4	1.400	1.857
5	1.479	2.205
6	1.540	2.500
	v_1	v_1
1	0.866	0.357
2	1.131	0.950
3	1.291	1.444
4	1.400	1.857
5	1.479	2.205
6	1.540	2.500

We note that v_0 is relatively insensitive to the profile type, its numerical values being close to 1 for "short-tailed" profiles ($m \approx 1$) and somewhat greater than 1 for very long-tailed profiles ($m \approx 5, 6$). On the other hand, v_1 is much more sensitive to profile type, varying from close to 1/3 for very short-tailed profiles, to close to 2.5 for very long-tailed profiles. This rule is confirmed by a numerical calculation

for the relatively long-tailed Woods-Saxon profile

$$f_{WS} = [1 + e^{(z-z_0)/a}]^{-1},$$

which gives $v_0=1.4085$, $v_1=2.2763$. The result for the "standard" profile, quoted in the text ($v_0=1.2042$, $v_1=1.2619$), is also in line with this rule.

Without more involved studies we cannot claim to have available reliable estimates of v_0, v_1 (especially the latter). In the text we have chosen the values associated with the standard profile. This "conservative" profile (neither extremely short-nor long-tailed) is unlikely to lead to a substantial error as regards v_0 , and places less weight than the Woods-Saxon profile on the uncertain curvature correction.

The uncertainty as regards the true value of the curvature correction is compounded by the fact that our derivation provides only the "geometrical" part of the curvature correction coefficient in eq. (15). This part results from curving the nuclear surface while keeping the profile function fixed. In general, the profile itself may change as the surface becomes curved. If the quantity whose leptodermous expansion is being considered responds linearly to a change in profile, this results in a further contribution to the curvature correction coefficient. In the case of the leptodermous expansion for the binding energy there is no linear response to a change in profile, since the (surface) energy of the originally plane surface is stationary with respect to all degrees of freedom (including profile changes). The result is that the associated correction skips one order in $A^{-1/3}$ and would only appear in the term proportional to A^0 . But, since there is no reason why the level density parameter a should be stationary with respect to profile changes, a further correction at the $A^{1/3}$ level is to be expected. To estimate it would require a discussion of the subtle question of how the profile of a nuclear surface changes with curvature.

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