

Exchange energy of an electron gas of arbitrary dimensionality

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EXCHANGE ENERGY OF AN ELECTRON GAS OF ARBITRARY DIMENSIONALITY*

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Abstract. Procedures are presented for obtaining the complete low temperature asymptotic behavior of fractional integrals (of Riemann–Liouville type) of squares of Fermi–Dirac integrals. These integrals occur in consideration of the properties of electron systems. The development is presented in the context of calculating the exchange thermodynamic potential for a d -dimensional neutralized homogeneous electron gas interacting via a $1/r$ potential.

Key words. Riemann–Liouville fractional integral, asymptotic expansion, exchange energy

1. Introduction. The study of the thermodynamics of the electron gas in three dimensions has a long history. Because of recent interest in systems such as semiconductor inversion layers, having restricted dimensionality, the two-dimensional analogue is receiving similar scrutiny. Several investigations of the first order exchange energy of these systems are available, the most recent being that of Isihara and Toyoda [1] (cf. also [1a]). The analytic methods used give only the leading terms of the low temperature expansion, however, and the main purpose of this note is to present the complete asymptotic series. We can do this most succinctly if the dimensionality d of the system is left arbitrary and we specialize to $d = 2, 3$ at the end of the calculation. To our knowledge this device has been used previously only by May [2] who examined the specific heat of the ideal Fermi and Bose gases and showed that they coincide for $d = 2$. Our result can also be applied for $d = 1$, where the model has been used for certain one-dimensional organic metals and the general expression may be of interest to renormalization group theorists. Specifically, we calculate the first order exchange contribution to the thermodynamic potential of a uniform neutralized electron gas under the usual assumption that the electrons interact by the $1/r$ potential in all dimensions.

2. Formulation of the problem. The general expression for the quantity we wish to calculate is

$$(1) \quad \log \Xi_x = \frac{v\beta}{(2\pi)^{2d}} \int d\mathbf{q} d\mathbf{p} u(\mathbf{q})f(\mathbf{p})f(\mathbf{p} + \mathbf{q})$$

in the sense that $\log \Xi = \log \Xi_0 + e^2 \log \Xi_x + \dots$, where Ξ is the grand partition function, v is the (d -dimensional) volume, e is the electron charge, $u(\mathbf{q})$ is the Fourier transform of $1/r$, $\beta = 1/k_B T$ where k_B is the Boltzmann constant and $f(\mathbf{p})$ is the Fermi function [3]

$$(2) \quad f(\mathbf{p}) = \{1 + \exp[-\beta(k_F^2 - p^2)]\}^{-1} = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \frac{\pi \exp[\beta(k_F^2 - p^2)s]}{\sin \pi s}, \quad 0 < c < 1.$$

Units where $\hbar = 2m = 1$ are used and k_F denotes the Fermi momentum. Inserting (2) into (1) leads to the $2d$ -dimensional integral

$$(3) \quad J_d(s_1, s_2) = \int d\mathbf{p} d\mathbf{q} u(\mathbf{q}) e^{-\beta p^2 s_1} e^{-\beta|\mathbf{p} + \mathbf{q}|^2 s_2}.$$

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In view of (hyper-)spherical symmetry, we have

$$(4) \quad \int d\mathbf{k} = \frac{2\pi^{(d-1)/2}}{\Gamma((d-1)/2)} \int_0^\infty k^{d-1} dk \int_0^\pi \sin^{d-2} \theta d\theta.$$

Thus, for example, the d -dimensional Fourier transform of the Coulomb potential is

$$(5) \quad u(\mathbf{q}) = \int \frac{d\mathbf{r}}{r} e^{i\mathbf{q} \cdot \mathbf{r}} = \frac{2\pi^{(d-1)/2}}{\Gamma((d-1)/2)} \int_0^\infty r^{d-2} dr \int_0^\pi \sin^{d-2} \theta d\theta e^{iqr \cos \theta}.$$

Assuming initially that $1 < d < 3$, both integrations are elementary and we find

$$(6) \quad u(\mathbf{q}) = \frac{(4\pi)^{d/2}}{2\pi^{1/2}} \frac{\Gamma((d-1)/2)}{q^{d-1}}$$

which is valid for all $d > 1$ by analytic continuation. In the same way the \mathbf{q} integral in (3) can be evaluated in terms of θ , where θ is the angle between \mathbf{p} and \mathbf{q} . The substitution $x = \cos \theta$ leads to an integral of the form

$$(7) \quad I = \int_{-1}^1 e^{-zx} (1-x^2)^{a-1} dx,$$

which is a special case of Poisson's integral representation for the modified Bessel function, so we have

$$(8) \quad I = 2^{3a-3/2} \frac{\Gamma(a+1/2)\Gamma^2(a)}{\Gamma(2a)} z^{-(a-1/2)} I_{a-1/2}(z)$$

and making the substitution $q^2 = t$, an integral is obtained which is a standard Laplace transform; thus the \mathbf{q} -integral becomes

$$(9) \quad Q = \frac{4^{d-1} \pi^{d-1/2}}{2\sqrt{\beta s_2}} \frac{\Gamma^2((d-1)/2)}{\Gamma(d-1)} {}_1F_1\left(\frac{1}{2}, \frac{d}{2}; \beta s_2 p^2\right).$$

Therefore, after performing the elementary angular integration (3) becomes

$$(10) \quad J_d(s_1, s_2) = \frac{4^{d-1} \pi^{(3d-1)/2}}{\sqrt{\beta s_2}} \frac{\Gamma^2((d-1)/2)}{\Gamma(d/2)\Gamma(d-1)} \int_0^\infty p^{d-1} e^{-\beta(s_1+s_2)p^2} {}_1F_1\left(\frac{1}{2}, \frac{d}{2}; \beta s_2 p^2\right) dp.$$

Finally the substitution $p^2 \rightarrow t$ leads to a tabulated Laplace transform giving

$$(11) \quad J_d(s_1, s_2) = 4^{d-3/2} \pi^{(3d-1)/2} \beta^{-(d+1)/2} \frac{\Gamma^2((d-1)/2)}{\Gamma(d-1)} \frac{(s_1+s_2)^{(1-d)/2}}{\sqrt{s_1 s_2}}.$$

The insertion of (11) and (2) into (1) leaves us with a double contour integral which can be factored by writing

$$(12) \quad (s_1 + s_2)^{-(d-1)/2} = \frac{1}{\Gamma((d-1)/2)} \int_0^\infty t^{(d-3)/2} e^{-(s_1+s_2)t} dt.$$

The two contour integrals then have the form [3], [4]

$$(13) \quad \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\pi e^{as}}{s^{1/2} \sin \pi s} ds = F_{-1/2}(a), \quad 0 < c < 1,$$

where $F_p(a)$ is the usual Fermi integral of order p ,

$$(14) \quad F_p(a) = \frac{1}{\Gamma(p+1)} \int_0^\infty \frac{x^p dx}{1+e^{x-a}}.$$

This function, with $p = -\frac{1}{2}$, plays a central role in the remainder of the calculation. Its properties are surveyed in [3]; we shall drop the subscript and denote it simply by $F(a)$. We therefore have, after a simple change of variable in the final t -integration,

$$(15) \quad \log \Xi_x = \frac{v}{2^{d+1}} \beta^{(1-d)/2} \frac{\pi^{-d/2}}{\Gamma(d/2)} \int_{-\infty}^{\eta} (\eta - t)^{(d-3)/2} [F(t)]^2 dt$$

where $\eta = \beta k_F^2$. Expression (15) is valid for $d > 1$ and for $d = 2, 3$ reduces to the formulas presented in reference [1].

3. Asymptotic analysis. We are interested in the behavior of the exchange energy at low temperatures and are therefore concerned with an asymptotic expansion of (15) as $\eta \rightarrow \infty$. The integral in (15)

$$(16) \quad G_{\mu}(\eta) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{\eta} (\eta - t)^{\mu-1} [F(t)]^2 dt$$

is the Riemann–Liouville fractional integral of order μ , of $[F(t)]^2$, and its asymptotic behavior can be found by the method in [5, § 4.10] using Mellin transform theory. This is described in the Appendix. Instead we present here an alternative procedure using the two-sided Laplace transform. The reason for presenting both approaches is that they each leave certain constants in the expansions either unspecified or in terms of complicated integrals. By comparing the results obtained in these two ways, these constants can be uniquely determined and the asymptotic series worked out completely.

From [3] we know that $[F(x)]^2 = O(e^{2x})$ as $x \rightarrow -\infty$, and as $x \rightarrow \infty$

$$(17) \quad [F(x)]^2 \sim \frac{4x}{\pi} + \sum_{k=0}^{\infty} a_k x^{-2k-1},$$

where it can be shown by similar methods that

$$(18) \quad a_k = \frac{4}{\pi^2} \sum_{n=0}^{k+1} \Gamma\left(2n - \frac{1}{2}\right) \Gamma(2k - 2n + 3/2) (1 - 2^{1-2n}) (1 - 2^{-1-2k+2n}) \zeta(2n) \zeta(2k - 2n + 2)$$

and in particular

$$(19) \quad a_0 = -\frac{\pi}{3}, \quad a_1 = -\frac{5\pi^3}{36}.$$

Therefore, in the strip $0 < \text{Re } s < 2$ we have

$$(20) \quad \bar{G}_{\mu}(s) = \int_{-\infty}^{\infty} e^{-s\eta} G_{\mu}(\eta) d\eta = \frac{1}{\Gamma(\mu)} \int_{-\infty}^{\infty} [F(t)]^2 dt \int_0^{\infty} e^{-s\eta} (\eta - t)^{\mu-1} d\eta = \frac{g(s)}{s^{\mu}},$$

where

$$(21) \quad g(s) = \int_{-\infty}^{\infty} e^{-st} [F(t)]^2 dt.$$

We therefore have the representation

$$(22) \quad G_{\mu}(\eta) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{g(s)}{s^{\mu}} e^{ns} ds, \quad 0 < c < 2.$$

The desired asymptotic expansion of $G_{\mu}(\eta)$ for $\eta \rightarrow \infty$ can be found by a standard method [6] in which we insert for $g(s)$ in (22) its development about $s = 0$. The

“dictionary” of necessary formulas is given in Table 1. Here the left column shows a specific term of the development about $s = 0$; the right column shows the corresponding term of the asymptotic expansion as $\eta \rightarrow \infty$. ($\psi(z)$ denotes the logarithmic derivative of the gamma function.)

TABLE 1
Inverse Laplace transforms

$f(s)$	$(1/2\pi i) \int_{c-i\infty}^{c+i\infty} f(s) e^{s\eta} ds$
s^λ	$\begin{cases} \left[\frac{1}{\Gamma(-\lambda)} \right] \eta^{-\lambda-1}, & \lambda \neq 0, 1, 2, \dots \\ 0, & \lambda = 0, 1, 2, \dots \end{cases}$
$s^\lambda \log s$	$\begin{cases} -\left[\frac{1}{\Gamma(-\lambda)} \right] \eta^{-\lambda-1} [\log \eta - \psi(-\lambda)], & \lambda \neq 0, 1, 2, \dots \\ (-1)^{\lambda+1} \lambda! \eta^{-\lambda-1}, & \lambda = 0, 1, 2, \dots \end{cases}$

In order to obtain the needed development of $g(s)$ it is convenient to use an alternative integral representation which we can obtain from Parseval’s formula. We have

$$(23) \quad f(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-sx/2} F(x) e^{ixu} dx = \frac{1}{\pi\sqrt{2}} \int_0^{\infty} t^{-1/2} dt \int_{-\infty}^{\infty} dx \frac{e^{-(s/2-iu)x}}{1 + e^{-x} e^t}.$$

Following the substitution $y = e^{-x+t}$ in the x integral, the integrals separate and we easily obtain

$$(24) \quad f(u) = \left(\frac{\pi}{2}\right)^{1/2} \frac{(s/2-iu)^{-1/2}}{\sin [\pi/2(s-2iu)]}.$$

By Parseval’s relation

$$(25) \quad \begin{aligned} \int_{-\infty}^{\infty} e^{-sx} [F(x)]^2 dx &= \int_{-\infty}^{\infty} f(u) f(-u) du \\ &= \pi \int_{-\infty}^{\infty} \frac{(s^2/4+u^2)^{-1/2}}{\cosh(2\pi u) - \cos(\pi s)} du. \end{aligned}$$

Next, by noting the representation [7, Eq. 1.9 (14)]

$$(26) \quad [\cosh(2\pi u) - \cos(\pi s)]^{-1} = \frac{1}{\pi} \csc(\pi s) \int_0^{\infty} \frac{\sinh[(1-s)x/2]}{\sinh(x/2)} \cos(xu) dx$$

we find

$$(27) \quad \begin{aligned} g(s) &= 2 \csc(\pi s) \int_0^{\infty} \frac{\sinh[x(1-s)/2]}{\sinh(x/2)} dx \int_0^{\infty} \frac{\cos(ux)}{\sqrt{\frac{1}{4}s^2+u^2}} du \\ &= 2 \csc(\pi s) \int_0^{\infty} K_0\left(\frac{1}{2}sx\right) \frac{\sinh[x(1-s)/2]}{\sinh(x/2)} dx. \end{aligned}$$

Finally, after an elementary transformation and use of the fact that [7, Eq. 4.16 (23)]

$$(28) \quad \int_0^\infty K_0(ax) e^{-ax} dx = \frac{1}{a}$$

we have the desired representation

$$(29) \quad g(s) = 4 \csc(\pi s) \left[s^{-1} - \int_0^\infty K_0\left(\frac{sx}{2}\right) \sinh\left(\frac{sx}{2}\right) \frac{e^{-x}}{1-e^{-x}} dx \right].$$

To expand (29) for small s we begin with [8, eqs. 5.41(1), 5.42(1)]

$$(30) \quad J_{1/2}(z)H_0^{(1)}(z) = \sum_{m=0}^\infty \frac{(-1)^m (z/2)^{2m+1/2} (m+3/2)_m}{(m!)^2 \Gamma(m+3/2)} \cdot \left[1 + \frac{i}{\pi} \left\{ 2 \log\left(\frac{z}{2}\right) + 2\psi\left(2m + \frac{3}{2}\right) - 2\psi\left(m + \frac{3}{2}\right) - 2\psi(m+1) \right\} \right].$$

Next we note that

$$(31) \quad J_{1/2}(iz) = \sqrt{\frac{2}{\pi iz}} i \sinh z, \quad H_0^{(1)}(iz) = \frac{2}{\pi i} K_0(z)$$

which gives us an expansion for $K_0(z) \sinh z$. Then with $z = sx/2$, and use of the identities

$$(32) \quad \frac{(m+3/2)_m}{(m!)^2 \Gamma(m+3/2)} = \frac{4}{\pi} \frac{2^{4m} \Gamma(2m+3/2)}{[(2m+1)!]^2},$$

$$\psi(m+1) + \psi(m+3/2) = 2\psi(2m+2) - 2 \log 2,$$

we find after an elementary integration

$$(33) \quad g(s) = \frac{4}{\pi s^2} \frac{\pi s}{\sin(\pi s)} \pi^{-1/2} \sum_{m=0}^\infty \frac{\Gamma(2m-1/2)}{(2m-1)!} \zeta(2m) s^{2m} \cdot \left[\log(s) + \psi(2m-1/2) - \psi(2m) + \frac{\zeta'(2m)}{\zeta(2m)} \right], \quad |s| < 1,$$

where it is understood that the $m = 0$ term of the series is $\sqrt{\pi}$. Finally we have the series

$$(34) \quad \pi s \csc(\pi s) = 2 \sum_{m=0}^\infty (1 - 2^{1-2m}) \zeta(2m) s^{2m}, \quad |s| < 1.$$

Now the two series in (33) must be multiplied together. Using the well-known values $\zeta(2) = \pi^2/6$ and $\zeta(4) = \pi^4/90$ we find to order $s^4 \log s$

$$(35) \quad g(s) = \frac{4}{\pi s^2} + \frac{\pi}{3} \log\left(\frac{s}{4}\right) + \left(\pi + \frac{2}{\pi} \zeta'(2) \right) + \frac{5\pi^3}{72} s^2 \log\left(\frac{s}{4}\right) + \left(\frac{65\pi^3}{432} + \frac{\pi}{3} \zeta'(2) + \frac{5}{4\pi} \zeta'(4) \right) s^2 + O(s^4 \log s).$$

The present expansion is inserted into (22). Term-by-term integration and the use of Table 1 then yields the desired asymptotic expansion of $G_\mu(\eta)$ up to relative order

$\eta^{-6} \log \eta$. The expansion thus obtained is inserted into (15) yielding

$$\begin{aligned}
 \log \Xi_x &= \frac{v}{2^{d-3}} \beta^{(1-d)/2} \frac{\pi^{-(d+2)/2}}{(d^2-1)\Gamma(d/2)} \eta^{(d+1)/2} \\
 &\cdot \left\{ 1 - \frac{\pi^2}{48} (d^2-1) \eta^{-2} \log \eta + \frac{\pi^2}{48} (d^2-1) \left[\psi\left(\frac{d-1}{2}\right) - \log 4 + 3 + \frac{\zeta'(2)}{\zeta(2)} \right] \eta^{-2} \right. \\
 (36) \quad &- \frac{5\pi^4}{4608} (d^2-1)(d-3)(d-5) \eta^{-4} \log \eta + \frac{5\pi^4}{4608} (d^2-1)(d-3)(d-5) \\
 &\cdot \left. \left[\psi\left(\frac{d-5}{2}\right) - \log 4 + \frac{13}{6} + \frac{4}{5} \frac{\zeta'(2)}{\zeta(2)} + \frac{1}{5} \frac{\zeta'(4)}{\zeta(4)} \right] \eta^{-4} + O(\eta^{-6} \log \eta) \right\}.
 \end{aligned}$$

This method allows one to obtain as many terms as desired in the asymptotic expansion, but necessitates the multiplication of two infinite series and is therefore limited in practice. It does however furnish the explicit value of all constants which enter into the expansion. In the Appendix we describe an alternative procedure which gives the complete expansion as a single series, but does not by itself identify all the coefficients in the expansion; however, they can be found by comparison with the formulas obtained above. From (A18) we quote the result

$$\begin{aligned}
 G_\mu(\eta) &\sim \frac{4}{\pi\Gamma(\mu+2)} \eta^{\mu+1} + \sum_{k=0}^{\infty} \frac{a_k}{(2k)!\Gamma(\mu-2k)} \{\log \eta + \psi(2k+1) - \psi(\mu-2k)\} \eta^{\mu-2k-1} \\
 (37) \quad &+ \sum_{k=0}^{\infty} \frac{c_{2k}}{(2k)!\Gamma(\mu-2k)} \eta^{\mu-2k-1}, \quad \eta \rightarrow \infty,
 \end{aligned}$$

where c_{2k} is given by (A19) and (A20).

All the coefficients in these expansions are known to many decimal places except for the logarithmic derivative of the Riemann zeta function. A seven-place table of the latter is available, however [9]. For convenience we list a few values here

$$\begin{aligned}
 \psi(1) &= \gamma = 0.5772156649 \dots, \\
 \zeta'(2)/\zeta(2) &= -0.569960993 \dots, \\
 (38) \quad \zeta'(4)/\zeta(4) &= -0.063669765 \dots, \\
 c_0 &= 0.4885480063 \dots, \\
 c_2 &= 5.3160859668 \dots.
 \end{aligned}$$

4. Discussion. The exchange contribution to the internal energy is

$$(39) \quad E_x^d = -\frac{e^2}{v} \left(\frac{\partial \log \Xi_x}{\partial \beta} \right)_\eta$$

where e is the electron charge, so that we have for low temperatures

$$\begin{aligned}
 E_x^d &= \frac{e^2}{2^{d-2}} \frac{\pi^{-(d+2)/2}}{(d+1)\Gamma(d/2)} k_F^{d+1} \\
 &\cdot \left\{ 1 - \frac{\pi^2}{48} (d^2-1) \eta^{-2} \log \eta + \frac{\pi^2}{48} (d^2-1) \left[\psi\left(\frac{d-1}{2}\right) - \log 4 + 3 + \frac{\zeta'(2)}{\zeta(2)} \right] \eta^{-2} \right. \\
 (40) \quad &- \frac{5\pi^4}{4608} (d^2-1)(d-3)(d-5) \eta^{-4} \log \eta + \frac{5\pi^4}{4608} (d^2-1)(d-3)(d-5) \\
 &\cdot \left. \left[\psi\left(\frac{d-5}{2}\right) - \log 4 + \frac{13}{6} + \frac{4}{5} \frac{\zeta'(2)}{\zeta(2)} + \frac{1}{5} \frac{\zeta'(4)}{\zeta(4)} \right] \eta^{-4} + O(\eta^{-6} \log \eta) \right\}.
 \end{aligned}$$

In particular,

$$(41a) \quad E_x^1 = \frac{e^2 k_F^2}{\pi^2} \left\{ 1 - \frac{\pi^2}{12\eta^2} - \frac{5\pi^4}{144} \eta^{-4} + O(\eta^{-6}) \right\},$$

$$(41b) \quad E_x^2 = \frac{e^2 k_F^3}{3\pi^2} \left\{ 1 - \frac{\pi^2 \log \eta}{16 \eta^2} - 0.56735753 \eta^{-2} - \frac{5\pi^4}{512} \eta^{-4} \log \eta \right. \\ \left. + 0.96536423 \eta^{-4} + O(\eta^{-6} \log \eta) \right\},$$

$$(41c) \quad E_x^3 = \frac{e^2 k_F^4}{4\pi^3} \left\{ 1 - \frac{\pi^2 \log \eta}{6 \eta^2} + 0.76740941 \eta^{-2} + \frac{5\pi^4}{144} \eta^{-4} + O(\eta^{-6}) \right\}.$$

For $d = 2, 3$ these results agree well with the expressions given by Isihara and Toyoda [1], differing only slightly in the value of the coefficient of the third terms. This work corrects an erroneous calculation by one of the authors [10], where Hospitals' rule was applied inconsistently in that a constant of integration was ignored. While the first two terms of (41c) were given correctly, the remainder of the expansion was not.

The results in (40) and (41) are not the physical value of the exchange energy. To obtain this, (36) must be combined with the kinetic contribution to the thermodynamic potential, which is

$$(42) \quad \log \Xi_0 = \frac{v\beta 2^{1-d} \pi^{-d/2} k_F^{d+2}}{\Gamma((d+4)/2)} \left\{ 1 + \frac{\pi^2}{24\eta^2} d(d+2) + O(\eta^{-4}) \right\}.$$

Next, k_F must be determined to order e^2 in terms of the density ρ by means of the relation

$$(43) \quad \rho = \frac{1}{2} (\beta v)^{-1} \left(\frac{\partial \log \Xi}{k_F \partial k_F} \right)_{\beta, v}.$$

When this is carried out, the resulting expression is inserted into

$$(44) \quad E^d = -\frac{1}{v} \frac{\partial}{\partial \beta} [\log \Xi_0 + e^2 \log \Xi_x]_{v, \eta}.$$

The physical exchange energy is then the term in (44) proportional to e^2 . Thus, in the zero temperature limit we have per unit volume

$$(45) \quad E_x^d = -\frac{e^2 \pi^{-(d+2)/2}}{2^{d-3} (d^2 - 1) \Gamma(d/2)} k_0^{d+1}$$

and

$$(46) \quad k_0 = 2\sqrt{\pi} \left[\frac{1}{2} \Gamma\left(\frac{d+2}{2}\right) \rho \right]^{1/d} = 2r_s^{-1} \left[\frac{\Gamma^2((d+2)/2)}{2} \right]^{1/d}$$

where r_s is the standard density parameter (radius of the spherical volume/electron). Hence the exchange energy per electron is

$$(47) \quad E_x^d = -\frac{4d}{\pi(d^2 - 1)} \left[\frac{\Gamma^2((d+2)/2)}{2} \right]^{1/d} \left(\frac{e^2}{r_s} \right).$$

A number of values of $-2E_x^d r_s / e^2 \equiv B(d)$ are listed in Table 2. One might expect E_x^d to vary nonmonotonically with d , since it is related to the density of states in k -space

TABLE 2
 Reduced exchange energy for integer and half-integer dimensions

d	$B(d)$	d	$B(d)$
1	∞	3	0.9163
3/2	1.7201	7/2	0.8527
2	1.2004	4	0.8075
5/2	1.0155	9/2	0.7735
		5	0.7467
		∞	0.4684

and thus to the volume

$$(48) \quad V(d) = \pi^{d/2} / \Gamma\left(\frac{d+2}{2}\right)$$

of the unit sphere which has a maximum at $d \cong 5.26$. However, this variation is compensated for by the dimensionality dependence of the Coulomb form factor in (6) as shown by the monotonic decrease of E_x^d in Table 2. These results have been applied to study the dimensionality dependence of the specific heat [11]. With minor changes the procedures described here are applicable to Bose–Einstein systems, where the Fermi integrals (14) are replaced by the Bose–Einstein integrals

$$(49) \quad B_p(a) = \frac{1}{\Gamma(p+1)} \int_0^\infty \frac{x^p dx}{e^{x+a} - 1}$$

Appendix. The fractional integral of order μ , of $[F(t)]^2$, is defined by

$$(A1) \quad G_\mu(x) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^x (x-t)^{\mu-1} [F(t)]^2 dt,$$

and includes the special cases

$$(A2) \quad \begin{aligned} G_0(x) &= [F(x)]^2, \\ G_k(x) &= \frac{1}{(k-1)!} \int_{-\infty}^x (x-t)^{k-1} [F(t)]^2 dt, \quad k = 1, 2, 3, \dots \end{aligned}$$

It is easily seen that $G'_k(x) = G_{k-1}(x)$, hence, $G_k(x)$ is the repeated integral of order k , of $[F(x)]^2$.

We write $G_\mu(x)$ as the sum of

$$(A3) \quad G_\mu^{(1)}(x) = \frac{1}{\Gamma(\mu)} \int_{-\infty}^0 (x-t)^{\mu-1} [F(t)]^2 dt$$

and

$$(A4) \quad G_\mu^{(2)}(x) = \frac{1}{\Gamma(\mu)} \int_0^x (x-t)^{\mu-1} [F(t)]^2 dt.$$

The asymptotic expansion of $G_\mu^{(1)}(x)$ is readily obtained through repeated integration by parts yielding

$$(A5) \quad G_\mu^{(1)}(x) \sim \sum_{k=0}^{\infty} \frac{G_{k+1}(0)}{\Gamma(\mu - k)} x^{\mu-1-k}, \quad x \rightarrow \infty$$

$$G_{k+1}(0) = \frac{(-1)^k}{k!} \int_{-\infty}^0 t^k [F(t)]^2 dt.$$

To treat the constituent $G_\mu^{(2)}(x)$ we apply the Mellin transform technique developed in [5]. We begin by writing

$$(A6) \quad G_\mu^{(2)}(x) = x^\mu I(x), \quad I(x) = \int_0^\infty [F(xt)]^2 f(t) dt,$$

$$f(t) = \frac{1}{\Gamma(\mu)} (1-t)^{\mu-1} \theta(1-t),$$

where $\theta(\tau)$ denotes the unit step function defined by $\theta(\tau) = 0$ for $\tau < 0$, $\theta(\tau) = 1$ for $\tau > 0$. Now by Parseval's relation for the Mellin transform

$$(A7) \quad I(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-s} M[F^2; s] M[f; 1-s] ds$$

where the path of integration must lie in the strip of analyticity in the s -plane common to the two Mellin transforms. It is easily found that

$$(A8) \quad M[f; 1-s] = \frac{\Gamma(1-s)}{\Gamma(\mu + 1-s)}$$

is analytic for $\text{Re } s < 1$, but the Mellin transform of F^2 does not exist due to behavior $[F(t)]^2 = O(1)$ as $t \rightarrow 0$, and $[F(t)]^2 = O(t)$ as $t \rightarrow \infty$. To get around this problem we write

$$(A9) \quad [F(t)]^2 = h_1(t) + h_2(t),$$

$$h_1(t) = [F(t)]^2 \theta(1-t), \quad h_2(t) = [F(t)]^2 \theta(t-1).$$

Then $M[h_1; s]$ is analytic for $\text{Re } s > 0$, while $M[h_2; s]$ is analytic for $\text{Re } s < -1$. Now we have

$$(A10) \quad I(x) = \frac{1}{2\pi i} \int_{c_1-i\infty}^{c_1+i\infty} x^{-s} M[h_1; s] \frac{\Gamma(1-s)}{\Gamma(\mu + 1-s)} ds$$

$$+ \frac{1}{2\pi i} \int_{c_2-i\infty}^{c_2+i\infty} x^{-s} M[h_2; s] \frac{\Gamma(1-s)}{\Gamma(\mu + 1-s)} ds$$

where $0 < c_1 < 1$, $c_2 < -1$. In order to recombine h_1 and h_2 , $M[h_2; s]$ must be analytically continued into the half-plane $\text{Re } s \geq -1$. To that purpose we introduce

$$(A11) \quad S_k(t) = \left[\frac{4t}{\pi} + \sum_{n=0}^k a_n t^{-2n-1} \right] \theta(t-1),$$

then

$$(A12) \quad M[h_2; s] = M[S_k; s] + M[h_2 - S_k; s] = -\frac{4}{\pi(s+1)} - \sum_{n=0}^k \frac{a_n}{s-2n-1} + M[h_2 - S_k; s]$$

where $M[h_2 - S_k; s]$ is analytic for $\text{Re } s < 2k + 3$. Thus we have $M[h_2; s]$ as a meromorphic function in the strip $-1 \leq \text{Re } s < 2k + 3$ where k can be as large as one likes. This fact can be used to shift the contour of the second integral in (A10) to coincide with that of the first by adding the residue at the intervening pole:

$$(A13) \quad \text{Res}_{s=-1} x^{-s} M[h_2; s] \frac{\Gamma(1-s)}{\Gamma(\mu+1-s)} = -\frac{4x}{\pi\Gamma(\mu+2)}.$$

Thus we find

$$(A14) \quad I(x) = \frac{4x}{\pi\Gamma(\mu+2)} + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-s} M[F^2; s] \frac{\Gamma(1-s)}{\Gamma(\mu+1-s)} ds, \quad 0 < c < 1.$$

From (A12) it is seen that $M[F^2; s]$ has simple poles at $s = 1, 3, 5, \dots$ with residues $-a_0, -a_1, -a_2, \dots$, respectively. Therefore the integrand in (A14) has double poles at $s = 2k + 1$ and simple poles at $s = 2k + 2$, where $k = 0, 1, 2, \dots$. The residues at these poles are determined by a straightforward calculation, viz.,

$$(A15) \quad \text{Res}_{s=2k+1} x^{-s} M[F^2; s] \frac{\Gamma(1-s)}{\Gamma(\mu+1-s)} = -\frac{a_k x^{-2k-1}}{(2k)! \Gamma(\mu-2k)} [\log x + \psi(2k+1) - \psi(\mu-2k)] - \frac{d_{2k} x^{-2k-1}}{(2k)! \Gamma(\mu-2k)},$$

$$(A16) \quad \text{Res}_{s=2k+2} x^{-s} M[F^2; s] \frac{\Gamma(1-s)}{\Gamma(\mu+1-s)} = \frac{d_{2k+1} x^{-2k-2}}{(2k+1)! \Gamma(\mu-2k-1)},$$

where

$$(A17) \quad d_{2k} = \lim_{s \rightarrow 2k+1} \left[M[F^2; s] + \frac{a_k}{s-2k-1} \right], \quad d_{2k+1} = M[F^2; 2k+2].$$

The complete asymptotic expansion of $I(x)$ is obtained now by shifting the line of integration in (A14) arbitrarily far to the right and adding up the residues (A15) and (A16) over $k = 0, 1, 2, \dots$. Then the corresponding asymptotic expansion of $G_\mu^{(2)}(x)$ is found through (A6).

By combining the expansions of $G_\mu^{(1)}(x)$ and $G_\mu^{(2)}(x)$ we establish the asymptotic expansion of $G_\mu(x)$,

$$(A18) \quad G_\mu(x) \sim \frac{4x^{\mu+1}}{\pi\Gamma(\mu+2)} + \sum_{k=0}^{\infty} \frac{a_k}{(2k)! \Gamma(\mu-2k)} x^{\mu-2k-1} [\log x + \psi(2k+1) - \psi(\mu-2k)] + \sum_{k=0}^{\infty} \frac{(-1)^k c_k}{k! \Gamma(\mu-k)} x^{\mu-k-1}, \quad x \rightarrow \infty.$$

Here the coefficients c_k are determined by combining $G_{k+1}(0)$ in (A5) and d_k in (A17); it is found that c_k can be expressed in terms of the modified moment of $[F(t)]^2$,

$$(A19) \quad c_{2k} = \int_{-\infty}^{\infty} t^{2k} \left\{ [F(t)]^2 - \left(\frac{4t}{\pi} + \sum_{n=0}^{k-1} a_n t^{-2n-1} \right) \theta(t) - a_k t^{-2k-1} \theta(t-1) \right\} dt, \\ c_{2k+1} = \int_{-\infty}^{\infty} t^{2k+1} \left\{ [F(t)]^2 - \left(\frac{4t}{\pi} + \sum_{n=0}^k a_n t^{-2n-1} \right) \theta(t) \right\} dt.$$

The present expansion (A18) should be compared to the asymptotic expansion of $G_\mu(x)$ as obtained from (22) through term-by-term integration of the complete series-expansion of $g(s)$ and the use of Table 1. Then by identifying the coefficients of corresponding terms of the two asymptotic expansions it is found that

$$\begin{aligned}
 c_{2k} &= -a_k \psi(2k+1) + \frac{8}{\pi} (2k)! (1-2^{-1-2k}) \zeta(2k+2) \\
 &+ \frac{8}{\pi^{3/2}} (2k)! \sum_{n=1}^{k+1} \frac{\Gamma(2n-1/2)}{(2n-1)!} \left[\psi(2n-1/2) - \psi(2n) + \frac{\zeta'(2n)}{\zeta(2n)} \right] \\
 &\cdot (1-2^{-1-2k+2n}) \zeta(2n) \zeta(2k-2n+2), \\
 c_{2k+1} &= 0.
 \end{aligned}
 \tag{A20}$$

Thus we have effectively evaluated the modified moments of the squared Fermi integral $F_{-1/2}(t)$. The underlying integrals come up in a variety of other contexts. The corresponding integrals for $[F_p(t)]^2$ with $p \neq -\frac{1}{2}$ may be evaluated in the same manner.

Finally, it is pointed out that the expansion (A18) also holds in the special case $\mu = k = 0, 1, 2, \dots$, thus yielding the asymptotic expansion of $G_k(x)$ introduced in (A2). For $\mu = 0$, (A18) reduces to the asymptotic expansion (17) of $[F(x)]^2$. For $\mu = 1$ and $\mu = 2$, (A18) simplifies to

$$\begin{aligned}
 G_1(x) &\sim \frac{2x^2}{\pi} + a_0 \log x + c_0 - \sum_{k=1}^{\infty} \frac{a_k}{2k} x^{-2k}, \quad x \rightarrow \infty \\
 G_2(x) &\sim \frac{2x^3}{3\pi} + a_0 x (\log x - 1) + c_0 x + \sum_{k=1}^{\infty} \frac{a_k}{2k(2k-1)} x^{-2k+1}, \quad x \rightarrow \infty.
 \end{aligned}
 \tag{A21}$$

The present results can also be derived by direct termwise integration of the asymptotic expansion of $[F(t)]^2$.

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