CRITICAL PHENOMENA IN SYSTEMS OF FINITE THICKNESS

II. IDEAL BOSE GAS

By Michael N. Barber†

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Abstract

The grand potential pressure of an ideal boson film which is infinite in \( d-1 \) dimensions \( (d > 2) \) but of finite thickness \( L \) in the \( d \)th dimension is analysed in the limit \( L \to \infty \), to order \( L^{-4} \). Across the film (i) periodic, (ii) antiperiodic, and (iii) hard wall boundary conditions are applied. The corresponding shifts in the critical temperature \( T_{\text{cr}}(L) \) are found to vary, for large \( L \), as (i) \( L^{-d+2} \), (ii) \( L^{-1} \), \( L^{-2} \ln L \), and \( L^{-2} \) for \( d = 3, 4 \), and \( \geq 5 \) respectively, and (iii) \( L^{-1} \ln L \) and \( L^{-1} \) for \( d = 3 \) and \( \geq 4 \). With hard wall boundary conditions, the critical temperature of a sufficiently thick film exceeds that of the bulk, while the other boundary conditions depress \( T_{c} \). The bulk critical region is asymptotically "rounded" on a scale set by the bulk correlation length matching the thickness \( L \) in accord with the scaling theory of finite-size effects.

I. INTRODUCTION

In Part I (Barber and Fisher 1973a), consideration was given to the effects of finite size and surfaces on the critical behaviour of the spherical model (Berlin and Kac 1952; Joyce 1972) of a ferromagnet. On the whole, the analytic results obtained were in accord with the scaling theory of finite-size effects in the critical region which has been developed recently by Fisher (1970; see also Fisher and Barber 1972a). In the present paper we investigate the analogous problem for the ideal Bose gas.† Admittedly the spherical model and ideal Bose gas are essentially equivalent in the critical region (Gunton and Buckingham 1968), but there is sufficient difference, both in mathematical detail and physical application, to make separate discussions illuminating.

To be specific, in this paper we will consider the behaviour of an ideal Bose gas in a \( d \)-dimensional Euclidean domain of infinite extent in \( d' = d-1 \) dimensions \( (d' \geq 2) \) but of finite thickness \( L \) in the \( d \)th dimension. Such a geometry will be referred to as a \( d' \)-dimensional film. As in Part I, interest will centre on the critical (or, for \( d = 3 \) and \( d' = 2 \), quasi-critical) behaviour in the asymptotic regime \( L \to \infty \). For \( d = 3 \) this corresponds to a "thick" film of infinite lateral extent.

Since the early work of Osborne (1949) and Ziman (1953), the behaviour of finite assemblies of non-interacting bosons has received considerable attention (Mills 1964; Goble and Trainor 1966, 1967, 1968; Carmi 1968; Kreuger 1968;...

† Department of Applied Mathematics, Research School of Physical Sciences, Australian National University, Canberra, A.C.T. 2601.
‡ A preliminary account of some of these results was given by Barber and Fisher (1971).

Sonin 1970a, 1970b; Pathria 1971, 1972). The aim of most of this work has not been to analyse the effects of finite size on the critical behaviour per se, but rather to attempt to construct a simple model of liquid helium in a restricted geometry, and in particular as a film. It was realized early (Ziman 1953), however, that an ideal Bose gas did not exhibit a Bose condensation unless infinite in at least three dimensions. On the other hand, in a real helium film superfluidity seems to persist to a few layers, although the specific heat anomaly appears rounded (Brewer 1970). The absence of a true condensation in a finite assembly of bosons has led to various definitions of a "quasi-condensation temperature", such as the "accumulation temperature" of Osborne (1949) and Ziman (1953), at which the chemical potential ceases to rise significantly and there is a rapid accumulation of particles into the ground state. Alternatively, one may consider the maximum of the (rounded) specific heat (Goble and Trainor 1967) or the appearance of some degree of long-range (but not infinite) off-diagonal order (Kreuger 1968). Such definitions have their utility, but their connection to the apparent onset temperature of superfluidity in a real helium film is not clear. More recently, the impossibility of long-range order in a two-dimensional film, even of interacting bosons, has been rigorously established (Hohenberg 1967; Chester et al. 1969; Jasnow and Fisher 1971), and hence the relevance of any calculation on an ideal boson film to real helium is probably limited. Nevertheless, the ideal Bose gas remains one of the few mathematically tractable models of a many-body system which exhibits a phase transition. Analytic calculations are therefore possible of finite-size effects, which allow a detailed test of more general theories, in particular the scaling theory of Fisher (1970). This aspect, rather than the construction of a specific model for any real system, has been a motivating factor in this series of papers.

In Section II of this paper, we formulate the problem of an ideal Bose gas as a film of finite thickness and analyse in Section III the free energy for a thick film \((L \to \infty)\). These basic results are then used to discuss the asymptotic behaviour (characterized by the exponents \(\lambda\) and \(\theta\)) of (i) the relative shift \(\varepsilon(L)\) defined by

\[
\varepsilon(L) = \{T_{c,d} - T_{c,d}(L)\}/T_{c,d} \sim L^{-\lambda}, \quad L \to \infty,
\]

and (ii) the fractional rounding \(\delta(L)\) defined by

\[
\delta(L) = \{T_{d}^{c}(L) - T_{c,d}(L)\}/T_{c,d} \sim L^{-\theta}, \quad L \to \infty.
\]

In these definitions, \(T_{c,d}(L)\) is the critical or quasi-critical temperature of the \(d'\)-dimensional film and \(T_{c,d} = T_{c,d}(\infty)\) is that of the bulk \(d\)-dimensional system while \(T_{d}^{c}(L)\) is a temperature at which the thermodynamic quantities first show a significant deviation from their limiting bulk behaviour. A more detailed discussion of the general aspects of critical phenomena in finite systems is given by Fisher and Ferdinand (1967), Fisher (1970), and Fisher and Barber (1972a). The thermodynamic properties, in particular the specific heat, of an ideal boson film will be considered in more detail in Part III (Barber and Fisher 1973b).

The values of \(\lambda\) and \(\theta\) for different choices of dimensionality and boundary conditions applied across the film are summarized in Table I(a) of Section IV. As
expected, they are of the same functional form as for the spherical model. Most notably, we find that
\[ \theta = v_d^{-1}, \] (3)
for all boundary conditions, where \( v_d \) is the exponent characterizing the divergence of the bulk correlation length (Fisher 1967). This result is in agreement with the scaling hypothesis (Fisher and Ferdinand 1967) that the rounding temperature \( T^*_d(L) \) is determined by the bulk correlation length \( \xi(T) \) matching the thickness of the film. On the other hand, the behaviour of the shift is considerably more complex and, as in the spherical model, reveals new subtleties.

II. FORMULATION

(a) Review of Basic Results

The basic theory of a non-interacting Bose gas is well known and standard (see e.g. London 1954). As an example of a system with a cooperative transition, it has been discussed by Gunton and Buckingham (1968) and Cooper and Green (1968). From these general results the grand potential pressure \( p \) of an ideal Bose gas in a \( d \)-dimensional domain \( \Omega \) of volume \( V_\Omega \) is
\[ p = -\frac{1}{\beta V_\Omega} \sum_k \ln[1 - \exp\{-\beta(e_k - \mu)\}], \] (4)
where \( \beta = 1/k_B T \) is the inverse temperature, \( k_B \) is Boltzmann's constant, and \( e_k = \hbar^2 k^2/2m \) is the energy of the single-particle state \( k \). The chemical potential \( \mu \) is determined as a function of temperature by the density constraint
\[ \langle N \rangle/V_\Omega = \rho = (\partial p/\partial \mu)_T = V_\Omega^{-1} \sum_k [1 - \exp\{-\beta(e_k - \mu)\}]^{-1}. \] (5)
Since \( \mu \) must satisfy \( \varepsilon_0 - \mu \geq 0 \), where \( \varepsilon_0 \) is the single-particle ground state energy, it is useful to introduce the dimensionless "potential"
\[ \phi = -\beta(\mu - \varepsilon_0) \geq 0. \] (6)

It is convenient for our purposes to specifically let \( \Omega \) be a \( d \)-dimensional Euclidean domain, bounded by mutually orthogonal \((d-1)\)-dimensional hyperplanes and of volume
\[ V_\Omega = L_1 \times L_2 \times \ldots \times L_d. \] (7)
In this geometry, the single-particle wavefunctions \( \Psi_k(x) \), with \( x = (x_1, \ldots, x_d) \), factorize as
\[ \Psi_k(x) \rightarrow \Psi_{k_1, \ldots, k_d}(x) = \prod_{i=1}^d \psi_{k_i}(x_i), \] (8)
while the energy
\[ e_k \rightarrow e_{k_1, \ldots, k_d} = \sum_{i=1}^d \hbar^2 k_i^2/2m. \] (9)
Substituting equations (6), (7), and (9) into (4) and expanding the logarithm yields

$$\beta p = \sum_{j=1}^{\infty} j^{-1} \exp(\phi j) \prod_{i=1}^{d} L_{i}^{-1} \sum_{k_{i}} \exp\{-A^2(k_i^2 - k_{i,0}^2)/4\pi\},$$

where \( k_{i,0} \) is the minimum value of \( k_i \) and we have introduced the thermal de Broglie wavelength

$$\Lambda = (2\pi h^2 \beta / m)^{1/4}.$$  \hfill (11)

(b) **Boundary Conditions**

The allowed values of \( k_i \) which appear in the summation in equation (10) are determined by the boundary conditions applied in the \( i \)th dimension. Three types of boundary conditions will be of special interest:

(i) periodic, \( \psi(x_i) = \psi(x_i + L) \);

(ii) antiperiodic, \( \psi(x_i) = -\psi(x_i + L) \);

(iii) hard walls, \( \psi(x_i = 0) = \psi(x_i = L) = 0 \).

The case of hard walls is, of course, the most realistic. Antiperiodic boundary conditions are of interest since in the ordered state the local order parameter suffers a "twist", and this enables one to identify a helicity modulus, which in a Bose system is proportional to the superfluid density \( \rho_s(T) \) (Fisher *et al.* 1973). Such an approach has been utilized by the author to calculate the superfluid density of an ideal Bose gas (unpublished data).

For non-interacting bosons, the problem of determining the allowed values of \( k_i \) now reduces to solving a one-dimensional free-particle Schrödinger equation, subject to the appropriate boundary conditions. Hence we find that

$$k_i = \pi r_i / L_i, \quad r_i \in \mathcal{L}_\tau,$$  \hfill (12)

where \( \tau = 0, \frac{1}{2}, \) and 1 denote the boundary conditions (i), (ii), and (iii) respectively above and the sets of integers \( \mathcal{L}_\tau \) are given explicitly as

$$\mathcal{L}_0 = (0, \pm 2, \pm 4, \ldots, \pm \infty),$$  \hfill (13a)

$$\mathcal{L}_\frac{1}{2} = (\pm 1, \pm 3, \pm 5, \ldots, \pm \infty),$$  \hfill (13b)

$$\mathcal{L}_1 = (1, 2, 3, \ldots, \infty).$$  \hfill (13c)

Note that for antiperiodic boundary conditions (\( \tau = \frac{1}{2} \)) the ground state (\( r_0 = \pm 1 \)) is doubly degenerate.

(c) **Bulk Behaviour**

To obtain the bulk behaviour, we may simply choose periodic boundary conditions in all dimensions and take the limit \( L_i \to \infty \). Hence equation (10) yields on
converting the sums to integrals
\[ \beta \rho = \Lambda^{-d} F_{4d+1}(\phi), \]
where
\[ F_{\sigma}(z) = \sum_{n=1}^{\infty} n^{-\sigma} \exp(-nz), \quad z \geq 0, \]
is the so-called Bose function (Erdelyi 1953; London 1954). For future reference we note that
\[ F_{\sigma}(0) = \zeta(\sigma), \]
with \( \zeta(z) \) the Riemann zeta function, while
\[ F_{\sigma}'(z) \equiv \frac{d}{dz} F_{\sigma}(z) = -F_{\sigma-1}(z). \]
The thermodynamic quantities now follow by the standard relations. In particular, the density constraint (5) becomes
\[ \rho = \Lambda^{-d} F_{4d}(\phi), \]
which determines \( \phi = \phi(T) \).

Following Gunton and Buckingham (1968), we now define a critical temperature \( T_{c,d} \) by
\[ \begin{align*}
\phi(T) &= 0, \quad T \leq T_{c,d}, \\
\phi(T) &> 0, \quad T > T_{c,d}.
\end{align*} \]
Thus from equations (11) and (18) we have
\[ k_B T_{c,d} = (2\pi h^2/m)[\rho/\zeta(\frac{1}{2}d)]^{2/d}, \]
which is nonzero for \( d \geq 3 \).

(d) Basic Results for a Finite Film

To obtain the form of the grand potential pressure for an ideal boson film of finite thickness \( L \), we proceed as in subsection (c) but take the limit \( L_i \to \infty \) only for \( i < d \). In the \( d \)th dimension we put \( L_d = L \) and specify the appropriate boundary conditions (see subsection (b)). If we introduce the dimensionless length parameter
\[ n = L/\sqrt{\pi \Lambda} = L/\pi(2h^2/mk_B T)^{1/2}, \]
the basic result for \( p \equiv p(\phi, \beta) \) in a film may be written as
\[ A^d \beta p(\phi, \beta) = P^f_{d}(\phi, n) \equiv \frac{\pi^{-\frac{1}{4}}}{n} \sum_{r \in \mathcal{L}_r} F_{\frac{1}{4}(d+1)}(\phi + \frac{1}{4}(r^2 - r_{0,r}^2)/n^2), \]
where the summation is over the sets \( \mathcal{L}_r \) defined by equations (13) and \( r_{0,r} = \min(r \in \mathcal{L}_r) \). The result (22) will be the basis of our analysis of the behaviour of an ideal boson film. Our immediate aim in the following section will be to analyse \( P^f_{d}(\phi, n) \) in the limit \( n \to \infty \) (that is, \( L \to \infty \)). The thermodynamic quantities then
follow as usual. In particular, the density constraint (5) may be written as

\[ A^d \rho = (\partial \beta p / \partial \phi)_\beta = P_{d-2}^1(\phi, n). \]  

(23)

III. ASYMPOTIC ANALYSIS

(a) Above the Critical Point

Although our primary interest is in the behaviour of \( P_d^0(\phi, n) \) in the critical region (i.e. for \( \xi(T) \sim L \)), it is useful and illuminating to analyse firstly the expression

\[ P_d^0(\phi, n) = \pi^{-\frac{d}{2}} \sum_{r = -\infty}^{\infty} F_{d+\frac{1}{2}}(\phi + r^2/n^2) \]  

(24)

for \( T \) fixed and greater than \( T_{c,d} \). In this regime, corresponding to \( \xi \ll L \), \( \phi \) is a positive constant. Clearly, we have

\[ \lim_{n \to \infty} P_d^0(\phi, n) = \pi^{-\frac{1}{2}} \int_{-\infty}^{\infty} F_{d+\frac{1}{2}}(\phi + x^2) \, dx = F_{d+1}(\phi). \]  

(25)

To analyse the corrections for large \( n \), we apply Poisson's summation formula (Lighthill 1964) to the sum in equation (24) and obtain

\[ P_d^0(\phi, n) = F_{d+1}(\phi) + 2\pi^{-\frac{1}{2}} \sum_{r = 1}^{\infty} \hat{F}_{d+\frac{1}{2}}(rn), \]  

(26)

where

\[ \hat{F}_d(y) = \int_{-\infty}^{\infty} F_d(\phi + x^2) \exp(-2\pi i xy) \, dx \]  

(27)

is the Fourier transform of \( F_d(\phi + x^2) \).

Now for \( |z| < 2\pi \) and \( |\arg z| < 2\pi \), the Bose functions \( F_\sigma(z) \) possess the convergent expansions (Erdelyi 1953)

\[ F_\sigma(z) = \Gamma(1-\sigma) z^{\sigma-1} + \sum_{n=0}^{\infty} (-z)^n \zeta(\sigma-n)/n!, \]  

(28a)

for non-integral \( \sigma \), and

\[ F_\sigma(z) = (-z)^{-1} \{ \psi(s) - \psi(1) - \ln z \}/(s-1)! + \sum_{n=0}^{\infty} (-z)^n \zeta(s-n)/n!, \]  

(28b)

for \( \sigma \) equal to an integer \( s \), the prime on the summation indicating the omission of the term \( n = s-1 \). In these formulae \( \Gamma(z) \) is the gamma function, \( \zeta(z) \) is the Riemann zeta function, and \( \psi(z) = d[\ln \Gamma(z)]/dz \). These expansions explicitly display the singularity at \( z = 0 \). From the general theory of Fourier transforms (Lighthill 1964) we then find

\[ \hat{F}_{d+\frac{1}{2}}(y) \approx \pi^{d-\frac{3}{2}} \phi^{d-\frac{1}{2}} y^{-\frac{1}{2} - \frac{3}{2} d} \exp(-2\pi \sqrt{\phi}), \quad y \to \infty. \]  

(29)

Substitution in equation (26) finally yields the required result

\[ P_d^0(\phi, n) \approx F_{d+1}(\phi) + 2\pi^{-\frac{1}{2} - d} \phi^{d-\frac{1}{2}} \exp(-2\pi n \sqrt{\phi}/n^{\frac{3}{2} d + \frac{1}{2}}), \quad n \to \infty, \ \phi > 0, \]  

(30)
from which we observe that for constant \( \phi > 0 \), or equivalently for fixed \( T > T_{c,d} \), the expression for \( P^0_d(\phi, n) \) approaches its limit \( F_{3d+1}(\phi) \) exponentially fast in \( n \), while for \( T \) close to \( T_{c,d} \), so that \( \phi \) is small, the exponential decrement will be small and hence the convergence slow. We can then expect to find some \( n \)-dependent scaling of \( \phi \) for which the asymptotic behaviour will in fact be distinct from that at fixed \( \phi > 0 \). Inspection of equation (30) suggests introduction of the variable

\[
x = \phi n^2 = -2\mu L^2 m/h^2.
\]

This \( L \)-scaling of the chemical potential \( \mu \) is completely analogous to the scaling of the spherical field found in Part I and to the scaling of the temperature found by Ferdinand and Fisher (1969) in their analysis of the specific heat anomaly in a finite two-dimensional Ising lattice. In both cases, the approach to the limiting behaviour is exponentially fast in \( n \) for \( T \) outside the scaled critical region.

As in Part I, we may now define the rounding or crossover temperature \( T^* \) (see Section I) more explicitly by

\[
x(T^*) = O(1) \quad \text{as} \quad n \to \infty.
\]

Since for the ideal Bose gas the correlation length is given by

\[
\xi_d(T) = \sqrt{(-\beta\mu)} = \sqrt{\phi},
\]

(Gunton and Buckingham 1968), we see that on combining equations (31) and (32) this definition of \( T^* \) is equivalent to

\[
\xi_d(T^*) = O(n) = O(L) \quad \text{as} \quad L \to \infty,
\]

which suggests that the Fisher and Ferdinand (1967) scaling hypothesis (see Section I) is correct for this model.

For other boundary conditions the leading correction terms are, in general, algebraic in \( n^{-1} \) rather than simply exponential (Barber and Fisher 1973b). However, equation (32) remains a valid definition of the rounding temperature. Thus in the remainder of our analysis we will only consider the behaviour in the scaled critical region, that is, we will analyse \( P^0_d(\phi, n) \) in the limit \( n \to \infty \) with \( x = \phi n^2 \) fixed. For simplicity we will consider the complete analysis (to order \( n^{-d} \)) only for the "realistic" case of \( d = 3 \), the analogous results for other values of \( d \) being merely quoted.

(b) Analysis in the Critical Region for \( d = 3 \)

To analyse \( P_3^0(x/n^2, n) \) for \( n \gg 1 \), it is convenient to write \( F_0(z) \) as an inverse Mellin transform (Titchmarsh 1948), namely

\[
F_0(z) = (2\pi)^{-1} \int_{c-i\infty}^{c+i\infty} z^{-p} \Gamma(p) \zeta(p) \, dp,
\]

where \( c = \text{Re} \, p > \max(0, 1-\sigma) \) and, as before, \( \Gamma(p) \) is the gamma function and \( \zeta(p) \).
the Riemann zeta function. If we now choose the contour such that,

\[ c = \text{Re } p > \frac{1}{2}, \]  

we may substitute equation (35) into (22) with \( d = 3 \). On interchanging the orders of summation and integration, which can be justified, we obtain

\[ P_3'(x/n^2, n) = \frac{\pi^{-\frac{3}{2}}}{2\pi i} \int_{c-i\infty}^{c+i\infty} n^{2p-1} \Gamma(p) \zeta(p+2) \eta'(p; x) \, dp, \]  

with the contour specified by equation (36). The auxiliary function \( \eta'(p; x) \) is defined by

\[ \eta'(p; x) = \sum_{r \in \mathcal{D}} (x + \frac{1}{4}r^2 - \frac{1}{4}r_0^2, r)^{-p}, \]  

where the sum is convergent for \( \text{Re } p > \frac{1}{2} \).

The required asymptotic expansion of \( P_3'(x/n^2, n) \) for large \( n \) may now be obtained from equation (37) by moving the contour to the left (in the complex \( p \) plane) and evaluating the residues at successive poles. To do so, we require an analytic continuation of \( \eta'(p; x) \) for \( \text{Re } p \leq \frac{1}{2} \). Let us first consider the case of periodic boundary conditions \( (\tau = 0) \). Here we have from equation (13a)

\[ \eta^0(p; x) = x^{-p} + 2 \sum_{l=1}^{\infty} (x + l^2)^{-p}, \quad \text{Re } p > \frac{1}{2}, \]  

which defines \( \eta^0(p; x) \) as an analytic function of \( p \) for \( \text{Re } p > \frac{1}{2} \). If we add and subtract \( l^{-2p} \) to the summand in this expression, we obtain

\[ \eta^0(p; x) = x^{-p} + 2\zeta(2p) + 2 \sum_{l=1}^{\infty} l^{-2p}((1+x/l^2)^{-p}-1), \]  

where the sum is now convergent for \( \text{Re } p > -\frac{1}{2} \). Since \( \zeta(2p) \) is analytic everywhere, except for a simple pole at \( p = \frac{1}{2} \), this is a suitable analytic continuation of \( \eta^0(p; x) \) for \( \frac{1}{2} > \text{Re } p > -\frac{1}{2} \). Similarly we obtain

\[ \eta^0(p; x) = x^{-p} + 2\zeta(2p) - 2xp\zeta(2p+2) + 2 \sum_{l=1}^{\infty} l^{-2p}((1+x/l^2)^{-p}-1+px/l^2), \]  

which may be used to define \( \eta^0(p; x) \) for \( -\frac{1}{2} > \text{Re } p > -1\frac{1}{2} \). Since \( \zeta(0) = -\frac{1}{2} \) and \( \zeta(-2) = 0 \) (Whittaker and Watson 1965), we find from equations (40) and (41) that \( \eta^0(p; x) \) vanishes at \( p = 0 \) and \( -1 \), and hence \( \Gamma(p) \eta^0(p; x) \) is analytic at \( p = 0 \) and \( -1 \). Consequently the only poles in the strip \( \frac{1}{2} > \text{Re } p > -1\frac{1}{2} \) of the integrand of equation (37) are at \( p = \pm \frac{1}{2} \) and \( -1 \). All are simple, and their residues can be evaluated by standard methods. We find

\[ P_3^0(x/n^2, n) = \zeta(2\frac{1}{2}) - x \zeta(1\frac{1}{2})/n^2 + H_3^0(x)/n^3 + O(n^{-4}), \]  

where

\[ H_3^0(x) = \frac{\pi^{-\frac{3}{2}}}{2\pi} \lim_{p \to -1} \Gamma(p) \eta^0(p; x) \]  

(43)
and the correction terms (of order $n^{-4}$) arise from the next pole of $\eta^0(p; x)$ at $p = -1\frac{1}{2}$.

To evaluate $H_0^0(x)$ explicitly, we make use of equation (41) together with the results (see Whittaker and Watson 1965)

$$\Gamma(1 + s) = -s^{-1} + O(1), \quad s \to 0,$$

$$\zeta'(0) = -\frac{1}{2} \ln(2\pi), \quad \zeta'(-2) = -\frac{1}{4} \pi^{-2} \zeta(3).$$  \hspace{1cm} (45a, b)

The result (45b) follows from the Riemann relation (Whittaker and Watson)

$$\zeta(1-s) = \pi^{-s} 2^{1-s} \Gamma(s) \zeta(s) \cos(\frac{1}{2} s \pi)$$  \hspace{1cm} (46)

on differentiating with respect to $s$ and then putting $s = 3$. Finally, on introducing the remnant function (Fisher and Barber 1972b)

$$R_{2,0}(x) = \sum_{i=1}^{\infty} I^2 \{(1 + x/|i|) \ln(1 + x/|l|) - x/|l|^2\}$$  \hspace{1cm} (47)

we obtain

$$H_0^0(x) = 2 \pi^{-\frac{1}{2}} R_{2,0}(x) - \pi^{-\frac{1}{2}} x \{1 - \ln(4\pi^2 x)\} + \pi^{-2\frac{1}{2}} \zeta(3).$$  \hspace{1cm} (48)

This completes our analysis of $P_{3}^0(x/n^2, n)$ for periodic boundary conditions ($\tau = 0$). A similar analysis is possible with antiperiodic ($\tau = \frac{1}{2}$) and hard wall ($\tau = 1$) boundary conditions. A more direct approach, however, is to notice that by rearranging their defining sums we may write

$$\eta^k(p; x) = 2^{2p} \eta^0(p; 4x - 1) - \eta^0(p; x - \frac{1}{4})$$  \hspace{1cm} (49)

and

$$\eta^l(p; x) = 2^{2p-1} \eta^0(p; 4x - 1) - \frac{1}{2} (x - \frac{1}{4})^{-p}.  \hspace{1cm} (50)$$

Hence, substitution into equation (37) yields

$$P_{3}^0(x/n^2, n) = 2 P_{3}^0((4x - 1)/(2n^2), 2n) - P_{3}^0((x - \frac{1}{4})/n^2, n)$$  \hspace{1cm} (51)

and

$$P_{3}^0(x/n^2, n) = P_{3}^0((4x - 1)/(2n^2), 2n) - C(n)/2\sqrt{\pi},$$  \hspace{1cm} (52)

with

$$C(n) = (2\pi)^{-1} \int_{c-i\infty}^{c+i\infty} n^{2p-1} (x - \frac{1}{4})^{-p} \Gamma(p) \zeta(p + 2) \, dp$$

$$= \zeta(2)/n + 2(\frac{1}{4} - x) \ln(n)/n^3 + (x - \frac{1}{4}) \ln(x - \frac{1}{4})/n^3 + O(n^{-5}), \quad as \quad n \to \infty.$$  \hspace{1cm} (53)

Thus, on substituting the asymptotic expansion (42) for $P_{0}^0$, we obtain

$$P_{3}^0(x/n^2, n) = \zeta(2\frac{3}{2}) + (\frac{1}{4} - x) \zeta(1\frac{1}{2})/n^2 + H_{3}^1(x)/n^3 + O(n^{-4})$$  \hspace{1cm} (54)

and

$$P_{3}^0(x/n^2, n) = \zeta(2\frac{1}{2}) - \frac{1}{2} \pi^{-\frac{1}{2}} \zeta(2)/n + (\frac{1}{4} - x) \zeta(1\frac{1}{2})/n^2$$

$$+ \pi^{-\frac{1}{2}} (x - \frac{1}{4}) \ln(n)/n^3 + H_{3}^1(x)/n^3 + O(n^{-4}),$$  \hspace{1cm} (55)
where

\[
H_\frac{1}{3}(x) = \frac{1}{3}H_\frac{3}{3}(4x-1) - H_\frac{3}{3}(x-\frac{1}{4})
= \frac{1}{3}\pi^{-\frac{1}{3}} R_{2,0}(4x-1) - 2\pi^{-\frac{1}{3}} R_{2,0}(x-\frac{1}{4}) + 2\pi^{-\frac{1}{3}} (x-\frac{1}{4}) \ln 2 - 3\zeta(3)/4\pi^{2\frac{1}{3}}
\]  

(56)

and

\[
H_\frac{1}{3}(x) = \frac{1}{3}H_\frac{3}{3}(4x-1) - \frac{1}{3}\pi^{-\frac{1}{3}} (\frac{1}{4} - x) \{1 - \ln(x-\frac{1}{4})\}
= \frac{1}{3}\pi^{-\frac{1}{3}} R_{2,0}(4x-1) + \frac{1}{3}\pi^{-\frac{2\frac{1}{3}}{3}} \zeta(3) - \pi^{-\frac{1}{3}} (\frac{1}{4} - x) \ln(4\pi).
\]  

(57)

(c) Extension to Arbitrary \(d\)

Proceeding as above, we introduce the integral representation (35) for \(F_\alpha(x)\) into equation (22), which yields for general \(d\)

\[
P_d^0(x/n^2, n) = \frac{\pi^{-\frac{1}{3}}}{2\pi i} \int_{c-i\infty}^{c+i\infty} n^{2p-1} \Gamma(p) \zeta(p + \frac{1}{4}d + \frac{1}{2}) \eta^\prime(p; x) \, dp,
\]  

(58)

with \(c = \text{Re} \, p > \frac{1}{4}\). If an analytic continuation of \(\eta^\prime(p; x)\) is now constructed for \(\text{Re} \, p \geq \frac{1}{2}(1-d)\) along the lines utilized in subsection (b), \(P_d^0(x/n^2, n)\) may be readily analysed to order \(n^{-d}\) for large \(n\). The details of the analysis are omitted here and the relevant results are merely quoted.

For periodic boundary conditions \((\tau = 0)\), we find

\[
P_d^0(x/n^2, n) = V_{2m+1}(x/n^2) + H_{2m}^0(x)/n^{2m+1} + O(n^{-2-2m}), \quad d = 2m+1; \quad (59a)
= V_{2m}(x/n^2) + 2(-x)^m \ln(n)/m! n^{2m} + H_{2m}^0(x)/n^{2m} + O(n^{-1-2m}), \quad d = 2m; \quad (59b)
\]

where

\[
V_d(z) = \sum_{k=0}^\lceil \frac{1}{2}(d-1) \rceil (-z)^k \zeta(\frac{1}{2}d + 1 - k)/k!
\]  

(60)

is a polynomial of degree \(\frac{1}{2}d-1\) if \(d\) is even and of degree \(\frac{1}{2}(d-1)\) if \(d\) is odd (here \([x]\) denotes, as usual, the integer part of \(x\)). The functions \(H_d^0(x)\) are defined by

\[
H_{2m}^0(x) = (-)^{1+m} R_{m+\frac{1}{2}, m}(x) + \pi^{-\frac{1}{3}} \Gamma(\frac{1}{2} - m) x^{m-\frac{1}{3}}
+ 2(-x)^m (C_E - \ln 2)/m! + 2h_{2m}^0(x),
\]  

(61a)

for \(d = 2m\), and

\[
H_{2m+1}^0(x) = 2(-)^{1+m} \pi^{-\frac{1}{3}} R_{m+1, m}(x)
+ \pi^{-\frac{1}{3}} (-x)^m \{\psi(m+1) + C_E - \ln(4\pi^2 x)\} + 2h_{2m+1}^0(x),
\]  

(61b)

for \(d = 2m+1\), where \(C_E\) is Euler's constant and

\[
h_d^0(x) = \pi^{-d} \sum_{k=0}^\lceil \frac{1}{2}(d-1) \rceil (-\pi^2 x)^k \Gamma(\frac{1}{2}d - k) \zeta(d-2k)/k!,
\]  

(62)
while the remnant functions $R_{\sigma,0}(x)$ are defined in general by (Fisher and Barber 1972b)

$$R_{\sigma,0}(x) = \{\Gamma(\sigma - |\sigma|)/\Gamma(\sigma)\} \sum_{i=1}^{\infty} l^{2\sigma-2} \{[1+x/l^2]^{\sigma-1}\} \mp_{\sigma+\frac{1}{2}}$$

(63a)

for $\sigma$ not a positive integer, and by

$$R_{s,0}(x) = \{(s-1)!\}^{-1} \sum_{r=1}^{\infty} r^{2s-1} \{[1+x/r^2]^{s-1}\} \ln(1+x/r^2)$$

(63b)

for integral $\sigma (= s)$. In these formulae, we have used the notation

$$[f(x)]_k = f(x) - \sum_{r=0}^{r<s-1} x^r f^{(r)}(0)/r!$$

(64)

with

$$f^{(r)}(0) = \left. d^r f(x)/dx^r \right|_{x=0}.$$  

(65)

The analogous expressions for antiperiodic ($\tau = \frac{1}{2}$) and hard wall ($\tau = 1$) boundary conditions may now be written:

$$P_d^\pm(x/n^2, n) = V_{2m+1}\{(x-\frac{1}{2})/n^2\} + H_{2m+1}^\pm(x)/n^{2m+1} + O(n^{-2-2m}),$$

$$d = 2m+1; \quad (66a)$$

$$= V_{2m}\{(x-\frac{1}{2})/n^2\} + 2(\frac{1}{4} - x)^m \ln(4n)/m! n^{2m+1} + H_{2m}^\pm(x)/n^{2m} + O(n^{-1-2m}),$$

$$d = 2m; \quad (66b)$$

and

$$P_d^\pm(x/n^2, n) = V_{2m}\{(x-\frac{1}{2})/n^2\} - V_{2m-1}\{(x-\frac{1}{2})/n^2\}/2n\sqrt{\pi}$$

$$+ 2(\frac{1}{4} - x)^m \ln(2n)/m! n^{2m} + H_{2m}^\pm(x)/n^{2m} + O(n^{-1-2m}),$$

$$d = 2m; \quad (67a)$$

$$= V_{2m+1}\{(x-\frac{1}{2})/n^2\} - \pi^{-\frac{1}{2}} V_{2m}\{(x-\frac{1}{2})/n^2\}/2n\sqrt{\pi}$$

$$- \pi^{-\frac{1}{2}} (\frac{1}{4} - x)^m \ln(n)/m! n^{2m+1} + H_{2m+1}^\pm(x)/n^{2m+1} + O(n^{-2-2m}),$$

$$d = 2m+1; \quad (67b)$$

with

$$H_{\frac{3}{2}}^\pm(x) = 2^{-d} H_{\frac{3}{2}}^0(4x-1) - H_{\frac{3}{2}}^0(x-\frac{1}{4})$$

(68)

and

$$H_{\frac{1}{2}}^\pm(x) = 2^{-d} H_{\frac{1}{2}}^0(4x-1) + h_{\frac{1}{2}}^\pm(x),$$

(69)

where

$$h_{\frac{1}{2}}^\pm(x) = -\frac{1}{2} \pi^{-\frac{3}{2}} \Gamma(\frac{1}{2} - m)(x-\frac{1}{4})^{m-\frac{1}{2}}, \quad d = 2m; \quad (70a)$$

$$= -\frac{1}{2} \pi^{-\frac{3}{2}} (\frac{1}{4} - x)^m \{C_k + \psi(m+1) - \ln(x-\frac{1}{4})\}/m!, \quad d = 2m+1. \quad (70b)$$
This completes our formal analysis of $P_d(x/n^2, n)$. In the next section we will use these results to analyse the asymptotic behaviour of the shift and rounding of the critical point. Before this, however, we now digress to establish in more detail the relation, for periodic boundary conditions, between the results of this subsection and those of subsection (a) above. In (a) we recall that $P_d^0(\phi, n)$ was analysed for $n \gg 1$, but with $\phi$ a positive constant. To relate the two sets of results, we consider the expression

$$
\Delta P_d^0(\phi) = P_d^0(\phi, n) - F_{d+1}(\phi).
$$

From equation (30) we have

$$
\Delta P_d^0(\phi) \approx 2\pi^{d-1/2} \phi^d \exp(-2\pi n \sqrt{\phi})/n^{d+1/2},
$$

for $n \gg 1$ and $\phi$ fixed.

In the other limit of interest we have

$$
\Delta P_d^0(x/n^2) = P_d^0(x/n^2, n) - F_{d+1}(x/n^2).
$$

The second term of this expression is easily expanded using equations (28), and hence, on substituting equations (59), we obtain

$$
\Delta P_d^0(x/n^2, n) = [H_{2m}^0(x) + (-x)^m \left\{ \ln x - \psi(m + 1) \right\}/m!] n^{-2m} + O(n^{-1-2m}),
$$

$$
n = 2m; \quad (74a)
$$

$$
= [H_{2m+1}^0(x) - x^{m+\frac{1}{2}} \Gamma(-\frac{1}{2} - m)] n^{-1-2m} + O(n^{-2-2m}),
$$

$$
n = 2m + 1; \quad (74b)
$$

as $n \to \infty$ with $x = \phi n^2$ fixed. It will now be shown that equation (72) is recovered by considering the limit $x \to \infty$ in the expressions (74). The functions $H_d^0(x)$ are defined by equations (61) in terms of the remnant functions $R_{\sigma, d}(x)$, whose analytic properties have been discussed in detail by Fisher and Barber (1972b). For convenience, their asymptotic expansions for large $x$, which are required in the present analysis, are summarized in the Appendix. Hence, we find

$$
\Delta P_d^0(x/n^2) \approx 2\pi^{d-1/2} x^{d-1/2} \exp(-2\pi \sqrt{x})/n^d, \quad x \to \infty,
$$

(75)

which is precisely equation (72) with $\phi = x/n^2$. It is interesting to note that for the ideal Bose gas the limit $x \to \infty$ recovers the correct asymptotic behaviour for all values of $\phi$, in contrast to the spherical model (Part I) where the same procedure was only valid for small $\phi$. This is a reflection of the present relatively simple form of $P_d^0(x/n^2, n)$ compared with the analogous function for the spherical model.

IV. SHIFTS AND ROUNDING IN $d$-DIMENSIONS

Although the quantity

$$
n = L/\sqrt{\pi A},
$$

(76)

where $A$ is the thermal de Broglie wavelength, has been a convenient expansion
parameter and is, in some ways, the direct analogue of the number of layers in a lattice model (see Part I), it is a rather unphysical length parameter. A more natural and conventional choice is

\[ l = L \rho^{1/d} = n \sqrt{\pi \left\{ \xi \left( \frac{1}{2}d \right) \right\}^{1/d} \left( T/T_{c,d} \right)^{-1/4}}, \]

(77)

and this quantity will be used in our remaining discussion.

### Table 1

**Asymptotic Behaviour of Shift and Rounding of Critical Point for Ideal Boson Films**

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Shift ( \varepsilon_\delta(l) )</th>
<th>Rounding ( \delta_\delta(l) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d )</td>
<td>( \tau = 0 )</td>
<td>( \tau = \frac{1}{2} )</td>
</tr>
<tr>
<td>3</td>
<td>( a_d^0/l )</td>
<td>( a_d^1/l )</td>
</tr>
<tr>
<td>4</td>
<td>( a_d^0/l^2 )</td>
<td>( a_d^1 \ln(l)/l^2 )</td>
</tr>
<tr>
<td>( \geq 5 )</td>
<td>( a_d^0/l^{d-2} )</td>
<td>( a_d^1/l^{d-2} )</td>
</tr>
</tbody>
</table>

### (b) Amplitude of Shift

<table>
<thead>
<tr>
<th>Dimension</th>
<th>( \tau = 0 )</th>
<th>Amplitude ( a_d^\ast )</th>
<th>( \tau = \frac{1}{2} )</th>
<th>( \tau = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Arbitrary</td>
<td>( \sim -\frac{3}{4} { \zeta(1) }^{-2/3} \approx -0.3515 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>( 1/\sqrt{6} \approx 0.4082 )</td>
<td>( \frac{1}{4} \pi \zeta(3d-1)/(3d-2) )</td>
<td>( -\frac{3}{4} { \zeta(1) }^{-2/3} \approx -0.3515 )</td>
<td></td>
</tr>
<tr>
<td>( \geq 5 )</td>
<td>( \frac{4\pi^{1-4d} T(1/2d-1)(d-2)}{d(\zeta(1/2d))^{2/3d}} )</td>
<td>( \frac{1}{4} \pi \zeta(3d-1) )</td>
<td>( \sim \frac{1}{4} { \zeta(1) }^{-2/3} \approx -0.3515 )</td>
<td></td>
</tr>
</tbody>
</table>

### (a) Density Constraint and Critical Temperature

From Section II, the scaled field \( x \) is determined in the critical region by the density constraint (23), which may be written as

\[ A^d \rho = \zeta \left( \frac{1}{2}d \right) \left( T/T_{c,d} \right)^{-1/4} = P_{d-2}^\ast \left( x/n^2, n \right). \]

(78)

Now for \( d > 4 \) the finite film exhibits a true Bose condensation at a nonzero temperature \( T_{c,d}(l) \) which is determined by \( x = 0 \) or, explicitly from equations (77) and (78), by

\[ T_{c,d}(l)/T_{c,d} = \{ P_{d-2}^\ast (0, n_c)/\zeta (1/2d) \}^{-2/4}, \quad d \geq 4, \]

(79)

with

\[ n_c = \ln \{ \zeta (1/2d) \}^{-1/4} \{ T_{c,d}(l)/T_{c,d} \}^{1/4}. \]

(80)

### (b) Shift and Rounding of Critical Point

The shift \( \varepsilon_\delta(l) \) in the critical temperature defined by equation (1) now follows for \( d \geq 4 \) and \( n \gg 1 \) from the basic formulae (59), (66), and (67) of Section III on putting \( \phi = x = 0 \). In terms of \( l \), the asymptotic behaviour which determines the exponent \( \lambda \) is summarized in Table 1(a), the corresponding amplitudes \( a_d^\ast \) being given.
in Table 1(b). In three dimensions, a film of finite thickness has no sharp condensation (see Section I), but we will see below that an effective shift can be defined in a natural way.

To study the rounding \( \delta_\lambda^2(l) \), we rewrite the density constraint (78) using equations (59), (66), and (67) to leading order in the forms

\[
\zeta(1^{\frac{1}{2}}) n l = -\frac{3}{2} H_{\tau}^1(x) + O(n^{-1}), \quad d = 3; \quad (81)
\]

\[
\zeta(2) n^2 l = 2x \ln(n) + H_{\tau}^2(x) - H_{\tau}^2(0) + O(n^{-1}), \quad d = 4; \quad (82)
\]

where the functions \( H_{d-2}^1(x) \) are defined by equations (61) for \( \tau = 0 \), by (68) for \( \tau = \frac{1}{2} \), and by (69) for \( \tau = 1 \). Finally, for \( d \geq 5 \) we have

\[
\zeta(\frac{1}{2}d) n^2 l = 2d^{-1} x \zeta(\frac{1}{2}d-1) + O(n^{-1}). \quad (83)
\]

In these formulae, the shifted temperature deviations are defined generally for all \( d \geq 4 \) by

\[
i = \{T - T_{c,d}^\tau(l)\}/T_{c,d}, \quad (84)
\]

but in three dimensions \( (d = 3) \) by

\[
i = (T - T_{c,3})/T_{c,3}, \quad \tau = 0, \frac{1}{2}; \quad (85)
\]

\[
i = (T - T_{c,3})/T_{c,3} - \frac{3}{2} \pi^{-\frac{1}{2}} \ln(n)/n \zeta(1^{\frac{1}{2}}), \quad \tau = 1. \quad (86)
\]

The rounding interval \( \Delta T^*(l) \) now follows from the definition (32), which leads immediately to the asymptotic forms of \( \delta_\lambda^2(l) \) displayed in Table 1(a). For \( d \geq 4 \) we observe that the rounding is defined with respect to the shifted critical temperature. For \( d = 3 \), we may define an effective shift from the form of \( l \) which appears in the density constraint (81). Thus for hard wall boundary conditions \( (\tau = 1) \) equation (86) leads unambiguously to the form

\[
e_{\lambda,\delta}^1(l) \approx a_{\delta,\lambda}^1 \ln(l)/l, \quad l \to \infty, \quad (87)
\]

as quoted in Table 1(a) (the value of \( a_{\delta,\lambda}^1 \) being given in Table 1(b)). In the case of periodic \( (\tau = 0) \) or antiperiodic \( (\tau = \frac{1}{2}) \) boundary conditions, the situation is less definite. However, we may introduce into equation (85) an effective shift

\[
e_{\lambda,\delta}^2(l) \sim l^{-\frac{1}{2}}, \quad \tau = 0, \frac{1}{2}, \quad (88)
\]

with an arbitrary amplitude \( a_{\delta,\lambda}^2 \), by merely adding an appropriate constant to \( H_{\tau}^1(x) \) in equation (81). It is shown in Part III that this definition is consistent, at least in the asymptotic regime, with an effective shift defined in terms of the temperature at which the specific heat is a maximum. The only effect of making a specific physical definition of the quasi-critical temperature is to specify the amplitude \( a_{\delta,\lambda}^2 \).

The above results for \( \varepsilon \) and \( \delta \) are, as expected, formally identical with those found for the spherical model in Part I, although the amplitudes \( a_{\delta,\lambda}^\varepsilon \) of the shift are different. The asymptotic behaviour of \( e_{\delta}^\varepsilon(l) \) has also been investigated recently by
Pathria (1971) from a consideration of the density of states in a finite system (Pathria 1966). This approach, however, failed to give the amplitude $a_d^2$ for $d = 3$, $\tau = 1$ and $d = 4$, $\tau = \frac{1}{2}$ (see Table 1(b)), although the correct order of the shift was obtained. Pathria (1971) also considered the case of Neumann boundary conditions ($\nabla \psi = 0$ on the free surfaces).

Since, for the ideal Bose gas, the correlation length exponent $v$ has the values (Gunton and Buckingham 1968)

$$v(3) = 1; \quad v(4) = \frac{1}{2} (\times \log); \quad v(d) = \frac{1}{2}, \quad d \geq 5;$$

we obtain the relation (3) by inspection, in agreement with the scaling hypothesis. The behaviour of the shift is considerably more complex, however, with the values

$$\lambda = (d-2), \quad \tau = 0, \quad \text{all } d;$$

$$= \frac{1}{v}, \quad \tau = \frac{1}{2}, \quad \text{all } d; \tag{90a}$$

$$= 1(\times \log), \quad \tau = 1, \quad d = 3; \tag{90b}$$

$$= 1, \quad \tau = 1, \quad d \geq 4. \tag{90c}$$

The result (90b) for antiperiodic conditions is consistent with the assumption that the scaling hypothesis is the only criterion determining finite size effects in the critical region (Fisher 1970). On the other hand, the result (90d) for hard wall boundary conditions appears to agree with the simple mean field argument (Fisher and Ferdinand 1967; Fisher 1970). However, the amplitudes $a_d^2$ are negative, indicating that the critical temperature of a sufficiently thick film actually exceeds the bulk value $T_{c,d}$.

The above anomalous behaviour is, of course, similar to that found for the spherical model, although in that case the enhancement appeared to be weaker; for instance (see Part I), the critical temperature of a three-dimensional layer spherical model was found to lie above $T_{c,4}$ only for 24 or more layers. In the analogous Bose problem one may estimate from the asymptotic formulae that the critical temperature of the three-dimensional film exceeds $T_{c,4}$ for $L/l \gtrsim 3$. In view of the similarity of the two models, it is likely that the physical origin of this anomalous behaviour is analogous in both cases. In Part I, we discussed one possible mechanism in some detail. For completeness, we will briefly outline it again but in a language appropriate to the ideal Bose gas.

The basic point is that the chemical potential $\mu$ is determined so as to maintain the density constraint (5), and hence $\mu$ is necessarily a function of $T$, while also, since $\rho$ is assumed independent of the thickness $L$ in a film, $\mu$ must depend on $L$. Now, for an ideal Bose film with hard wall boundary conditions, the local particle density vanishes at the surfaces and, by continuity, the local density must therefore be depleted near the surfaces. Consequently, these regions, presumably of volume $L^{-1}$ relative to the bulk, must contribute less to the density constraint. To maintain the constraint, it is thus necessary to increase the chemical potential in the bulk by an increment of order $L^{-1}$. This encourages the onset of condensation, and hence the critical temperature is enhanced by an amount of order $L^{-1}$. 

This completes our discussion of the effects of finite size on the critical point
of an ideal boson film. Granted the explanation advanced above for the effects of
hard walls, we have seen that the exact results for the shifts and rounding are con­
sistent with the general scaling theory of finite-size effects (Fisher 1970; Fisher and
Barber 1972a). As for the spherical model, the exception is the $1/l^{d-2}$ shifts which
occur with periodic boundary conditions. However, as discussed in Part I, these are
certainly of higher order and correspond to $\epsilon_d^0(l) = 0$ in the scaling formulation.

In subsequent papers, we will make use of the basic asymptotic results developed
in Section III to discuss thermodynamic behaviour of a film in more detail (Part III,
Barber and Fisher 1973b) and to compute the helicity modulus of an ideal Bose fluid.

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APPENDIX

Asymptotic Expansions of Remnant Functions

The asymptotic expansions, for large z, of the remnant functions $R_{\sigma,\tau}(z)$ with $\tau = 0$ and $\sigma = \frac{k}{2}$ ($k = 1, 2, ...$) are included here for reference. These functions have been discussed in detail, for arbitrary real $\sigma$ and $\tau$, by Fisher and Barber (1972b). For $\tau = 0$, $R_{\sigma,0}(z)$ is defined by equations (63a) and (63b) for non-integral and integral values of $\sigma$ respectively.

For $z \neq 0$ and $|\arg z| < \pi$, we can write (Fisher and Barber 1972b)

$$R_{\sigma,0}(z) = P_{\sigma,0}(z) + Q_{\sigma,0}(z). \quad (A1)$$

The principal asymptotic part of equation (A1) is, with $s = 1, 2, ...$,

$$P_{\sigma,0}(z) = \frac{i}{2} \Gamma(s+\frac{1}{2}) - \frac{1}{2} \ln(z)/(s-1)!$$

$$- \frac{1}{4} (2\ln(2\pi) - C_E - \psi(s)) z^{s-1}/(s-1)!$$

$$+ \sum_{n=1}^{s-1} \frac{1}{n} \zeta(2l+1)(-\pi^2 z)^{-l}/(s-1-l)!,$$  \quad (A2)

$$P_{\sigma+\frac{1}{2},0}(z) = z^s \ln(z)/s! - (2\ln 2 - C_E + \psi(s+1)) z^s/s!$$

$$+ \pi^s z^{s-1}/\Gamma(s+\frac{1}{2}) + 2z^s \sum_{l=1}^{s} (l-1)! \zeta(2l)(-\pi^2 z)^{-l}/(s-l)!,$$  \quad (A3)

where $C_E$ is Euler's constant, $\zeta(s)$ is the Riemann zeta function, and $\psi(z)$ is the logarithmic derivative of the gamma function. The secondary part of equation (A1) is

$$Q_{\sigma,0}(z) = 2(-)^\sigma \pi^s (4/\pi)^{s-\sigma} [\sigma]_2^4(\sigma-\frac{1}{4}) \sum_{n=1}^{\infty} n^{\sigma-s} K_{\sigma-\frac{1}{4}}(2\pi n z^s),$"
where $K_s(x)$ is the modified Bessel function of the third kind and $[x]$ is the integer part of $x$. Since we have

$$K(z) \approx K_{\frac{3}{2}}(z) = (\pi/2z)^{\frac{3}{4}} \exp(-z), \quad z \to +\infty,$$

we find

$$Q_{\sigma,0}(z) \approx (-1)^{[\sigma+\frac{1}{2}]\pi^1-\sigma(4/\pi)^\sigma-[\sigma]z^{3(\sigma-1)}\exp(-2\pi\sqrt{z}),$$

as $z \to +\infty$. For $s = 1$, equations (A2) and (A3) reduce respectively to

$$P_{1,0}(z) = \pi \sqrt{z} - \ln(2\pi \sqrt{z}),$$

$$P_{1\frac{1}{2},0}(z) = z \ln z + (2C_E - \ln 4 - 1) + 2\sqrt{z} - \frac{1}{3}.$$