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Helicity modulus for an ideal Bose fluid

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Abstract. The concept of the helicity modulus, $Y_d(T)$, introduced by Fisher, Barber and Jasnow, is applied to the ideal Bose gas in d dimensions. Above the critical temperature $T_{c,d}$, Y is found to vanish identically, while for $T < T_{c,d}$,

$$Y_d(T) = (\hbar^2 \rho / m) [1 - (T/T_{c,d})^{1/d}],$$

where ρ is the total density. The relevance of these results to more general theories of superfluidity is discussed.

1. Introduction

The concept of the helicity modulus was introduced by Fisher, Barber and Jasnow (1973, to be referred to as FBJ), who discussed its role in the critical behaviour of isotropic systems with n -component order parameters ($n \geq 2$). Fundamentally, the helicity modulus $Y(T)$ is a measure of the response of the system to a helical or 'phase-twisting' field. In this context, Y can be used to define a phase-coherence length $\Lambda^{(Y)}(T)$, which has similar properties to a correlation length. In particular, $\Lambda^{(Y)}(T)$ diverges at the critical point. Since conventional definitions of a correlation length fail in the ordered phase of an isotropic system, this concept appears to have some utility (see FBJ §§ 3–5).

Alternatively, one can consider the helicity modulus to be the analogy, for an isotropic system, of the surface tension or interfacial free energy between two phases in a system with a scalar ($n = 1$) order parameter, e.g. an Ising model. This viewpoint yields the explicit definition (FBJ § 2)

$$Y(T) = \lim_{A(\Omega), L(\Omega) \rightarrow \infty} \{ [2L(\Omega) / \pi^2 A(\Omega)] [\mathcal{F}^{(1/2)}(T; \Omega) - \mathcal{F}^{(0)}(T; \Omega)] \}, \quad (1.1)$$

where $\mathcal{F}^{(\tau)}(T; \Omega)$ is the *total* free energy of the system in a domain Ω of cross-sectional area $A(\Omega)$ and length $L(\Omega)$, with respectively periodic ($\tau = 0$) and anti-periodic ($\tau = \frac{1}{2}$) boundary conditions applied across the length $L(\Omega)$. This definition was used by Barber and Fisher (1973a) to calculate $Y(T)$ for the spherical model (Berlin and Kac 1952) on a hypercubic lattice. As was first argued by Stanley (1968), this model corresponds to an n -component spin system in the limit $n \rightarrow \infty$.

The helicity modulus may also be defined for a continuum system. In particular, for a Bose fluid $Y(T)$ is simply related to the superfluid density $\rho_s(T)$ through (FBJ equation (2.10)):

$$\rho_s(T) = (m/\hbar^2)Y(T), \quad (1.2)$$

where m is the mass of a single particle and \hbar is Planck's constant divided by 2π . Thus the helicity modulus affords an *equilibrium* definition of $\rho_s(T)$.

In this paper, we apply the definition (1.1) to calculate Y and hence ρ_s for an *ideal* d -dimensional Bose fluid ($d \geq 3$). This calculation is most easily carried out for a d -dimensional Euclidean domain which is of infinite extent in $d' (= d - 1)$ dimensions ($d' \geq 2$) but of a finite thickness L in the d th dimension. We shall refer to this geometry as a 'film'. In terms of $f_d^a(T, \rho; L)$, the free energy per unit volume, where as before τ denotes the boundary conditions applied across the length L , (1.1) reduces to

$$Y_d(T) = \lim_{L \rightarrow \infty} \{ (2L^2/\pi^2) [f_d^{1/2}(T, \rho; L) - f_d^0(T, \rho; L)] \}. \tag{1.3}$$

Note that we explicitly indicate that the free energy densities are functions of the particle density $\rho = N/V(\Omega)$, and *both* free energies are to be computed at the *same* density. This point is important, since the ideal Bose gas is usually and most easily discussed in the grand canonical ensemble (see e.g. London 1954) with ρ replaced by its conjugate variable, the chemical potential μ .

Equation (1.3) forms the basis of our calculation, which is arranged as follows. In § 2, we summarise the relevant results of an earlier analysis (Barber 1973) of the free energies of ideal Bose fluids in partially finite geometries. The helicity modulus is extracted from these results in § 3 and a concluding discussion given in § 4. The final expressions for $Y_d(T)$ have been reported elsewhere (FBJ § 2) but the details of the analysis have not been presented before.

2. Free energies of ideal Bose gases in partially finite geometries

The thermodynamic properties of an ideal Bose fluid in a domain Ω of volume V_Ω are most easily derived from the grand potential (London 1954, Gunton and Buckingham 1968)

$$\beta p(\mu, T) = -V_\Omega^{-1} \sum_{\mathbf{k}} \ln\{1 - \exp[-\beta(\epsilon_{\mathbf{k}} - \mu)]\}, \tag{2.1}$$

where $\beta = (k_B T)^{-1}$, and $\epsilon_{\mathbf{k}}$ is the energy of the single-particle state \mathbf{k} . The chemical potential μ is determined as a function of temperature and density ρ by the *density constraint*

$$\rho = (\partial p / \partial \mu)_T. \tag{2.2}$$

Equation (2.1) has been specialised to the film geometry of interest here by Barber (1973). To summarise these results it is convenient to define a dimensionless length

$$l = L/\Lambda\sqrt{\pi} \tag{2.3}$$

and reduced chemical potential

$$\begin{aligned} \phi &= -\beta(\mu - \epsilon_0^>) > 0 & T > T_c \\ \phi &= -\beta(\mu - \epsilon_0^<)= 0 & T \leq T_c, \end{aligned} \tag{2.4}$$

where the thermal de Broglie wavelength is

$$\Lambda = (2\pi\hbar^2/mk_B T)^{1/2}. \tag{2.5}$$

The basic expression for $p(\mu, T)$ for a d' -dimensional film of thickness L and infinite lateral extent can then be written (Barber 1973)

$$\Lambda^d \beta p = P_d^\tau(\phi, l) = (\pi^{-1/2}/l) \sum_{r \in \mathcal{L}_\tau} F_{\frac{1}{2}(d+1)}[\phi + \frac{1}{4}(r^2 - r_{0,\tau}^2)/l^2] \quad (2.6)$$

where the so called Bose functions (Erdélyi 1953, London 1954) are defined by

$$F_\sigma(z) = \sum_{m=1}^{\infty} m^{-\sigma} \exp(-mz). \quad (2.7)$$

The sum in (2.6) is over the subsets of integers:

$$\begin{aligned} \mathcal{L}_0 &= (0, \pm 2, \pm 4, \dots, \pm \infty) & (\tau = 0) \\ \mathcal{L}_{1/2} &= (\pm 1, \pm 3, \pm 5, \dots, \pm \infty) & (\tau = \frac{1}{2}) \end{aligned} \quad (2.8)$$

with $r_{0,\tau} = \min\{|r|, r \in \mathcal{L}_\tau\}$.

The density constraint (2.2) follows by differentiation and can be written as

$$\Lambda^d \rho = P_{d-2}^\tau(\phi, l), \quad (2.9)$$

where we have used the result that

$$F'_\sigma(z) = dF_\sigma(z)/dz = -F_{\sigma-1}(z). \quad (2.10)$$

The condition (2.4) then determines (Barber 1973) a non-zero critical temperature $T_{c,d}^\tau(l)$ for all l and both τ if d exceeds three. However, if $d = 3$ and l is finite ϕ vanishes only at $T = 0$.

The free energy f_d which appears in (1.3) is related to $p(\mu, T)$ by a Legendre transformation. Explicitly we have

$$\beta f_d^\tau(T, \rho) = -\beta p(\mu, T) + \beta \rho \mu = -\beta p - \rho \phi + \rho \beta \epsilon_0^\tau \quad (2.11)$$

where $\beta \epsilon_0^\tau = \frac{1}{4} r_{0,\tau}^2 / 4l^2$. Thus (1.3) becomes, on using (2.4),

$$Y_d(T) = (k_B T \Lambda^2 / 2\pi) \{ \rho + 4\Lambda^{-d} \lim_{l \rightarrow \infty} [l^2 (Q_d^{1/2}(\phi_{1/2}, l) - Q_d^0(\phi_0, l))] \} \quad (2.12)$$

where

$$Q_d^\tau(\phi, l) = -P_d^\tau(\phi, l) - \Lambda^d \rho \phi \quad (2.13)$$

and we explicitly indicate that ϕ depends on the boundary conditions. Hence to evaluate Y_d , we require an expansion of $P_d^\tau(\phi, l)$ to order l^{-2} . For the most part, this analysis has been given elsewhere (Barber 1973). We shall refer to these results as required.

3. Derivation of the helicity modulus

We consider in turn the two temperature regimes: T above $T_{c,d}$ and T below $T_{c,d}$, where $T_{c,d}$ is the critical temperature of the bulk d -dimensional ideal gas given by (Gunton and Buckingham 1968)

$$\Lambda_c^d \rho = F_{\frac{1}{2}d}(0) = \zeta(\frac{1}{2}d) \quad (3.1)$$

with $\zeta(z)$ denoting the Riemann zeta function. Substituting (2.5) yields

$$k_B T_{c,d} = (2\pi\hbar^2/m)[\rho/\zeta(\frac{1}{2}d)]^{2/d}. \tag{3.2}$$

The identification (1.2) of $Y_d(T)$ with the superfluid density leads one to expect that the helicity modulus should vanish for $T \geq T_{c,d}$.

3.1. Helicity modulus above $T_{c,d}$

If T is above $T_{c,d}$, ϕ is positive for all l . From equation (30) of Barber (1973) we have

$$P_d^0(\phi, l) \approx F_{\frac{1}{2}d+1}(\phi) + 2\pi^{1-\frac{1}{2}d} \phi^{\frac{1}{2}d-1} \exp(-2\pi l\sqrt{\phi})/l^{\frac{1}{2}d+1} \quad l \rightarrow \infty, \phi > 0. \tag{3.3}$$

Hence

$$\phi_0 = \phi_\infty + O(\exp(-2\pi l\sqrt{\phi_\infty})), \tag{3.4}$$

where ϕ_∞ is the solution of the bulk constraint

$$\Lambda^d \rho = F_{\frac{1}{2}d}(\phi_\infty). \tag{3.5}$$

Combining (3.3) and (3.4) yields

$$Q_d^{(0)}(\phi, l) \approx -F_{\frac{1}{2}d+1}(\phi_\infty) - \Lambda^d \rho \phi_\infty + O(\exp(-2\pi l\sqrt{\phi_\infty})) \quad l \rightarrow \infty, \phi_\infty > 0. \tag{3.6}$$

In the case of anti-periodic boundary conditions, we may expand the summand in (2.6) as

$$F_{\frac{1}{2}(d+1)}(\phi + \frac{1}{4}r^2/l^2) + \frac{1}{4}l^{-2}F_{\frac{1}{2}(d-1)}(\phi + \frac{1}{4}r^2/l^2) + O(l^{-4}), \tag{3.7}$$

where we have used (2.10). Since, for positive ϕ , $F_\sigma(\phi + z)$ is analytic in z , the sums over $\mathcal{L}_{1/2}$ can be converted to integrals with exponentially small error to yield

$$P_d^{1/2}(\phi, l) = F_{\frac{1}{2}d+1}(\phi) + \frac{1}{4}l^{-2}F_{\frac{1}{2}d}(\phi) + O(l^{-4}) \quad l \rightarrow \infty, \phi > 0. \tag{3.8}$$

The density constraint (2.9) now implies that

$$\phi_{1/2} = \phi_\infty + \frac{1}{4}l^{-2} + O(l^{-4}), \tag{3.9}$$

where ϕ_∞ is again given by (3.5). Hence

$$Q_d^{1/2}(\phi_{1/2}, l) \approx -F_{\frac{1}{2}d+1}(\phi_\infty) - \Lambda^d \rho \phi_\infty - \frac{1}{4}\Lambda^d \rho l^{-2} + O(l^{-4}), \quad l \rightarrow \infty, \phi_\infty > 0. \tag{3.10}$$

Substituting this result and (3.6) in (2.12) yields the expected result that

$$Y_d(T) = 0 \quad T > T_{c,d}. \tag{3.11}$$

3.2. Helicity modulus beneath the critical temperature

In the regime T less than $T_{c,d}$ it is necessary to consider separately the cases $d > 3$ and $d = 3$. In the first, we make use of the result (Barber 1973) that $T_{c,d}^\tau(l)$ for both $\tau = 0$ and $\tau = \frac{1}{2}$ is a monotonic increasing function of l . Thus given any $T < T_{c,d} = \lim_{l \rightarrow \infty} T_{c,d}^\tau(l)$ we can find a value of l , say \hat{l} , for which

$$T < \min(T_{c,d}^0(l), T_{c,d}^{1/2}(l)), \quad l > \hat{l}. \tag{3.12}$$

Hence for $l > \hat{l}$, we can put $\phi_0 = \phi_{1/2} = 0$ in (2.6) and (2.13). Thus (2.12) becomes

$$Y_d(T) = (k_B T \Lambda^2 / 2\pi) \left(\rho + 4\Lambda^{-d} \lim_{l \rightarrow \infty} (l^2 \Delta Q(l)) \right), \tag{3.13}$$

with

$$\Delta Q(l) = (\pi^{-1/2}/l) \sum_{s=-\infty}^{\infty} \{F_{\frac{1}{2}(d+1)}(s^2/l^2) - F_{\frac{1}{2}(d+1)}[s(s+1)/l^2]\}. \tag{3.14}$$

The analysis of $\Delta Q(l)$ for large l is given in the appendix, where we show that

$$l^2 \Delta Q(l) = -\frac{1}{4} \zeta(\frac{1}{2}d) + O(l^{-1}), \quad l \rightarrow \infty. \tag{3.15}$$

Substituting this result in (3.13) yields

$$\begin{aligned} Y_d(T) &= (k_B T \Lambda^2 / 2\pi) [\rho - \Lambda^{-d} \zeta(\frac{1}{2}d)] \\ &= (k_B T \rho \Lambda^2 / 2\pi) [1 - (T/T_{c,d})^{1/d}], \quad d > 3 \end{aligned} \tag{3.16}$$

where we have used (3.1) and (2.5).

For $d = 3$, the above argument is inapplicable, since for finite l , the finite-thickness system does not have a non-zero critical temperature. Thus the field ϕ remains positive for all $l(<\infty)$ and $T > 0$. However, the analysis of Barber (1973) (see also Barber and Fisher 1973b) establishes that for fixed $T < T_{c,3}$ and large l , ϕ can be written as

$$\phi = x/l^2. \tag{3.17}$$

The 'scaled field' x is determined by the density constraint (2.9) which reduces to (Barber 1973)

$$(\Lambda_c^3 - \Lambda^3)\rho = H^r(x)/l + O(l^{-2}), \quad l \rightarrow \infty, x = O(1). \tag{3.18}$$

The functions $H^r(x)$ are given by

$$H^0(x) = 2\pi^{-1/2} \ln[2 \sinh(\pi x^{1/2})] \tag{3.19}$$

and

$$H^{1/2}(x) = 2\pi^{-1/2} \ln\{2 \cosh[\pi(x - \frac{1}{4})^{1/2}]\}. \tag{3.20}$$

If we define a reduced scaled temperature variable

$$\theta = \frac{1}{2} \sqrt{\pi} \rho l (\Lambda_c^3 - \Lambda^3) = \frac{1}{2} \sqrt{\pi} l \zeta(3/2) [1 - (T_{c,3}/T)^{3/2}], \tag{3.21}$$

we can invert (3.18) to give

$$x = W^r(\theta) + O(l^{-1}), \tag{3.22}$$

with

$$W^0(\theta) = [\sinh^{-1}(\frac{1}{2} \exp \theta)]^2 / \pi^2, \tag{3.23}$$

and

$$W^{1/2}(\theta) = \frac{1}{4} + [\cosh^{-1}(\frac{1}{2} \exp \theta)]^2 / \pi^2. \tag{3.24}$$

We observe that θ is negative for $T < T_{c,3}$ and tends to $-\infty$ as $l \rightarrow \infty$ with T fixed. In this limit, we find explicitly that

$$x_0 \approx \frac{1}{4} \pi^{-2} \exp(-2|\theta|), \quad \tau = 0, \tag{3.25a}$$

and

$$x_{1/2} \approx \frac{1}{2} \pi^{-1} \exp(-|\theta|), \quad \tau = \frac{1}{2}. \tag{3.25b}$$

These results imply that for both boundary conditions, $\phi_r(T, l)$ becomes exponentially small as l tends to infinity at fixed $T < T_{c,3}$.

To complete the derivation of $Y_3(T)$, we require the expansions of $P_3^r(x/l^2, l)$ to order l^{-2} . These are given in equations (42) and (54) of Barber (1973), from which we obtain

$$l^2(P_3^{1/2} - P_3^0) = \zeta(3/2)(\frac{1}{4} + x_0 - x_{1/2}) + O(l^{-1}). \tag{3.26}$$

Substituting this result, together with (3.27) and (3.35), in (2.12) finally yields

$$\begin{aligned} Y_3(T) &= (k_B T \Lambda^2 / 2\pi) [\rho - \Lambda^{-3} \zeta(3/2)] \\ &= (k_B T \Lambda^2 \rho / 2\pi) [1 - (T/T_{c,3})^{3/2}], \quad T \leq T_{c,3}. \end{aligned} \tag{3.27}$$

4. Discussion

In the preceding section we evaluated the helicity modulus, defined by (1.3), for ideal Bose gases in d dimensions. The pertinent results are contained in (3.11), (3.17) and (3.27), which may be summarised as ($d \geq 3$):

$$Y_d(T) = \begin{cases} 0 & T > T_{c,d} \\ (k_B T \Lambda^2 \rho / 2\pi) [1 - (T/T_{c,d})^{1/d}] & T \leq T_{c,d}. \end{cases} \tag{4.1}$$

The critical temperature $T_{c,d}$ is given by (3.2). From (1.2) and (2.5), we find that the superfluid density $\rho_s(T)$ of an ideal Bose gas is simply

$$\rho_s(T) = \rho n_0(T), \tag{4.2}$$

where

$$n_0(T) = 1 - (T/T_{c,d})^{1/d} \quad T \leq T_{c,d}, \tag{4.3}$$

is the condensate fraction in the bulk system (see e.g. London 1954).

Several aspects of these results are worth comment. The first concerns the critical behaviour of $Y_d(T)$ near $T_{c,d}$. In this regime the behaviour of the helicity modulus can be described (see FBJ § 2) by an exponent ν defined by

$$Y(T) \sim |(T - T_c)/T_c|^\nu \quad \text{as } T \rightarrow T_c^-. \tag{4.4}$$

Various arguments (see FBJ §§ 5 and 6) then relate ν to more conventional exponents by the Josephson relation (Josephson 1966):

$$\nu = 2\beta - \eta. \tag{4.5}$$

Here β describes the vanishing of the order parameter $\Psi_0(T)$ as $T \rightarrow T_c^-$, ν the divergence of the correlation length as $T \rightarrow T_c^+$ and η the decay of the correlation function at T_c . For the ideal Bose gas (Gunton and Buckingham 1968)

$$\Psi_0(T) = \sqrt{n_0(T)} \tag{4.6}$$

and hence

$$\beta = \frac{1}{2}, \quad \text{for all } d. \tag{4.7}$$

The correlation exponents have the values (see Gunton and Buckingham 1968, Barber 1973)

$$\eta = 0 \quad \text{for all } d \quad (4.8)$$

$$\nu = \begin{cases} (d-2)^{-1} & d < 4 \\ 1 & d \geq 4, \end{cases} \quad (4.9)$$

with an additional logarithmic factor for $d = 4$.

From (4.1) we find that for the ideal Bose gas

$$\nu = 1 \quad \text{for all } d, \quad (4.10)$$

which satisfies the Josephson relation (4.5). On the other hand, there exist additional arguments (see FBJ §§ 3 and 5) which predict that

$$\nu = (d-2)\nu \quad (4.11)$$

a relation first proposed for $d = 3$ by Ferrell *et al* (1967). This relation, however, is inconsistent with the exponent values (4.9) and (4.10) if d exceeds 4, and misses logarithmic factors for $d = 4$. This failure is, of course, nothing more than a direct reflection of the well known failure of hyperscaling or d -dependent scaling in more than four dimensions. Nevertheless, its validity in three dimensions, strengthens the arguments of FBJ, that a phase coherence length $\Lambda^{(Y)}(T)$ defined by

$$\Lambda^{(Y)}(T) = [k_B T / Y(T)]^{1/(d-2)} \quad (4.12)$$

can play the role of a correlation length in the ordered phase of an isotropic system. Whilst this definition has been used on an essentially *ad hoc* basis by Ferrell *et al* (1967, 1968) in their treatment of dynamic scaling, its further justification awaits the calculation of $Y(T)$ for more realistic systems.

Finally, it is informative to contrast the low temperature behaviour of $Y(T)$ for the ideal Bose gas with that expected in interacting systems. Two features of (4.1) and (4.2) are special to the ideal gas. Firstly, at $T=0$, there is no *depletion*, i.e. $\rho_s(0) = \rho$. Secondly the leading low temperature behaviour

$$Y(T) - Y(0) \sim \rho_s(T) - \rho \sim T^{1/d} \quad (4.13)$$

is the same as that of the condensate fraction. Neither of these results is expected to be true for a system of interacting bosons (see e.g. Khalatnikov 1965). It would therefore be of considerable interest to apply the definition (1.1) to either a weakly interacting Bose gas treated within the approximation of Bogoliubov (1947, reprinted in Pines 1961) or to an isotropic magnet within spin-wave theory. Some progress along these lines has been made recently (Jasnow, private communication) but further work is required to fully test the utility of (1.1).

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Appendix. Analysis of $\Delta Q(l)$ for large l

It is convenient to rewrite (3.14) as

$$\Delta Q(l) = (2\pi^{-1/2}/l) \sum_{s=1}^{\infty} [F_{\sigma}(s^2/l^2) - F_{\sigma}(s(s+1)/l^2)] - \pi^{-1/2}\zeta(\sigma)/l, \tag{A.1}$$

where we have defined

$$\sigma = \frac{1}{2}(d+1) \geq 2. \tag{A.2}$$

Introducing the representation (Barber 1973)

$$F_{\sigma}(z) = (2\pi i)^{-1} \int_{c-i\infty}^{c+i\infty} z^{-p} \Gamma(p) \zeta(\sigma+p) dp, \tag{A.3}$$

where $\Gamma(p)$ is the gamma function and

$$c = \text{Re } p > \max(0, 1 - \sigma), \tag{A.4}$$

we obtain

$$\Delta Q(l) = -\pi^{-1/2}\zeta(\sigma)/l + (2\pi^{-1/2}/2\pi i) \int_{c-i\infty}^{c+i\infty} l^{2p-1} \Gamma(p) \zeta(\sigma+p) \omega(p) dp. \tag{A.5}$$

The function $\omega(p)$ is defined by

$$\omega(p) = \sum_{s=1}^{\infty} [s^{-2p} - s^{-p}(s+1)^{-p}]. \tag{A.6}$$

For large s , the summand of this expression varies as s^{-2p-1} and hence $\omega(p)$ is an analytic function of p for $\text{Re } p > 0$. We shall however require an analytic continuation to $\text{Re } p \geq -\frac{1}{2}$. This follows by rewriting (A.6) as

$$\begin{aligned} \omega(p) &= \sum_{s=1}^{\infty} s^{-2p} [1 - (1+1/s)^{-p}] \\ &= p\zeta(2p+1) - \frac{1}{2}p(p+1)\zeta(2p+2) \\ &\quad + \sum_{s=1}^{\infty} s^{-2p} [1 - p/s + p(p+1)/2s^2 - (1+1/s)^{-p}]. \end{aligned} \tag{A.7}$$

The sum in the final expression in (A.7) is now convergent for $\text{Re } p > -1$, while the zeta-functions indicate that $\omega(p)$ has a simple pole at $p = -\frac{1}{2}$ with a residue of $1/16$.

Thus, on closing the contour in (A.5) in the left-half of the complex p -plane and evaluating the residues at successive poles yields

$$\Delta Q(l) = -\pi^{-1/2}\zeta(\sigma)l^{-1} + 2\pi^{-1/2}\zeta(\sigma)\omega(0)l^{-1} + 2\pi^{-1/2}\Gamma(-\frac{1}{2})\zeta(\sigma-\frac{1}{2})l^{-2}/8 + O(l^{-3}). \tag{A.8}$$

From (A.7),

$$\omega(0) = \lim_{p \rightarrow 0} p\zeta(2p+1) = \frac{1}{2} \tag{A.9}$$

and hence

$$l^2 \Delta Q(l) = -\zeta(\sigma - \frac{1}{2})/4 + O(l^{-1}), \quad (\text{A.10})$$

from which (3.15) follows immediately.

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