Casimir effect for a sphere and a cylinder in front of a plane and corrections to the proximity force theorem

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Using a path integral approach we rederive a recently found representation of the Casimir energy for a sphere and a cylinder in front of a plane and derive the first correction to the proximity force theorem.

I. INTRODUCTION

In view of the rapid experimental progress in the Casimir force measurements and increasing interest in the field of nanotechnology there is a growing demand for reliable theoretical predictions. Beyond geometries allowing for a separation of variables one was left so far basically with the proximity force approximation for ideal reflecting surfaces or with the pairwise summation for dilute dielectric bodies. Also the basic formula for the interaction of dielectric bodies, the Lifshitz formula, is known for simple geometries only (for a review see [1]). There are a number of approximate methods trying to overcome these limitations. The oldest one is the semiclassical approach (see, for example, the recent papers [2,3] and references therein) which exists in several modifications including the optical path approximation [4]. Another method is the multiple reflection approximation which recently has been reconsidered in the context of the Casimir effect [5]. New developments are the multiscattering approach of [6] which was applied to the geometry of two spheres and of a sphere in front of a plane and the calculation in [7] for a cylinder and a plane using a path integral formulation together with a trace formula. Significant progress had been reached in the world line method [8] which is now able to provide corrections to the small separation behavior.

In the present paper we use the path integral approach developed in [9,10] and apply it to the geometry of a sphere and a cylinder in front of a plane for Dirichlet boundary conditions. We rederive the formulas obtained in [6,7] in a simpler way and calculate the first correction to the proximity force theorem.

The paper is organized as follows. In the next section we describe the method of [9,10] in detail. In the third section we apply the method to the geometry of a sphere in front of a plane. In the fourth section we discuss some other geometries. Conclusions are given in the final section. Throughout the paper we put $\hbar = c = 1$

II. FUNCTIONAL INTEGRATION AND BOUNDARY CONDITIONS

A simple, but powerful method to introduce boundary conditions into a quantum field theory is to use functional delta functions. This method was introduced in [9] for the calculation of the radiative corrections to the Casimir effect for parallel plates in a covariant gauge. We present it here in the simpler case for a scalar field theory with Dirichlet boundary conditions. The basic idea of the method is to restrict the space of fields over which the functional integration runs to such that fulfil the boundary conditions. Technically this can be achieved by representing the generating functional of the Green's functions as

$$Z(J) = \int D\phi \prod_{x \in S} \delta(\phi(x)) \exp\{-S\} \quad (1)$$

with an action

$$S = \int dx \left(\frac{1}{2} \phi(x)(-\partial^2 + m^2)\phi(x) + J(x)\phi(x) \right), \quad (2)$$

where we included the term with the source $J(x)$. This is the usual action for a scalar field with mass m. For simplicity we write all formulas in the Euclidean formulation.

The functional $Z(J)$, (1), taken without the delta function is the generating functional of the corresponding field theory without boundary conditions. Obviously, in (1) more complicated actions can be inserted, especially such which include interactions. However, in connection with the Casimir effect we restrict ourselves here to a free field theory, i.e., to a quadratic action. Also we mention that the initial space where the field ϕ is defined does not need to be flat or free of boundaries. The method to implement boundary conditions through functional delta functions is completely general, at last on the formal level taken in this section.

The next step in the method is the use of a Fourier representation for the delta function,

$$\prod_{x \in S} \delta(\phi(x)) = \int Db \exp\left(i \int_S dz b(z)\phi(f(z)) \right), \quad (3)$$

where we described the surface S by a function $f(z)$ such

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that $x = f(z) \in S$ and the coordinates z are a suitable parametrization of S. In fact, (3) is a functional integral over a scalar field $b(z)$ defined on the surface S. Using (3) in the generating functional (1) we represent $Z(J)$ in the form

$$Z(J) = \int D\phi Db \exp(-\tilde{S}) \qquad (4)$$

with

$$\tilde{S} = \frac{1}{2} \int dx \phi(x)(-\partial^2 + m^2)\phi(x)$$
$$- i \int dx \int_S dz \phi(x) H(x,z) b(z) + \int dx J(x)\phi(x). \qquad (5)$$

Here we introduced the new notation,

$$H(x,z) = \delta(x - f(z)), \qquad (6)$$

projecting the argument x on the surface S. Obviously, $\tilde{S}$ is quadratic in the fields $\phi(x)$ and $b(z)$, hence $\tilde{S}$ can be diagonalized,

$$\tilde{S} = \frac{1}{2} \int dx (\phi(x) - \phi_0(x))(-\partial^2 + m^2)(\phi(x) - \phi_0(x))$$
$$+ \frac{1}{2} \int_S dz \int_S dz' (b(z) - b_0(z)) K(z,z') (b(z) - b_0(z))$$
$$- \frac{1}{2} \int dx \int dy J(x)^S D(x,y) J(y), \qquad (7)$$

with

$$\phi_0(x) = \int dx' D(x,x') \left(i \int_S dz H(x',z) b(z) - J(x') \right),$$
$$b_0(z) = -i \int_S dz' \int dx dx' K^{-1}(z,z') H(x,z') D(x,x') J(x'), \qquad (8)$$

and

$$K(z,z') = \int dx \int dy H(x,z) D(x,y) H(y,z')$$
$$= D(f(x), f(y)). \qquad (9)$$

The function $D(x,y)$ is the inverse of the kernel of the free action,

$$(-\partial^2 + m^2) D(x,y) = \delta(x - y). \qquad (10)$$

It is just the usual propagator of the free field theory defined by the action S, (2). Instead, the new quantity

$$^S D(x,y) = D(x,y)$$
$$- \int_S dz \int_S dz' D(x, f(z)) K^{-1}(z,z') D(f(z'), y), \qquad (11)$$

which we introduced in (7), is the propagator of the given

field theory with boundary conditions. Finally, $K^{-1}(z,z')$ is the inverse of $K(z,z')$ on the surface S,

$$\int_S dz' K(z,z') K^{-1}(z', z'') = \delta(z - z''). \qquad (12)$$

This inversion and further operations like the trace or the determinant with $K(z,z')$ are to be understood as done with an operator $\hat{K}$ whose integral kernel in a space of suitable functions defined on the surface S is just $K(z,z')$.

With Eq. (12) it is easy to check that $^S D(x,y)$, (11), is indeed the propagator which fulfills the boundary conditions. First we remark that it is a propagator. Obviously Eq. (10) is fulfilled for $x \notin S$. Inserted into Eq. (10), the first term delivers the necessary delta function. The second term delivers a delta function too which is, however, nonvanishing for $x \in S$ only. This is not a problem because in the presence of boundary conditions the equation has to be fulfilled outside the boundary only. So it remains to check that the boundary conditions are fulfilled. Put x on the surface S, i.e., consider $x \in S$. Then in the second term we can apply (12) and we get zero as required by the Dirichlet condition.

The calculation of the inverse on S of K is the main step in the method. All steps before are merely a formal rewriting. The inversion of K on S, however, is equivalent to solve the wave equation with boundary conditions and, in this sense, not much progress is archived.

After rewriting the exponential in the form given by Eq. (7), it is quadratic in the fields. The integrals are Gaussian and after integration we represent $Z(J)$, (1), in the form

$$Z(J) = C(\det(\partial^2 + m^2))^{-(1/2)} (\det K(z,z'))^{-(1/2)}$$
$$\times \exp\left\{ -\frac{1}{2} \int dx \int dy J(x)^S D(x,y) J(y) \right\}, \qquad (13)$$

where C is a constant. In this formula the first determinant comes from the integration over ϕ. It is the usual one appearing also without boundary condition. Of course, it is independent on the boundary conditions. The second determinant comes from the integration over b. It does depend on the boundary conditions. The source term has the standard form and it generates the usual Feynman rules with the boundary dependent propagator $^S D(x,y)$ instead of the usual one. In this way the field theory with boundary conditions was constructed in [9].

The last step in the method, which was done in [10], is to consider the free energy

$$F = -\frac{1}{T} \ln Z(0), \qquad (14)$$

where T is the total time which is the logarithm of the generating functional at zero source term. In [10] this was done for a theory with finite temperature, but of course we can use it at zero temperature too. In this way we get for the boundary dependent part of the Casimir energy

$$E_{\text{Casimir}} = -\frac{1}{T}\ln(\det K(z, z'))^{-(1/2)} = \frac{1}{2T}\,\text{tr}\ln K. \quad (15)$$

The trace in this formula is to be taken in the space of functions on the boundary surface S and K is the operator in this space, whose integral kernel is the function $K(z, z')$, defined in Eq. (9). In this way the Casimir energy is represented by an expression on the surface S. The contribution of the free space, which contains the highest ultraviolet divergences, had been dropped in (15).

Let us mention that the evaluation of the trace in (15) is a problem of the same difficulty as the inversion of K or the solution of the wave equation with boundary condition, and again, so far we have only a formal rewriting of the original problem.

III. A SPHERE AND A CYLINDER IN FRONT OF A PLANE

In this section we apply the general formula (15) for the Casimir energy to the geometry of a sphere and of a cylinder in front of a plane. We start with the remark that the derivation in the preceding section is valid also if the initial space is not the full $\mathbb{R}^4$ but only a half of it with $z \le a$ and if the field $\phi(x)$ satisfies Dirichlet (or other) boundary conditions on the plane $z = a$: $\phi_{|_{z=a}} = 0$. In that case, for the propagator $D(x, x')$, (10), which has to fulfill Dirichlet boundary conditions at $z = a$ we take

$$D(x, x') \rightarrow D_D(x, x') = D(x - x') - D(\tilde{x} - x'), \quad (16)$$

where $\tilde{x} = (x, y, 2a - z, t)$ is the coordinate reflected on the plane $z = a$ and

$$D(x - x') = \int \frac{d^4 k}{(2\pi)^4} \frac{e^{-k(x-x')}}{k^2 + m^2} \quad (17)$$

is the free space propagator. Here m is the mass of the field ϕ but in the following we restrict ourselves to massless fields.

In the next step we use the stationarity of the problem and turn to the Fourier transform in the time coordinate, $x_4 \rightarrow \omega$. In this way the Casimir energy (15) can be represented as

$$E = \frac{1}{2\pi} \int_0^\infty d\omega \, \text{tr}\ln K_\omega \quad (18)$$

with (cf. (9))

$$K_\omega(z, z') = D_{D,\omega}(f(z), f(z')) \quad (19)$$

and

$$D_{D,\omega}(x, x') = D_\omega(x - x') - D_\omega(\tilde{x} - x'). \quad (20)$$

as well as the free space propagator after Fourier transform in the time direction,

$$D_\omega(x - x') = \int \frac{d^3 k}{(2\pi)^3} \frac{e^{-k(x-x')}}{\omega^2 + k^2}. \quad (21)$$

In (18) the trace is now only over the surface S and we used the symmetry of K_ω under $\omega \rightarrow -\omega$. We note that the function K_ω, (19) is even in $\omega \rightarrow -\omega$. We take this into account in all integration over ω below.

Now let us consider a sphere of radius R centered in the origin so that the distance from its center to the plane is a. In terms of spherical coordinates (r, θ, φ) it is described by constant r and the angles provide a parametrization of S, $z = (\theta, \varphi)$. A basis of functions in this space are the spherical harmonics $| l, m\rangle = Y_{l,m}(\theta, \phi)$. Now we calculate the trace in (18) in this basis, i.e., we represent the energy by

$$E = \frac{1}{2\pi} \int_0^\infty d\omega \, \text{tr}_{l,m} \ln K_{lm,l'm'}, \quad (22)$$

with

$$K_{lm,l'm'} = \langle l, m \mid D_D(x, x') \mid l, m\rangle$$
$$= \int d\theta_x \sin\theta_x d\varphi_x \int d\theta_{x'} \sin\theta_{x'} d\varphi_{x'} Y_{l,m}(\theta_x, \varphi_x)$$
$$\times D_D(x, x') Y^*_{l'm'}(\theta_{x'}, \varphi_{x'}),$$

and $r_x = r_{x'} = R$. Now the trace is over the indices of the infinite dimensional matrix $\ln K_{lm,l'm'}$. An equivalent representation is in terms of the determinant of this matrix,

$$\text{tr}\ln K_{lm,l'm'} = \ln \det(K_{lm,l'm'}). \quad (23)$$

Next we use the well-known explicit expansion of the free space propagator,

$$D_\omega(x - x') = \sum_{l,m} Y_{l,m}(\theta_x, \varphi_x) d_l(r, r') Y^*_{l'm'}(\theta_{x'}, \varphi_{x'}), \quad (24)$$

with

$$d_l(r, r') = \frac{1}{\sqrt{rr'}} j_l(\omega r_<) h_l^{(1)}(\omega r_>), \quad (25)$$

where $j_l(z)$ and $h_l^{(1)}(z)$ are the spherical Bessel functions to represent K in the form

$$K_{l,l'} = \delta_{l,l'} d_l(R, R) - \langle lm \mid D_\omega(\tilde{x} - x') \mid l'm\rangle, \quad (26)$$

where because of the azimuthal symmetry we could introduce

$$K_{lm,l'm'} = \delta_{m,m'} K_{l,l'}. \quad (27)$$

The last step is to separate a distance independent contribution by writing

$$\ln K_{l,l'} = \ln(\delta_{l,l'} d_l(R, R)) + \ln\left(\delta_{l,l'} - \frac{1}{d_l(R, R)}\langle lm \right.$$
$$\left. \mid D_\omega(\tilde{x} - x') \mid l'm\rangle\right). \quad (28)$$

The distance a enters this expression only trough $\tilde{x}$ in the second term in the right-hand side whereas the first is independent of a. In fact, it is this term which contains

the surface divergences which are still present in the Casimir energy given by Eq. (22). But dropping it we come to

$$E = \frac{1}{2\pi} \int_0^\infty d\omega \, \text{tr}_{l,m} \ln(\delta_{l,l'} - A_{l,l'}), \qquad (29)$$

where we introduced the notation

$$A_{l,l'} = \frac{1}{d_l(R,R)} \langle lm \mid D_\omega(\tilde{x} - x') \mid l'm \rangle. \qquad (30)$$

The energy E, (29), is the ultraviolet finite, distance dependent part of the Casimir energy which be means of $F = -\frac{\partial}{\partial a} E$ is alone responsible for the force.

The representation (29) is still to some extend symbolic. In fact, a precise formula is

$$E = \frac{1}{2\pi} \int_0^\infty d\omega \sum_{m=-\infty}^{\infty} \ln \det(\delta_{l,l'} - A_{l,l'}), \qquad (31)$$

where $(\delta_{l,l'} - A_{l,l'})$ is a infinite dimensional matrix with l, $l' \geq |m|$.

Another way to represent the trace in an explicit formula is to expand the logarithm,

$$E = \frac{1}{2\pi} \int_0^\infty d\omega \sum_{s=0}^{\infty} \frac{-1}{s+1}$$
$$\times \sum_{m=-\infty}^{\infty} \sum_{l=|m|}^{\infty} \sum_{l_1=|m|}^{\infty} \cdots \sum_{l_s=|m|}^{\infty} A_{l,l_1} A_{l_1,l_2} \ldots A_{l_s,l}, \quad (32)$$

whereby the convergence of the sum over s is assumed.

Let us mention that the representations (31) and (32) of the Casimir energy are exact. Their basic merit is that they are free of ultraviolet divergences. Hence they can be used also for direct numerical approximation. Examples of that are given in [6,7].

A further simplification appears because the matrix elements $A_{l,l'}$ can be written explicitly in terms of modified Bessel functions and $3j$-symbols. In fact, the formula

$$A_{l,l'} = \sqrt{\frac{\pi}{2}} \sqrt{\frac{(2l+1)(2l'+1)}{2a\omega}} (-1)^{l+l'} \frac{I_{l'+(1/2)}(\omega R)}{K_{l+(1/2)}(\omega R)}$$
$$\cdot \sum_{l''=|l-l'|}^{l+l'} (-i)^{l''} (2l''+1) K_{l''+(1/2)}(2a\omega)$$
$$\times \begin{pmatrix} l'' & l & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'' & l & l' \\ 0 & -m & m \end{pmatrix} \qquad (33)$$

holds. Its derivation is given in Appendix A.

Similar formulas as for the sphere can be written for a cylinder in front of a plane. For comparison we consider besides the $(3 + 1)$-dimensional also the $(2 + 1)$-dimensional case, i.e., a circle in a front of a line on a plane. We denote the energies by $E_{(3+1)}^{\text{cyl}}$ and $E_{(2+1)}^{\text{cyl}}$ correspondingly.

We start from the formula (18) for the energy which for $E_{(2+1)}^{\text{cyl}}$ does not change,

$$E_{(2+1)}^{\text{cyl}} = \frac{1}{2\pi} \int_0^\infty d\omega \, \text{tr} \ln K_\omega. \qquad (34)$$

For $(3 + 1)$ dimensions using the translational invariance along the axis of the cylinder it must be substituted by

$$E_{(3+1)}^{\text{cyl}} = \frac{1}{2\pi} \int_0^\infty d\omega \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \, \text{tr} \ln K_\gamma \qquad (35)$$

with $\gamma = \sqrt{\omega^2 + k_z^2}$ where k_z is the momentum parallel to the axis of the cylinder. Obviously the integration over k_z can be done,

$$E_{(3+1)}^{\text{cyl}} = \frac{1}{4\pi} \int_0^\infty d\omega \, \omega \, \text{tr} \ln K_\omega, \qquad (36)$$

so that the difference is just the additional factor $\omega/2$ in (36) as compared to (34). We note that $E_{(3+1)}^{\text{cyl}}$ is the energy per unit length of the cylinder.

Next we have to consider the function K_ω in two dimensions. A basis of functions on a circle is simply $|m\rangle = \exp\{im\varphi\}/\sqrt{2\pi}$ and the free space propagator has the decomposition

$$D_\omega^{(2+1)}(x - x') = \sum_m |m\rangle d_m^{(2+1)}(r,r')\langle m' | \qquad (37)$$

with

$$d_m^{(2+1)}(r,r') = I_m(\omega r_<) K_m(\omega r_>). \qquad (38)$$

In this way we obtain in place of (26)

$$K_{m,m'} = \delta_{m,m'} d_m^{(2+1)}(R,R) - \langle m \mid D_\omega^{(2+1)}(\tilde{x} - x') \mid m' \rangle, \qquad (39)$$

where $D_\omega^{(2+1)}(\tilde{x} - x')$ is the same as (21) in a dimension lower by one,

$$D_\omega^{(2+1)}(x - x') = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-k(x-x')}}{\omega^2 + k^2}, \qquad (40)$$

and $\tilde{x} = (x, 2a - y)$ is the reflected coordinate in the (x, y)-plane.

Separating again the distance independent contribution we represent the energy in the form

$$E_{(3+1)}^{\text{cyl}} = \frac{1}{4\pi} \int_0^\infty d\omega \, \omega \sum_m \ln(\delta_{m,m'} - A_{m,m'}), \qquad (41)$$

with

$$A_{m,m'} = \frac{1}{d_m^{(2+1)}(r,r)} \langle m \mid D_\omega^{(2+1)}(\tilde{x} - x') \mid m' \rangle. \qquad (42)$$

In the $(2 + 1)$-dimensional case we have the same formula except for the factor ω dropped,

$$E_{(2+1)}^{\text{cyl}} = \frac{1}{2\pi} \int_0^\infty d\omega \sum_m \ln(\delta_{m,m'} - A_{m,m'}). \qquad (43)$$

Like in the case of a sphere, the matrix elements $A_{m,m'}$ can be calculated explicitly (see Appendix A) and expressed in terms of Bessel functions,

$$A_{m,m'} = \frac{1}{K_m(\omega r)} K_{m+m'}(2\omega a) I_m(\omega r), \qquad (44)$$

a formula which coincides with the corresponding ones in [6,7].

IV. CYLINDER AT SMALL SEPARATION FROM A PLANE

In this section we consider a cylinder at small separation from a plane. We start with Dirichlet boundary conditions. Here we consider first the case of $(3 + 1)$ dimensions, i.e., the usual space. Then we reduce the dimension by one, i.e., we consider the $(2 + 1)$-dimensional case which is a circle in front of a line on a plane. Finally, we consider the case of Neumann boundary conditions. Since in the cylindrical case the polarizations of the electromagnetic field separate into TM modes fulfilling Dirichlet boundary conditions and TE modes fulfilling Neumann boundary conditions this gives at once the result for the electromagnetic field.

A. Dirichlet case

Starting point is the formula (41). We rescale $\omega \to \omega/r$ so that the energy is now given by

$$E_{(3+1)}^{\text{cyl}} = \frac{1}{4\pi r^2} \int_0^\infty d\omega \, \omega \, \text{tr} \ln(\delta_{m,m'} - A_{m,m'}(\omega)), \quad (45)$$

where $A_{m,m'}$ is now given by

$$A_{m,m'}(\omega) = \frac{1}{K_m(\omega)} K_{m+m'}(2\omega(1 + \epsilon)) I_{m'}(\omega), \qquad (46)$$

with

$$\epsilon = \frac{L}{R}, \qquad (47)$$

where $L = a - R$ is the separation between the cylinder and the plane and we are interested in the small distance behavior, i.e., in $\epsilon \to 0$.

To start with, we expand the logarithm in Eq. (45). Below, this turns out to be justified because in the orders in ϵ we are interested in, this series converges. The energy is now given by

$$E_{(3+1)}^{\text{cyl}} = \frac{-1}{4\pi R^2} \sum_{s=1}^\infty \frac{1}{s+1} \int_0^\infty d\omega \, \omega \sum_m \sum_{n_1} \cdots \sum_{n_s} \mathcal{M} \quad (48)$$

with

$$\mathcal{M} = A_{m,m+n_1}(\omega) A_{m+n_1,m+n_2}(\omega) \ldots A_{m+n_{s-1},m+n_s}(\omega)$$
$$\times A_{m+n_s,m}(\omega). \qquad (49)$$

In (48) the summations over m and the n_i's run over the integers.

Now the small distance behavior of the energy comes from the region in the integration resp. sums of large all, ω, m and the n_i's. We use the uniform asymptotic expansion of the Bessel functions and substitute the sums by integrals. Further we use the symmetry under $m \to -m$ and obtain in the sense of an asymptotic expansion

$$E_{(3+1)}^{\text{cyl}} = \frac{-1}{2\pi R^2} \sum_{s=1}^\infty \frac{1}{s+1}$$
$$\times \int_0^\infty d\omega \, \omega \int_0^\infty dm \int_{-\infty}^\infty dn_1 \ldots \int_{-\infty}^\infty dn_s \, \mathcal{M}, \qquad (50)$$

where for the $A_{m,m'}(\omega)$ in $\mathcal{M}$ still Eq. (46) holds, however, with the Bessel functions replaced by their well known uniform asymptotic expansions which are displayed in Appendix B. From the expressions in the exponential factors in

$$A_{m,m'} \sim e^{-\tilde{\eta}}, \qquad (51)$$

which combine into

$$\tilde{\eta} = (m + m')\eta\left(\frac{2\omega(1 + \epsilon)}{m + m'}\right) - m\eta\left(\frac{\omega}{m}\right) - m'\eta\left(\frac{\omega}{m'}\right), \qquad (52)$$

(see Eqs. (46) and (B1)), it follows that for small ϵ the dominating contribution into (50) comes from $\omega \sim m \sim 1/\epsilon$, $n_i \sim 1/\sqrt{\epsilon}$. Hence we substitute

$$\omega = \frac{t\sqrt{1 - \tau^2}}{\epsilon}, \qquad m = \frac{t\tau}{\epsilon}, \qquad n_i \to n_i \sqrt{\frac{4t}{\epsilon}}, \qquad (53)$$

where the factor $\sqrt{4t}$ was introduced for later convenience. With these substitutions the energy becomes

$$E_{(3+1)}^{\text{cyl}} = \frac{-\epsilon^{-3}}{2\pi R^2} \sum_{s=0}^\infty \frac{1}{s+1}$$
$$\times \int_0^\infty \frac{dt}{t} t^3 \int_0^1 d\tau \int_{-\infty}^\infty dn_1 \ldots \int_{-\infty}^\infty dn_s \left(\frac{4t}{\epsilon}\right)^{s/2} \mathcal{M}. \qquad (54)$$

Now we change the notations for the $A_{m,m'}(\omega)$,

$$A_{m+n,m+n'}(\omega) \to A_{n,n'}^{\text{as}} \qquad (55)$$

indicating the dependence on the variables n and n'. Using the asymptotic expansions of the Bessel functions entering by means of Eq. (46), we obtain the expansion

$$A_{n,n'}^{\mathrm{as}} = \sqrt{\frac{\epsilon}{4\pi t}} e^{-\eta^{\mathrm{as}}} (1 + \sqrt{\epsilon} a_{n,n'}^{(1/2)}(t,\tau) + \epsilon a_{n,n'}^{(1)}(t,\tau) + \dots),$$

$$(56)$$

with

$$\eta^{\mathrm{as}} = 2t + (n - n')^2. \tag{57}$$

Details including the explicit form of the functions $a_{n,n'}^{(1/2)}(t,\tau)$ and $a_{n,n'}^{(1)}(t,\tau)$ are shown in Appendix B.

Next we insert (56) for the $A_{m,m'}(\omega)$ into $\mathcal{M}$ in (49) and after a re-expansion we obtain

$$\mathcal{M} = \left(\frac{\epsilon}{4\pi t}\right)^{(s+1/2)} e^{-2(s+1)t - \eta_1} \left(1 + \sqrt{\epsilon} \sum_{i=0}^{s} a_{n_i,n_{i+1}}^{(1/2)}(t,\tau)\right.$$

$$+ \epsilon \left(\sum_{0 \leq i < j \leq s} a_{n_i,n_{i+1}}^{(1/2)}(t,\tau) a_{n_j,n_{j+1}}^{(1/2)}(t,\tau)\right.$$

$$\left.\left.+ \sum_{i=0}^{s} a_{n_i,n_{i+1}}^{(1)}(t,\tau)\right) + \dots\right), \tag{58}$$

with

$$\eta_1 = \sum_{i=0}^{s} (n_i - n_{i+1})^2. \tag{59}$$

Here, in order to include all contributions into the sum signs, we have to put $n_0 = n_{s+1} = 0$ formally.

The above formulas allow us to represent the energy E, Eq. (54), in the form

$$E_{(3+1)}^{\mathrm{cyl}} = \frac{-1}{2\pi L^2} \sqrt{\frac{R}{L}} \sum_{s=0}^{\infty} \frac{1}{s+1} \int_0^\infty \frac{dt}{t} \frac{t^{5/2} e^{-2(s+1)t}}{\sqrt{4\pi}}$$

$$\times \int_0^1 d\tau \int_{-\infty}^\infty \frac{dn_1}{\sqrt{\pi}} \dots \int_{-\infty}^\infty \frac{dn_s}{\sqrt{\pi}} \mathcal{M}^{\mathrm{as}}, \tag{60}$$

with

$$\mathcal{M}^{\mathrm{as}} = e^{-\eta_1} \left(1 + \sqrt{\epsilon} \sum_{i=0}^{s} a_{n_i,n_{i+1}}^{(1/2)}(t,\tau)\right.$$

$$+ \epsilon \left(\sum_{0 \leq i < j \leq s} a_{n_i,n_{i+1}}^{(1/2)}(t,\tau) a_{n_j,n_{j+1}}^{(1/2)}(t,\tau)\right.$$

$$\left.\left.+ \sum_{i=0}^{s} a_{n_i,n_{i+1}}^{(1)}(t,\tau)\right) + \dots\right). \tag{61}$$

In this representation it is possible to carry out the integrations over τ and over t and we obtain

$$E_{(3+1)}^{\mathrm{cyl}} = \frac{-1}{2\pi L^2} \sqrt{\frac{R}{L}} \sum_{s=0}^{\infty} \frac{1}{s+1} \int_{-\infty}^\infty \frac{dn_1}{\sqrt{\pi}} \dots \int_{-\infty}^\infty \frac{dn_s}{\sqrt{\pi}}$$

$$\times e^{-\eta_1} \left\{\frac{\Gamma(5/2)}{\sqrt{4\pi}(2(s+1))^{5/2}}\right.$$

$$+ \epsilon \left(\sum_{0 \leq i < j \leq s} b(n_i, n_{i+1}, n_j, n_{j+1})\right.$$

$$\left.\left.+ \sum_{i=0}^{s} d(n_i, n_{i+1}) + \dots\right) + \dots\right\}, \tag{62}$$

with

$$b(n_i, n_{i+1}, n_j, n_{j+1}) = \int_0^\infty \frac{dt}{t} \frac{t^{5/2} e^{-2(s+1)t}}{\sqrt{4\pi}}$$

$$\times \int_0^1 d\tau a_{n_i,n_{i+1}}^{(1/2)}(t,\tau) a_{n_j,n_{j+1}}^{(1/2)}(t,\tau), \tag{63}$$

and

$$d(n_i, n_{i+1}) = \int_0^\infty \frac{dt}{t} \frac{t^{5/2} e^{-2(s+1)t}}{\sqrt{4\pi}} \int_0^1 d\tau a_{n_i,n_{i+1}}^{(1)}(t,\tau). \tag{64}$$

The quite lengthy explicit formulas for b and d are shown at the end of Appendix B, Eqs. (B14) and (B15). In Eq. (62) we dropped the contribution proportional to $\sqrt{\epsilon}$. It can be seen that it contains only odd powers of the n_i's and vanishes under the integration over the n_i's.

The next step is to perform the integrations over the n_i's in Eq. (62). In the leading order in ϵ this is quite simple. We rewrite the quadratic form η_1, Eq. (59), by noticing that obviously the formula

$$n_1^2 + \sum_{i=1}^{s-1} (n_i - n_{i+1})^2 + n_s^2$$

$$= \frac{2}{1}\left(n_1 - \frac{2}{1} n_2\right)^2 + \frac{3}{2}\left(n_2 - \frac{3}{2} n_3\right)^2 + \dots$$

$$+ \frac{s}{s-1}\left(n_{s-1} - \frac{s-1}{s} n_s\right)^2 + \frac{s+1}{s} n_s^2 \tag{65}$$

holds. It immediately delivers

$$\int_{-\infty}^\infty \frac{dn_1}{\sqrt{\pi}} \dots \int_{-\infty}^\infty \frac{dn_s}{\sqrt{\pi}} e^{-\eta_1} = \frac{1}{\sqrt{s+1}}, \tag{66}$$

and we obtain the energy for a cylinder in front of a plane in leading order in small separation,

$$E_{(3+1)}^{\mathrm{cyl\ PFT}} = \frac{-1}{2\pi L^2} \sqrt{\frac{R}{L}} \sum_{s=0}^{\infty} \frac{\Gamma(5/2)}{\sqrt{4\pi}} \frac{1}{(s+1)^4}$$

$$= \frac{-1}{2\pi L^2} \sqrt{\frac{R}{L}} \frac{3\zeta(4)}{32\sqrt{2}} = -\frac{\pi^3}{1920\sqrt{2}} \frac{1}{L^2} \sqrt{\frac{R}{L}}, \tag{67}$$

which coincides with the known result from applying the

proximity force theorem. Note that in order to restore dimensions it has to be multiplied with $\hbar$ and c. Also note that this is the energy per unit length of the cylinder.

Now we turn to the remaining terms in Eq. (62). Of course, all integrations there over the n_i's are Gaussian. But the combinatorics is somewhat involved so that we delegate these calculations into Appendix C. The result is enjoyable simple,

$$
\int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} \left(\sum_{0 \le i < j \le s} b(n_1, n_{i+1}, n_j, n_{j+1}) \right.
$$
$$
\left. + \sum_{i=0}^{s} d(n_i, n_{i+1}) \right) = \frac{7}{384\sqrt{2}} \frac{1}{(1+s)^3}. \quad (68)
$$

The remaining sum over s in (62) is the same as in the leading order and finally for small distance L the energy becomes

$$
E_{(3+1)}^{\text{cyl}} = \frac{-1}{2\pi L^2} \sqrt{\frac{R}{L}} \frac{3\zeta(4)}{32\sqrt{2}} \left\{ 1 + \frac{7}{36} \frac{L}{R} + O\left(\left(\frac{L}{R} \right)^2 \right) \right\}, \quad (69)
$$

a formula, which represents the first correction to the proximity force theorem.

Using the method shown above it is easy to repeat the calculation for $(2 + 1)$ dimensions. The first change is in the substitution (53) where it is now meaningful not to use the variable τ but to define

$$
\omega = \frac{t \sin\varphi}{\epsilon}, \qquad m = \frac{t \cos\varphi}{\epsilon}, \qquad n_i \rightarrow n_i \sqrt{\frac{4t}{\epsilon}}, \quad (70)
$$

with $\varphi \in [0, \frac{\pi}{2}]$. Next we mention the changed formula (60)

$$
E_{(2+1)}^{\text{cyl}} = \frac{-1}{2L} \sqrt{\frac{R}{L}} \sum_{s=0}^{\infty} \frac{1}{s+1} \int_0^{\infty} \frac{dt}{t} \frac{t^{3/2} e^{-2(s+1)t}}{\sqrt{4\pi}} \int_0^{\pi/2} \frac{d\varphi}{\pi/2}
$$
$$
\times \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} \mathcal{M}^{\text{as}}, \quad (71)
$$

where besides the prefactor only the power of t changed and the integration over τ is changed for that over φ. The remaining steps go in complete parallel to the $(3 + 1)$-dimensional case and the result is

$$
E_{(2+1)}^{\text{cyl}} = \frac{-1}{2L} \sqrt{\frac{R}{L}} \frac{\zeta(3)}{8\sqrt{2}} \left\{ 1 + \frac{1}{4} \frac{L}{R} + O\left(\left(\frac{L}{R} \right)^2 \right) \right\}. \quad (72)
$$

B. Neumann case

Let us consider the changes which come in for Neumann boundary conditions first in the general formulas of Sec. II. Basically it is sufficient to change in formula (6) the delta function for its normal (to the surface S) derivative, $H \rightarrow \partial_{n_x} \delta(x - f(z))$. As a consequence, the definition of $K(z, z')$, (9), changes for

$$
K(z, z') = \partial_{n_x} \partial_{n_{x'}} D(f(x), f(x')), \quad (73)
$$

where the normal derivatives must be taken before putting the argument onto the surface. The next changes is in formula (16) because on the plane at $z = a$ we have to take Neumann conditions too. It amounts simply in a different sign,

$$
D(x, x') \rightarrow D_N(x, x') = D(x - x') + D(\tilde{x} - x'). \quad (74)
$$

As next changes we mention formula (38) where the Bessel functions must be substituted by their derivatives,

$$
d_m^{(2+1)}(r, r') = I_m'(\omega r_<) K_m'(\omega r_>). \quad (75)
$$

and Eq. (41) which looks now

$$
E_{(3+1)}^{\text{cyl,N}} = \frac{1}{4\pi} \int_0^{\infty} d\omega\, \omega \sum_m \ln(\delta_{m,m'} + A_{m,m'}) \quad (76)
$$

with

$$
A_{m,m'} = \frac{1}{K_m'(\omega R)} K_{m+m'}(2\omega a) I_m'(\omega R) \quad (77)
$$

Now we trace the changes in the asymptotic expansion for small separations. First we consider the asymptotic expansion of $A_{m,m'}$, (77), using the asymptotic expansions of the derivatives of the Bessel functions,

$$
\left\{ {I_m'(mz) \atop K_m'(mz)} \right\} = \pm \frac{\pi^{\mp(1/2)}}{\sqrt{2m}} \frac{(1+z^2)^{1/4}}{z} e^{\pm m\eta(z))} \left(1 \pm \frac{v_1(t)}{m} + \cdots \right) \quad (78)
$$

with $v_1(t) = (-9t + 7t^3)/24$. The first observation is that the minus sign in the expansion of $K_m'(mz)$ just compensates the sign change in (76). The second remark is that in the expansion of the factors in front of the exponential, (B6) in the Dirichlet case, just n and n' change their places which does not affect the expression under the trace in (76). The final remark is that the only change comes from the Debye polynomial $v_1(t)$ which appears in two places instead of $u_1(t)$. The further calculation runs then in exactly the same way as in the Dirichlet case, but the result is different, namely, for the formula which corresponds to (68) we obtain

$$
\int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} \left(\sum_{0 \le i < j \le s} b(n_1, n_{i+1}, n_j, n_{j+1}) \right.
$$
$$
\left. + \sum_{i=0}^{s} d(n_i, n_{i+1}) \right) = \frac{7}{384\sqrt{2}} \frac{1}{(1+s)^3} - \frac{1}{12\sqrt{2}(s+1)}, \quad (79)
$$

i.e., we get a contribution which is the same as in the Dirichlet case and an additional contribution. Inserted into the energy this gives

$$E^{\text{cyl,N}}_{(3+1)} = \frac{-1}{2\pi L^2}\sqrt{\frac{R}{L}\frac{3\zeta(4)}{32\sqrt{2}}}\left\{1 + \left(\frac{7}{36} - \frac{8}{9}\frac{\zeta(2)}{\zeta(4)}\right)\frac{L}{R} + O\left(\left(\frac{L}{R}\right)^2\right)\right\},\tag{80}$$

a formula, which represents the first correction to the proximity force theorem for Neumann boundary conditions.

We note that the mentioned compensation of the signs ensures that the leading order contribution, i.e., the proximity force theorem, gives the same answer for both types of boundary conditions as expected. Less obvious is the behavior of the Neumann contribution in what it has in addition to the Dirichlet case (which equals the first term in the right-hand side of Eq. (79)). This is the second term in the right-hand side of Eq. (79), which results in a much less convergent sum over s. In the $(3 + 1)$ dimensional case the sum is still convergent, but in the $(2 + 1)$ dimensional case not. Carrying out the corresponding calculation we obtain

$$\frac{1}{32\sqrt{2}(s + 1)^2} - \frac{1}{4\sqrt{2}}\tag{81}$$

in place of the right-hand side of Eq. (79). Now the sum over s is logarithmic divergent. In fact this implies that the correction to the proximity force theorem in $(2 + 1)$ dimensions for Neumann boundary conditions is proportional to $\frac{L}{R}\ln(L/R)$.

Finally we collect the energies for Dirichlet and Neumann boundary conditions together to the first correction to the proximity force theorem for the electromagnetic fields,

$$\begin{aligned}E^{\text{cyl,electromgn.}}_{(3+1)} &= \frac{-1}{2\pi L^2}\sqrt{\frac{R}{L}\frac{3\zeta(4)}{16\sqrt{2}}}\\&\quad\times\left\{1 + \left(\frac{7}{36} - \frac{4}{9}\frac{\zeta(2)}{\zeta(4)}\right)\frac{L}{R} + O\left(\left(\frac{L}{R}\right)^2\right)\right\}\\&= -\frac{1}{L^2}\sqrt{\frac{R}{L}\frac{\pi^3}{960\sqrt{2}}}\\&\quad\times\left\{1 + \underbrace{\left(\frac{7}{36} - \frac{20}{3\pi^2}\right)}_{=-0.48103}\frac{L}{R} + O\left(\left(\frac{L}{R}\right)^2\right)\right\}.\end{aligned}\tag{82}$$

V. SPHERE AND CYLINDER AT LARGE SEPARATION FROM A PLANE

The limiting case of large separation between a sphere and a cylinder and a plane is known and we display it here for completeness. For a sphere the starting point is Eq. (32) with $A_{l,l'}$ given by Eq. (33). The main contribution comes from small ω and small orbital momenta. We substitute

$$\omega \rightarrow \frac{\omega}{2a}\tag{83}$$

and expand $A_{l,l'}$ for small R/a. simply by expanding the two Bessel functions in (33) which depend on r. The leading order is

$$A_{l,l'} = \delta_{l,0}\delta_{l',0}\frac{R}{2a}e^{-\omega} + \ldots.\tag{84}$$

Inserted into E, (32), this gives immediately the large distance limit

$$E = -\frac{r}{8\pi a^2}\left(1 + \frac{3}{4}\frac{R}{a} + O\left(\left(\frac{R}{a}\right)^2\right)\right),\tag{85}$$

where we included the first correction too (note $a = L + R$). This result agrees with [6].

The corresponding procedure for a cylinder is similar. We start from Eq. (43) or from Eq. (48) in dependence on the dimension and with $A_{m,m'}$ given by Eq. (44). Again, the dominating contribution comes from small momenta. We do the substitution (83) and expand $A_{m,m'}$. Here, however, a peculiarity shows up because of the logarithmic behavior of the Bessel function $K_m(\omega\frac{r}{2a})$ in the denominator for $m = 0$. The expansion is

$$A_{m,m'} = \frac{\delta_{m,0}\delta_{m',0}K_0(\omega)}{-\gamma - \ln(\omega R/4a)} + O\left(\left(\frac{R}{a}\right)^2\right),\tag{86}$$

where γ is Euler's constant. Inserting into (32) and integrating over ω we get

$$\begin{aligned}E^{\text{cyl}}_{(2+1)} &= \frac{\pi}{8a}\frac{1}{\ln(R/2a)}\left(1 - \frac{2\ln2}{\ln(R/2a)}\right.\\&\quad\left.+ O\left(\left(\frac{1}{\ln(R/2a)}\right)^2\right)\right) + O\left(\left(\frac{R}{a}\right)^2\right)\end{aligned}\tag{87}$$

and

$$\begin{aligned}E^{\text{cyl}}_{(3+1)} &= \frac{1}{8\pi a^2}\frac{1}{\ln(R/2a)}\left(1 - \frac{\pi^2/12}{(\ln(R/2a))^2}\right.\\&\quad\left.+ O\left(\left(\frac{1}{\ln(R/2a)}\right)^3\right)\right) + O\left(\left(\frac{R}{a}\right)^2\right).\end{aligned}\tag{88}$$

In the $(3 + 1)$-dimensional case the next-to-leading order is zero.

We note that the logarithmic behavior of the large distance limit is related to the corresponding behavior of the Greens function in two dimensions. Because the logarithmic behavior is present in $E^{\text{cyl}}_{(2+1)}$, i.e., for a circle on a plane, it seems unlikely that it is related to the length of the cylinder as discussed for the three dimensional case in [7].

VI. CONCLUSIONS

In the foregoing sections we showed the derivation of the expression for the Casimir energy in terms of the determinant of the projection $K(z, z')$ of the free space propagator on the boundary surface S which was known from [9,10] and independently rederived and applied to the calculation at large distance in [6,7] which can be considered as a significant progress because it opened the way for

direct numerical calculation of the Casimir force for non-simple geometries. In the present paper we showed that also the short distance behavior can be calculated by this method and derived the first corrections to the force proximity theorem including the electromagnetic case. In $(3 + 1)$ dimensions the corrections are power like, in $(2 + 1)$ dimensions the corrections contain a logarithm for Neumann conditions.

In general, corrections to the limiting behavior for both large and small distances, can be calculated as expansion in the corresponding small parameter. These expansions are asymptotic ones. For the small distance behavior this is clear from Sec. IV where we substituted the sums over the orbital momenta of the photon propagator by the corresponding integrals. Obviously, exponentially small contributions are neglected in this way. For the long distance expansion this follows from the denominators in the corresponding matrix elements, (33) and (44). Consider the energy as a function of the expansion parameter $\delta = r/2a$ (after the rescaling (83)) in the complex plane of δ. Consider a movement of δ encircling the origin. At some time pole of the integrand will cross the path of the integration over ω causing an additional contribution. Hence, the energy as a function of δ has a cut starting from $\delta = 0$.

The new method for the Casimir force for nonsimple geometry which so far gave the possibility to calculate the large and the small distance behavior, has the potential in it for the calculation of the Casimir force at all distances with desired precision. Also, it obviously can be generalized to much more boundary conditions than Dirichlet or Neumann ones. In the present paper we considered primarily Dirichlet conditions in order to keep the representation as simple as possible. The generalizations to Neumann are obvious, one has to change the sign in (16) and to add a derivative to $H(x, z)$, Eq. (6) as done, for example, in [7]. In the path integral approach this was considered from a more general point of view in [11].

The short distance expansion in Sec. IV sheds light also on the quasi classic, optical path and similar approximations. Indeed, the dominating contributions come solely from large momentum, however in an expansion over the number of reflections, like the expansion of the logarithm in Sec. IV shows, all terms contribute. Therefore, in order to get some approximation, say in the first order of the small parameter, all reflections must be included.

ACKNOWLEDGMENTS

Note added.—Since the submission of this paper, Gies and Klingmüller [12] confirmed the correction factor 7/36 in Eq. (69) for Dirichlet boundary conditions in the cylinder-plane geometry by numerical world line methods.

APPENDIX A

In this appendix we show the calculation of the matrix elements (30) and (42) in Sec. III. We start with the cylindrical case. Using (40) we represent the matrix element in (42) in the form

$$W_{m,m'} \equiv \langle m \mid D_\omega^{(2+1)}(\tilde{x} - x') \mid m' \rangle$$

$$= \int \frac{d^2k}{(2\pi)^2} \frac{e^{2iak_2}}{\omega^2 + k^2} f_m(\tilde{k}) f_m^*(k) \qquad \text{(A1)}$$

with

$$f_m(k) = \int_0^{2\pi} \frac{d\varphi}{\sqrt{2\pi}} e^{-im\varphi + ikx}. \qquad \text{(A2)}$$

Here we used $\tilde{x} = (x_1, 2a - x_2)$ and defined $\tilde{k} = (k_1, -k_2)$ in order to rewrite $k(\tilde{x} - x') = 2ak_2 + \tilde{k}x - kx'$. Using polar coordinates in the k-plane, $k_1 = k \sin\varphi_k$, $k_2 = k \cos\varphi_k$, and an integral representation

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-im\varphi + iz\sin\varphi} = J_m(z) \qquad \text{(A3)}$$

of the Bessel function $J_m(z)$ for the functions $f_m(k)$ entering (A1) we obtain

$$W_{m,m'} = \int \frac{d^2k}{2\pi} \frac{e^{2iak_2}}{\omega^2 + k^2} J_m(kr) J_{m'}(kr) e^{-i(m+m')\varphi_k}. \qquad \text{(A4)}$$

The formula (A3) can also be used for the integration over the angle φ_k,

$$W_{m,m'} = \int_0^\infty \frac{dk k}{\omega^2 + k^2} J_m(kr) J_{m'}(kr) J_{m+m'}(2ka). \qquad \text{(A5)}$$

The last integration can be done by extending it over the whole k axis and closing the contour picking up the pole in $k = i\omega$. With the relations $J_m(z) = \frac{1}{2}(H_m^{(1)}(z) + H_m^{(2)}(z))$, $H_m^{(1)}(-z) = (-1)^{m+1} H_m^{(2)}(z)$, $J_m(-z) = (-1)^m J_m(z)$ one obtains

$$W_{m,m'} = \frac{i\pi}{2} J_m(i\omega r) J_{m'}(i\omega r) H_{m+m'}^{(1)}(2i\omega a), \qquad \text{(A6)}$$

or in terms of the modified Bessel functions,

$$W_{m,m'} = I_m(\omega r) I_{m'}(\omega r) K_{m+m'}(2\omega a), \qquad \text{(A7)}$$

which after division by $d_m^{(2+1)}(r, r)$, (38), gives (44).

Now we turn to the spherical case and consider the matrix elements in (30). Using (21) we represent them in the form

$$D_{l,l'} \equiv \langle lm \mid D_\omega(x - \tilde{x}) \mid l'm \rangle$$

$$= \int \frac{d^3k}{(2\pi)^3} \frac{e^{-2iak_3}}{\omega^2 + k^2} f_{lm}^*(k) f_{l'm}(\tilde{k}) \qquad \text{(A8)}$$

with $\tilde{k} = (k_1, k_2, -k_3)$ and

$$f_{lm}(k) \equiv e^{-ikx} \mid lm \rangle = \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi e^{-ikx} Y_{lm}(\theta, \varphi)$$
$$= 4\pi(-i)^l j_l(kr) Y_{lm}(\theta_k, \varphi_k), \qquad (A9)$$

whereby in the last line the decomposition of a plane wave into spherical waves,

$$e^{ikz} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\theta_z, \varphi_z) Y_{lm}(\theta_k, \varphi_k), \qquad (A10)$$

was used. Here, $j_l(z)$ are the spherical Bessel functions. Writing the integration over k in spherical coordinates and using again (A10) an integral over a product of three hypergeometric functions appears which can be written in terms of $3j$-symbols,

$$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi Y_{lm}(\theta, \varphi) Y_{l'm'}(\theta, \varphi) Y_{l''m''}(\theta, \varphi)$$
$$= \sqrt{\frac{(2l+1)(2l'+1)(2l''+1)}{4\pi}} \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & l'' \\ m & m' & m'' \end{pmatrix}$$
$$(A11)$$

and we arrive at

$$D_{l,l'} = \frac{2}{\pi} \sqrt{(2l+1)(2l'+1)} \int_0^\infty \frac{dk k^2}{\omega^2 + k^2} j_l(kr) j_{l'}(kr)$$
$$\cdot \sum_{l''=|l-l'|}^{l+l'} i^{l+l'-l''}(2l''+1) j_{l''}(2ak)$$
$$\times \begin{pmatrix} l'' & l & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'' & l & l' \\ 0 & -m & m \end{pmatrix}. \qquad (A12)$$

Using $j_l(z) = \frac{1}{2}(h_l^{(1)}(z) + h_l^{(2)}(z))$, the integration can be extended to the whole k axis and closed picking up the pole in $k = i\omega$. The result can be inserted into (30) and we obtain

$$A_{l,l'} = \sqrt{(2l+1)(2l'+1)} \frac{j_{l'}(ir\omega)}{h_l^{(1)}(ir\omega)} \cdot \sum_{l''=|l-l'|}^{l+l'} i^{l+l'-l''}(2l''+1)$$
$$\times h_{l''}^{(1)}(2ia\omega) \begin{pmatrix} l'' & l & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'' & l & l' \\ 0 & -m & m \end{pmatrix} \qquad (A13)$$

which coincides with the corresponding formula in [6]. Passing now to the modified Bessel functions and dividing by $d_l(r, r)$, (25), we obtain just formula (33).

APPENDIX B

In this appendix we calculate the uniform asymptotic expansion of $A_{m,m'}(\omega)$, Eq. (46), using (B1) and obtain $A_{m,m'}^{as}$, Eq. (56), and the coefficients $a_{n,n'}^{(1/2)}(t, \tau)$ and $a_{n,n'}^{(1)}(t, \tau)$ therein.

We remind the uniform asymptotic expansion of the Bessel functions,

$$\begin{Bmatrix} I_m(mz) \\ K_m(mz) \end{Bmatrix} = \frac{\pi^{\mp(1/2)}}{\sqrt{2m}} \frac{\exp(\pm m\eta(z))}{(1+z^2)^{1/4}} \left(1 \pm \frac{u_1(t)}{m} + \dots\right) \qquad (B1)$$

with $\eta(z) = \sqrt{1+z^2} + \ln(z/(1+\sqrt{1+z^2}))$ and $u_1(t) = (3t - 5t^3)/24$ with $t = 1/\sqrt{1+z^2}$, the first of the Debye polynomials. Since we intend to calculate the first next-to-leading order only the restriction to $u_1(t)$ is sufficient.

We start with the exponential factor and do the substitution (53) there. Up to order ϵ we get

$$\tilde\eta = 2t + (n - n')^2 + \sqrt{\frac{\epsilon}{t}} \tau(2t - (n - n')^2)(n + n')$$
$$+ \epsilon\left(-\tau^2 + \frac{1-\tau^2}{t}(n + n')^2\right.$$
$$\left. - \frac{1-3\tau^2}{12t^2}((n - n')^4 + 6(n^2 - n'^2)^2)\right). \qquad (B2)$$

The expansion of the exponential is

$$e^{-\tilde\eta} = e^{-\eta_0}(1 + \sqrt{\epsilon}\eta_{n,n'}^{(1/2)} + \epsilon\eta_{n,n'}^{(1)} + O)\epsilon^2)) \qquad (B3)$$

with

$$\eta_{n,n'}^{(1/2)} = -\frac{1}{\sqrt{t}}\tau(2t - (n - n')^2)(n + n'). \qquad (B4)$$

and

$$\eta_{n,n'}^{(1)} = -t\tau^2 + (1 - \tau^2)(n + n')^2 - \frac{1-3\tau^2}{12t}(n - n')^2$$
$$\times (7n^2 + 10nn' + 7n'^2). \qquad (B5)$$

Next we consider the factors in front of the exponential in $A_{n,n'}^{as}$. From (46) and (B1) they collect into

$$C_{m,m'} = \frac{1}{\sqrt{2\pi}}\left(\frac{m}{m'}\frac{1}{m+m'}\right)^{1/2}\left(\frac{1+z_1^2}{1+z_2^2}\frac{1}{1+z_3^2}\right)^{1/4} \qquad (B6)$$

with $z_1 = \omega/m$, $z_2 = \omega/m'$ and $z_1 = 2\omega(1+\epsilon)/(m+m')$. Here, again, we do the substitution (53) and the expansion for small ϵ gives

$$C_{m,m'} \rightarrow c_{m,m'} = \sqrt{\frac{\epsilon}{4\pi t}}(1 + \sqrt{\epsilon}c_{n,n}^{(1/2)} + \epsilon c_{n,n'}^{(1)} + \dots) \qquad (B7)$$

with

$$c_{n,n'}^{(1/2)} = \frac{\tau}{2\sqrt{t}}(n - 3n') \qquad (B8)$$

and

$$c_{n,n'}^{(1)} = \frac{-1+\tau^2}{2} + \frac{1}{8t}(6n^2 - 4nn' - 10n'^2$$
$$+ (-11n^2 + 2nn' + 29n'^2)\tau^2). \qquad (B9)$$

We note hat these contributions are not symmetric under $n \leftrightarrow n'$.

Finally we have to consider the contributions from the Debye polynomials. To the given order we note

$$D = \frac{1 + \frac{u_1(t_1)}{m} + \dots}{1 - \frac{u_1(t_2)}{m'} + \dots} \left(1 - \frac{u_1(t_3)}{m + m'} + \dots \right) \quad \text{(B10)}$$

with $t_i = \sqrt{1 + z_i^2}$. Doing here the substitution (53) we obtain

$$D \to 1 + \epsilon d^{(1)} + \dots \quad \text{(B11)}$$

with

$$d^{(1)} = \frac{3 - 5\tau^2}{16t}. \quad \text{(B12)}$$

Taking (B3), (B7), and (B11) together and reexpanding again we obtain finally for $a_{n,n'}^{(1/2)}(t, \tau)$ and $a_{n,n'}^{(1)}(t, \tau)$ in Eq. (56)

$$a_{n,n'}^{(1/2)}(t, \tau) = \frac{(n - 3n' + 2(n + n')(n^2 - 2n'n + n'^2 - 2t))\tau}{2\sqrt{t}},$$

$$a_{n,n'}^{(1)}(t, \tau) = \frac{(n - 3n')(n + n')(n^2 - 2n'n + n'^2 - 2t)\tau^2}{2t} + \frac{3 - 5\tau^2}{16t} + \frac{1}{8t}[(6 - 11\tau^2)n^2 + 2n'(\tau^2 - 2)n + 4t(\tau^2 - 1)$$

$$+ n'^2(29\tau^2 - 10)] + \frac{1}{12t}[-7(3\tau^2 - 1)n^4 + 4n'(3\tau^2 - 1)n^3 + 6((3\tau^2 - 1)n'^2 + 2t(\tau^2 - 1))n^2$$

$$+ 4nn'((3\tau^2 - 1)n'^2 + 6t(\tau^2 - 1)) + 6(n + n')^2(n^2 - 2n'n + n'^2 - 2t)^2\tau^2 + 12t^2\tau^2 + 12n'^2t(\tau^2 - 1)$$

$$- 7n'^4(3\tau^2 - 1)]. \quad \text{(B13)}$$

At the end of this appendix we display the explicit forms of the functions b, (63), and d, (64), introduced in Eq. (62):

$$b(x, y, z, w) = \frac{1}{384\sqrt{2}(s + 1)^{7/2}}[4(s + 1)(4(s + 1)x^3 - 4(s + 1)yx^2 + 2(-2(s + 1)y^2 + s - 2)x + y(4(s + 1)y^2$$

$$- 6(s + 1) - 6))w^3 + 4(s + 1)(-4(s + 1)x^3 + 4(s + 1)yx^2 + (4(s + 1)y^2 - 2(s + 1) + 6)x$$

$$+ y(-4(s + 1)y^2 + 6(s + 1) + 6))zw^2 + (-4(s + 1)(2(s + 1)(2z^2 + 3) + 6)x^3$$

$$+ 4(s + 1)y(2(s + 1)(2z^2 + 3) + 6)x^2 + (4(2y^2 - 1)(2z^2 + 3)(s + 1)^2 + 24(y^2 + z^2 + 1)(s + 1) + 60)x$$

$$+ y(-4(2y^2 - 3)(2z^2 + 3)(s + 1)^2 - 24(y^2 - z^2 - 3)(s + 1) + 60))w + z(8(s + 1)(2sz^2 + 2z^2 + s - 2)x^3$$

$$- 8(s + 1)y(2sz^2 + 2z^2 + s - 2)x^2 + (-4(2y^2 - 1)(2z^2 + 1)(s + 1)^2 + 24(y^2 - z^2 - 1)(s + 1) + 60)x$$

$$+ y(4(2y^2 - 3)(2z^2 + 1)(s + 1)^2 - 24(y^2 + z^2 - 1)(s + 1) + 60))], \quad \text{(B14)}$$

$$d(x, y) = \frac{1}{384\sqrt{2}(s + 1)^{7/2}}[8(s + 1)^2x^6 - 16(s + 1)^2yx^5 - 8(s + 1)((s + 1)y^2 - s + 2)x^4 + 32(s + 1)^2y(y^2 - 1)x^3$$

$$- 2(4(s + 1)^2y^4 - 8(s + 1)(s + 4)y^2 + (4 - 7s)s - 4)x^2 + 4y(-4(s + 1)^2y^4 + 8(s + 1)^2y^2 - s(5s + 16) + 4)x$$

$$+ 8(s + 1)^2y^6 - 24(s + 1)(s + 2)y^4 + (40 - 2(s - 4)s)y^2 + 4(s - 1)s + 7]. \quad \text{(B15)}$$

APPENDIX C

In this appendix we calculate the integrals over the n_i's in Eq. (62). As mentioned in the text all these integrations are Gaussian and we are left with the corresponding combinatorics.

We note that a number of these integrations can be carried out independently of the functions $b(n_i, n_{i+1}, n_j, n_{j+1})$ and $d(n_i, n_{i+1})$ entering (62). In the following we divide the whole expression into a number of pieces and in each we first perform these integrations. The remaining ones, one to four in number, depend on the

details of these functions. They have been performed machined.

We start with the part involving $d(n_i, n_{i+1})$, (64), in (62). It is easier because it contains only one sum. First we separate the first and the last contributions to this sum,

$$\sum_{i=0}^{s} d(n_i, n_{i+1}) = d(0, n_1) + d(n_s, 0) + \sum_{i=1}^{s-1} d(n_i, n_{i+1}). \quad \text{(C1)}$$

Renaming the n_i's by numbering them in the reverse order

in the first term in the right-hand side we have

$$S_1 \equiv \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} (d(0, n_1) + d(n_s, 0)) e^{-\eta_1}$$

$$= \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} (d(0, n_s) + d(n_s, 0)) e^{-\eta_1}.$$

$$(C2)$$

Now we apply formula (65). However, in order to avoid confusion with the notations we rewrite it,

$$m_1^2 + \sum_{i=1}^{s-1} (m_i - m_{i+1})^2 + m_u^2$$

$$= \frac{2}{1} \left(m_1 - \frac{2}{1} m_2 \right)^2 + \frac{3}{2} \left(m_2 - \frac{3}{2} m_3 \right)^2 + \dots$$

$$+ \frac{u}{u-1} \left(m_{u-1} - \frac{u-1}{u} m_u \right)^2 + \frac{u+1}{u} m_u^2. \quad (C3)$$

With $u = s - 1$, $m_1 = n_1, \dots, m_u = n_{s-1}$ the first $(s - 1)$ integrations can be carried out, one by one. The first is that over n_1, which must be shifted, $n_1 \to n_1 + \frac{2}{1} n_2$ and gives just $(\frac{1}{2})^{1/2} \sqrt{\pi}$. The second integrations needs the shift $n_2 \to n_2 + \frac{3}{2} n_3$ and gives $(\frac{2}{3})^{1/2} \sqrt{\pi}$ and so on. The shifts of the variables which do not enter the functions d (and, below, b) are obvious and we do not mention them in the following. Finally, renaming $n_s = x$ we obtain

$$S_1 = \frac{1}{\sqrt{s+1}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} (d(0, x) + d(x, 0))$$

$$\times \exp\left(-\frac{s+1}{s} x^2 \right). \quad (C4)$$

The last integration was carried out machined (like the similar ones below) and the result reads

$$S_1 = \frac{1}{12\sqrt{2}(s+1)^2} - \frac{3}{8\sqrt{2}(s+1)^3} + \frac{37}{64\sqrt{2}(s+1)^4}$$

$$- \frac{1}{4\sqrt{2}(s+1)^5}. \quad (C5)$$

Next we calculate the contribution from the sum over i in (C1). To this end we represent η_1 in the form

$$\eta_1 = n_1^2 + (n_1 - n_2)^2 + \dots + (n_{i-1} - n_i)^2 + n_i^2 - n_i^2$$

$$+ (n_i - n_{i+1})^2 - n_{i+1}^2 + n_{i+1}^2 + (n_{i+1} - n_{i+2})^2$$

$$+ \dots + n_s^2 \quad (C6)$$

and apply (C3) to $n_1, \dots, n_i$ with $u = i$ and $m_1 = n_1, \dots, m_u = n_i$ and to $n_{i+1}, \dots, n_s$ with $u = s - i$ and $m_1 = n_s, \dots, m_u = n_{i+1}$ so that it takes the form

$$\eta_1 = \frac{2}{1} \left(n_1 - \frac{1}{2} n_2 \right)^2 + \dots + \frac{i}{i-1} \left(n_{i-1} - \frac{i-1}{i} n_i \right)^2$$

$$+ \frac{2}{1} \left(n_s - \frac{s-1}{2} n_2 \right)^2 + \dots$$

$$+ \frac{s-i}{s-i-1} \left(n_{i+2} - \frac{s-i-1}{s-i} n_{i+1} \right)^2$$

$$+ \frac{s-i+1}{s-i} n_{i+1}^2 + \frac{i+1}{i} \left(n_i - \frac{i}{i+1} n_{i+1} \right)^2$$

$$+ \frac{s+1}{(i+1)(s-i)} n_{i+1}^2. \quad (C7)$$

With this formula the integrations over $n_1, \dots, n_i$ and over $n_{i+1}, \dots, n_s$ can be done and renaming $n_i = x$ and $n_{i+1} = y$ we obtain

$$S_2 \equiv \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} \sum_{i=1}^{s-1} d(n_i, n_{i+1}) e^{-\eta_1}$$

$$= \sum_{i=1}^{s-1} \frac{1}{\sqrt{i(s-i)}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} d(x, y)$$

$$\cdot \exp\left(-\frac{i+1}{i} \left(x - \frac{i}{i+1} y \right)^2 - \frac{s+1}{(i+1)(s-i)} y^2 \right). \quad (C8)$$

The last two integrations and the sum over i give

$$S_2 = -\frac{1}{16\sqrt{2}(s+1)^2} + \frac{127}{384\sqrt{2}(s+1)^3} - \frac{103}{192\sqrt{2}(s+1)^4}$$

$$+ \frac{1}{4\sqrt{2}(s+1)^5}. \quad (C9)$$

Taken together the expressions simplify to some extend,

$$S_1 + S_2 = \frac{1}{48\sqrt{2}(s+1)^2} - \frac{17}{384\sqrt{2}(s+1)^3}$$

$$+ \frac{1}{24\sqrt{2}(s+1)^4}. \quad (C10)$$

Now we calculate the contributions of the double sum in (62). Again we separate the first and the last terms,

$$S_3 = \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} \sum_{0 \le i < j \le s} b(n_i, n_{i+1}, n_j, n_{j+1})$$

$$= \int_{-\infty}^{\infty} \frac{dn_1}{\sqrt{\pi}} \cdots \int_{-\infty}^{\infty} \frac{dn_s}{\sqrt{\pi}} (b(0, n_1, n_s, 0)$$

$$+ \sum_{0 < j < s} b(0, n_1, n_j, n_{j+1}) + \sum_{0 < i < s} b(n_i, n_{i+1}, n_s, 0)$$

$$+ \sum_{0 < i < j < s} b(n_i, n_{i+1}, n_j, n_{j+1}))$$

$$\equiv S_{3,1} + S_{3,2} + S_{3,3} + S_{3,4}. \quad (C11)$$

For $S_{3,1}$ we rewrite η_1 in the form

$$\eta_1 = n_1^2 + (n_2 - n_1)^2 + (n_2 - n_1 - (n_3 - n_1))^2 + \ldots$$
$$+ (n_{s-1} - n_1 - (n_s - n_1))^2 + (n_s - n_1)^2$$
$$- (n_s - n_1)^2 + n_s^2 \tag{C12}$$

and apply (C3) with $u = s - 1$, $m_1 = n_2 - n_1, \ldots, m_u = n_s - n_1$,

$$\eta_1 = \frac{2}{1}\left(n_2 - n_1 - \frac{1}{2}(n_3 - n_1)\right)^2 + \ldots$$
$$+ \frac{s-1}{s-2}\left(n_{s-1} - n_1 - \frac{s-2}{s-1}(n_s - n_1)\right)^2$$
$$+ \frac{s}{s-1}\left(n_1 - \frac{1}{s}n_s\right)^2 + \frac{s+1}{s}n_s^2. \tag{C13}$$

After integration over $n_2, \ldots, n_{s-1}$ and renaming $n_1 = x$ and $n_s = y$ we have

$$S_{3,1} = \frac{1}{\sqrt{s-1}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} d(0, x, y, 0)$$
$$\cdot \exp\left(-\frac{s}{s-1}\left(x - \frac{1}{s}y\right)^2 - \frac{s+1}{s}y^2\right). \tag{C14}$$

The last two integrations give

$$S_{3,1} = -\frac{s-1}{8\sqrt{2}(s+1)^5}. \tag{C15}$$

For $S_{3,2}$ we rewrite η_1 in the form

$$\eta_1 = n_1^2 + (n_1 - n_2)^2 + \ldots + (n_{i-1} - n_i)^2 + n_i^2 - n_i^2$$
$$+ (n_i - n_{i+1})^2 - (n_{i+1} - n_s)^2 + (n_{i+1} - n_s)^2$$
$$+ (n_{i+1} - n_s - (n_{i+2} - n_s))^2 + \ldots$$
$$+ (n_{s-2} - n_s - (n_{s-1} - n_s))^2 + (n_{s-1} - n_s)^2 + n_s^2 \tag{C16}$$

and apply (C3) to $n_1, \ldots, n_i$ with $u = i$, $m_1 = n_1, \ldots, m_u = n_i$ and to $n_{i+1} - n_s, \ldots, n_{s-1} - n_s$ with $u = s - i - 1$ and $m_1 = n_{i+1} - n_s, \ldots, m_u = n_{s-1} - n_s$ so that η_1 takes the form

$$\eta_1 = \frac{2}{1}\left(n_1 - \frac{1}{2}n_2\right)^2 + \ldots + \frac{i}{i-1}\left(n_{i-1} - \frac{i-1}{i}n_i\right)^2$$
$$+ \frac{2}{1}\left(n_{s-1} - n_s - \frac{1}{2}(n_{s-2} - n_s)\right)^2 + \ldots$$
$$+ \frac{s-i-1}{s-i-2}\left(n_{i+2} - n_s - \frac{s-i-2}{s-i-1}(n_{i+1} - n_s)\right)^2$$
$$+ \frac{i+1}{i}\left(n_i - \frac{i}{i+1}n_{i+1}\right)^2 + \frac{s}{(s-i-1)(i+1)}$$
$$\times \left(n_{i+1} - \frac{i+1}{s}n_s\right)^2 + \frac{s+1}{s}n_s^2. \tag{C17}$$

After integration over $n_1, \ldots, n_{i-1}$ and $n_{i+1}, \ldots, n_{s-1}$ and

renaming $n_1 = x$, $n_{i+1} = y$ and $n_s = z$ we have

$$S_{3,2} = \sum_{i=1}^{s-1} \frac{1}{\sqrt{i(s-i-1)}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}}$$
$$\times \int_{-\infty}^{\infty} \frac{dz}{\sqrt{\pi}} d(x, y, z, 0) \cdot \exp\left(-\frac{i+1}{i}\left(x - \frac{i}{i+1}y\right)^2\right.$$
$$\left. - \frac{s}{(s-i-1)(i+1)}\left(y - \frac{i+1}{s}z\right)^2 - \frac{s+1}{s}z^2\right). \tag{C18}$$

The last three integrations and the sum give

$$S_{3,2} = -\frac{s-1}{8\sqrt{2}(s+1)^4}. \tag{C19}$$

In the same way we calculate $S_{3,3}$. Here we rewrite η_1 in the form

$$\eta_1 = n_1^2 + (n_2 - n_1)^2 + (n_2 - n_1 - (n_3 - n_1))^2 \ldots$$
$$+ (n_{j-1} - n_1 - (n_j - n_1))^2 + (n_j - n_1)^2 +$$
$$- (n_j - n_1)^2 + (n_j - n_{j+1})^2 - n_{j+1}^2 + n_{j+1}^2$$
$$+ (n_{j+1} - n_{j+2})^2 + \ldots + n_s^2 \tag{C20}$$

and apply (C3) to $n_2, \ldots, n_{j-1}$ with $u = j - 1$, $m_1 = n_2 - n_1, \ldots, m_u = n_{j-1} - n_1$ and to $n_{j+1}, \ldots, n_s$ with $u = s - j$ and $m_1 = n_s, \ldots, m_u = n_{j+1}$ so that η_1 takes the form

$$\eta_1 = \frac{2}{1}\left(n_2 - n_1 - \frac{1}{2}(n_3 - n_1)\right)^2 + \ldots$$
$$+ \frac{j-1}{j-2}\left(n_{j-1} - n_1 - \frac{j-2}{j-1}(n_j - n_1)\right)^2$$
$$+ \frac{2}{1}\left(n_s - \frac{1}{2}n_{s-1}\right)^2 + \ldots$$
$$+ \frac{s-j}{s-j-1}\left(n_{j+2} - \frac{s-j-1}{s-j}n_{j+1}\right)^2 \tag{C21}$$

After integration over $n_2, \ldots, n_{j-1}$ and over $n_{j+2}, \ldots, n_s$ and renaming $n_1 = x$, $n_j = y$ and $n_s = z$ we have

$$S_{3,2} = \sum_{j=1}^{s-1} \frac{1}{\sqrt{(j-1)(s-j)}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}}$$
$$\times \int_{-\infty}^{\infty} \frac{dz}{\sqrt{\pi}} d(0, x, y, z) \cdot \exp\left(-\frac{s+1}{is}x^2\right.$$
$$- \frac{s}{(s-j+1)(j-1)}\left(y - \frac{s-j+1}{s}x\right)^2$$
$$\left. - \frac{s-j+1}{s-j}z^2\right). \tag{C22}$$

The last three integrations and the sum give

$$S_{3,3} = -\frac{(s-1)^2}{8\sqrt{2}(s+1)^4}.$$ (C23)

The last step is $S_{3,4}$, which in fact contains the double sum. Here we represent η_1 in the form

$$\eta_1 = n_1^2 + (n_1 - n_2)^2 + \ldots + (n_{i-1} - n_i)^2 + n_i^2 - n_i^2 + (n_i - n_{i+1})^2 + (n_{i+2} - n_{i+1})^2 + (n_{i+2} - n_{i+1} - (n_{i+3} - n_{i+1}))^2 + \ldots$$
$$+ (n_{j-1} - n_{i+1} - (n_j - n_{i+1}))^2 + (n_j - n_{i+1})^2 - (n_j - n_{i+1})^2 + (n_j - n_{j+1})^2 - n_{j+1}^2 + n_{j+1}^2 + (n_{j+1} - n_{j+2}))^2$$
$$+ \ldots + n_s^2.$$ (C24)

We apply (C3) 3 times, first, with $u = i$ and $m_1 = n_1, \ldots, m_u = n_i$, second, with $u = j - i - 1$ and $m_1 = n_{i+2} - n_{i+1}, \ldots, m_u = n_j - n_{i+1}$, and, third, with $u = s - j$ and $m_1 = n_s, \ldots, m_u = n_{j+1}$. So we write η_1 in the form

$$\eta_1 = \frac{2}{1}\left(n_1 - \frac{1}{2}n_2\right)^2 + \ldots + \frac{i}{i-1}\left(n_{i-1} - \frac{i-1}{i}n_i\right)^2 + \frac{2}{1}\left(n_{i+2} - n_{i+1} - \frac{1}{2}(n_{i+3} - n_{i+1})\right)^2 + \ldots$$
$$+ \frac{j-i-1}{j-i-2}\left(n_{j-1} - n_{i+1} - \frac{j-i-2}{j-i-1}(n_j - n_{i+2})\right)^2 + \frac{2}{1}\left(n_s - \frac{1}{2}n_{s-1}\right)^2 + \ldots + \frac{s-j}{s-j-1}\left(n_{j+2} - \frac{s-j-1}{s-j}n_{j+1}\right)^2$$
$$+ \frac{i+1}{i}\left(n_i - \frac{i}{i+1}n_{i+1}\right)^2 + \frac{j}{(i+1)(j-i-1)}\left(n_{i+1} - \frac{i+1}{j}n_j\right)^2 + \frac{s+1}{j(s-j+1)}n_j^2$$
$$+ \frac{s-j+1}{s-j}\left(n_{j+1} - \frac{s-j}{s-j+1}n_j\right)^2.$$ (C25)

All integration except for four, whose variables we rename for $n_i = x$, $n_{i+1} = y$, $n_j = z$ and $n_{j+1} = w$, can be done,

$$S_{3,4} = \sum_{0<i<j<s} \frac{1}{\sqrt{(j-i-1)(s-j)i}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dz}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{dw}{\sqrt{\pi}} d(x,y,z,w) \cdot \exp\left[-\frac{i+1}{i}\left(x - \frac{i}{i+1}y\right)^2 \right.$$
$$\left. - \frac{j}{(j-i+1)(i+1)}\left(y - \frac{i+1}{j}z\right)^2 - \frac{s+1}{(s-j+1)j}z^2 - \frac{s-j+1}{s-j}\left(w - \frac{s-j}{s-j+1}z\right)^2 \right].$$ (C26)

The last integrations give

$$S_{3,4} = -\sum_{0<i<j<s} \frac{(2i+1)(4j-3s-1)}{8\sqrt{2}(s+1)^5}$$ (C27)

and after the summations over i and j

$$S_{3,4} = \frac{(s-2)(s-1)(5s+3)}{48\sqrt{2}(s+1)^5}.$$ (C28)

Together we get for S_3, (C11),

$$S_3 = -\frac{(s-1)s}{48\sqrt{2}(s+1)^4}.$$ (C29)

Collecting together all parts we obtain finally

$$S_1 + S_2 + S_3 = \frac{7}{384\sqrt{2}(s+1)^3},$$ (C30)

which is the result quoted in Eq. (68).

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