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Casimir force for a sphere in front of a plane beyond proximity force approximation

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Abstract
For the configuration of a sphere in front of a plane, we calculate the first two terms of the asymptotic expansion for small separation of the Casimir force. We consider both Dirichlet and Neumann boundary conditions.

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1. Introduction and discussion

High precision measurements of the Casimir force are of remarkable actual interest. For instance, these measurements provide stronger constraints on hypothetical interactions in the sub-micrometer region [1] and give hope to measure thermal forces. The high precision is achieved in a setup where the force between a flat plate and a sphere is measured. The typical radius of the sphere is $R \approx 200\ \mu$m (although recently [2] a sphere with $R \approx 80\ \mu$m was used) and the separation ranges from contact till $L \approx 1\ \mu$m. This setup provides a large area of opposing surfaces avoiding difficulties of keeping the surfaces in parallel. The ratio of these two sizes,

$$\epsilon = \frac{L}{R} \sim 10^{-3}, \tag{1}$$

is a small parameter describing the deviation of the geometry from the plane parallel one.

The calculation of the Casimir force for arbitrarily shaped surfaces was a longstanding problem and one was left with unsatisfactory approximate methods. The most important of them is the proximity force approximation (PFA) known from [3]. The method takes the force density known from the plane parallel case and integrates it over the curved surface. Clearly, this method works only for small deviations and from the very setup it was impossible to get higher order corrections or information on the precision of the approximation. Nevertheless, the PFA worked remarkably well in the comparison of the precision measurements [2, 4] with the theoretical expectations. Along with this, from increasing the precision of the measurements there appears a call to go beyond [2].

The evaluation of the Casimir force is in general plagued by ultraviolet divergences. This is the case even for the force between distinct bodies despite its finiteness. The point is that divergences are present in intermediate steps. One has to introduce some regularization, say in a mode sum representation, to subtract the divergent terms (even if these do not depend on the separation) and to perform the limit of removing the regularization. This procedure works well in simple geometries with separate variables in the corresponding wave equation. However, for a more general geometry, where one would have to calculate eigenvalues numerically, this hampers the calculations quite a lot.

There exist approximate methods which give important results. For instance, the semiclassical approximation in [5, 6] has put the PFA on a solid base within quantum field theory. Also the optical path approximation [7] was very important in this context, since it also confirmed the leading-order PFA from a field-theory perspective and gave somewhat better results at next-to-leading order. The so-called 'worldline methods' played an exceptional role [8], where a functional integral representation of the Green function is computed numerically. Regrettably, this method is restricted to Dirichlet boundary conditions.

Progress happened recently with the representation of the Casimir interaction energy between two bodies in terms of a functional determinant which is free of ultraviolet divergences [9, 10]. For any fixed distance between the bodies, the energy is represented by multiple convergent sums and integrals. These allow for direct numerical evaluation [9]. However, for small ϵ like the value in (1), the computations become too complex and are restricted to $\epsilon \gtrsim 0.1$.

A solution of this problem was found in [11], where the first correction beyond the PFA was calculated for a cylinder in front of a plane. Technically, an asymptotic expansion for small ϵ of the representation in terms of a functional determinant was derived. In the leading order, the PFA was reobtained and in the next-to-leading order the first correction beyond the PFA was calculated analytically. This was done for Dirichlet and for Neumann boundary conditions:

$$\begin{aligned} E^{\text{cyl}}_{\text{Dirichlet}} &= -\frac{1}{L^2}\sqrt{\frac{R}{L}}\frac{\pi^3}{1920\sqrt{2}}\left\{1+\frac{7}{36}\frac{L}{R}+O\left(\left(\frac{L}{R}\right)^2\right)\right\},\\ E^{\text{cyl}}_{\text{Neumann}} &= -\frac{1}{L^2}\sqrt{\frac{R}{L}}\frac{\pi^3}{1920\sqrt{2}}\left\{1+\left(\frac{7}{36}-\frac{40}{3\pi^2}\right)\frac{L}{R}+O\left(\left(\frac{L}{R}\right)^2\right)\right\}. \end{aligned} \tag{2}$$

The sum of these two, by virtue of the wave guide geometry, at once delivers the result for the electromagnetic case. It is remarkable that the result for the Dirichlet boundary conditions was confirmed with good precision by the worldline methods in [12].

In the present paper, we use the method developed in [11] to calculate the Casimir interaction energy for a sphere in front of a plane. We perform the calculation for Dirichlet and for Neumann boundary conditions. The result is

$$\begin{aligned} E^{\text{sphere}}_{\text{Dirichlet}} &= -\frac{\pi^3}{1440}\frac{R}{L^2}\left\{1+\frac{1}{3}\frac{L}{R}+O\left(\left(\frac{L}{R}\right)^2\right)\right\},\\ E^{\text{sphere}}_{\text{Neumann}} &= -\frac{\pi^3}{1440}\frac{R}{L^2}\left\{1+\left(\frac{1}{3}-\frac{10}{\pi^2}\right)\frac{L}{R}+O\left(\left(\frac{L}{R}\right)^2\right)\right\}. \end{aligned} \tag{3}$$

With these formulae, we reconfirm the PFA in leading order. In the next-to-leading order, we analytically obtained the first correction beyond the PFA. Again, as in the cylindrical case, the Dirichlet case is confirmed by the 'worldline methods' calculation in [12]. Since in this geometry the polarizations of the electromagnetic field do not separate, (3) does not include the result for the electromagnetic case which is left as a future work. A general approach for this was considered in [13] along with specific calculations of the Casimir interaction between spheres over a wide range of separations, including rather short distances. However, if we expect the corresponding result to be of the same order as (3) one can conclude that these corrections do not affect the current high precision measurements of the Casimir force but must be taken into account in the future ones.

In the remaining part of this paper, we follow [11] and represent the calculations resulting in (3). The essentially new element is a certain asymptotic expansion of the Clebsch–Gordan coefficients which was not found in the literature.

2. Asymptotic expansion of the Casimir energy for small separation

The expression of the Casimir energy for a sphere in front of a plane in terms of a convergent functional determinant is known from [9–11]. Here we use the notations adopted in [11]. The energy under consideration is given by

$$E = \frac{1}{2\pi}\int_0^\infty \mathrm{d}\omega\, \mathrm{tr}_{l,m} \ln(\delta_{l,l'} - A_{l,l'}). \tag{4}$$

Here, the trace is over the orbital momenta l and m in a representation in the orbital momentum basis of the matrix elements:

$$A_{l,l'} = \sqrt{\frac{\pi}{2}}\sqrt{\frac{(2l+1)(2l'+1)}{2a\omega}}(-1)^{l+l'}\frac{I_{l'+\frac{1}{2}}(\omega R)}{K_{l+\frac{1}{2}}(\omega R)} \times \sum_{l''=|l-l'|}^{l+l'} (-i)^{l''}(2l''+1)K_{l''+\frac{1}{2}}(2a\omega)\begin{pmatrix} l'' & l & l' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l'' & l & l' \\ 0 & -m & m\end{pmatrix}, \tag{5}$$

where I_ν and K_ν are modified Bessel functions, $a = L + R$ is the distance from the plane to the center of the sphere and the symbols in brackets are the $3j$-symbols. It is convenient for the following to expand the logarithm in (4):

$$E = \frac{1}{2\pi}\int_0^\infty \mathrm{d}\omega \sum_{s=0}^{\infty}\frac{-1}{s+1}\sum_{m=-\infty}^{\infty}\sum_{l=|m|}^{\infty}\sum_{l_1=|m|}^{\infty}\cdots\sum_{l_s=|m|}^{\infty} A_{l,l_1}A_{l_1,l_2}\cdots A_{l_s,l}. \tag{6}$$

For fixed R and a, the integral and all sums in this formula are convergent. With $\epsilon = L/R$, (1), we note $a = R(1+\epsilon)$ and for small ϵ the convergence gets lost. As for the frequency ω, this can be seen from the arguments of the Bessel functions. Using their asymptotic behavior for a large argument, $I_\nu(z) \sim \exp(z)$ and $K_\nu(z) \sim \exp(-z)$, the integrand in the matrix element behaves like $\exp(-2\omega\epsilon)$ and ceases to decrease for $\epsilon = 0$. Similar arguments hold for the sums involved. As a consequence, a simple expansion for small ϵ does not work.

Next, we rewrite equation (6) by making the substitution $\omega \to \omega/R$ and by changing the summation indices in the products of the matrix elements:

$$E = -\frac{1}{2\pi R}\sum_{s=0}^{\infty}\frac{1}{s+1}\int_0^\infty \mathrm{d}\omega \sum_{m=-\infty}^{\infty}\sum_{l=|m|}^{\infty}\sum_{l_1=-l}^{\infty}\cdots\sum_{l_s=-l}^{\infty} A_{l,l+l_1}A_{l+l_1,l+l_2}\cdots A_{l+l_s,l}. \tag{7}$$

The strategy of the calculation for small ϵ is as follows. We assume that the dominating contribution comes from the large values of the frequency ω and all summation indices involved in (7). We are interested in the asymptotic expansion for small ϵ; hence, we substitute all sums by integrations. The error introduced in this way is supposed to be exponentially small like in the difference between the sum and the integral in the Abel–Plana formula. After that, we substitute the variables in (7):

$$\omega = \frac{t}{\epsilon}\sqrt{1-\tau^2}, \qquad l = \frac{t\tau}{\epsilon}, \qquad m = \sqrt{\frac{t}{\epsilon}}\tau\mu$$
$$l_1 = \sqrt{\frac{4t}{\epsilon}}n_1, \ldots, l_s = \sqrt{\frac{4t}{\epsilon}}n_s, \tag{8}$$

manifesting that the main contributions come from $\omega \sim 1/\epsilon$, from the 'main diagonal' matrix index $l \sim 1/\epsilon$, from the 'off-diagonal directions' $l_i \sim 1/\sqrt{\epsilon}\,(i = 1, \ldots, s)$ and from the magnetic quantum number $m \sim 1/\sqrt{\epsilon}$. The variable τ is the cosine of the angle in the (ω, l)-plane. After this, we expand the matrix elements for $\epsilon \to 0$ and calculate the remaining integrals.

In the new variables, the expression for the energy reads

$$E \simeq -\frac{\epsilon^{-2}}{4\pi R}\sum_{s=0}^{\infty}\frac{1}{s+1}\int_0^{\infty}\mathrm{d}t\, t\int_0^1\frac{\mathrm{d}\tau\,\tau}{\sqrt{1-\tau^2}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\mu}{\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{\mathrm{d}n_1}{\sqrt{\pi}}\cdots\int_{-\infty}^{\infty}\frac{\mathrm{d}n_s}{\sqrt{\pi}}\mathcal{M}, \tag{9}$$

where

$$\mathcal{M} = \left(\frac{4\pi t}{\epsilon}\right)^{\frac{s+1}{2}} A_{l,l+l_1}\cdots A_{l+l_s,l} \tag{10}$$

collects the information from the matrix elements.

In appendix A, we calculate the asymptotic expansion of the matrix elements (5) for $\epsilon \to 0$ with the variables substituted according to equation (8). Using equation (A.20) obtained there, we get for the asymptotic expansion of the energy the expression

$$E \simeq -\frac{\epsilon^{-2}}{4\pi R}\sum_{s=0}^{\infty}\frac{1}{s+1}\int_0^{\infty}\mathrm{d}t\, t\,\mathrm{e}^{-2(s+1)t}\int_0^1\frac{\mathrm{d}\tau\,\tau}{\sqrt{1-\tau^2}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\mu}{\sqrt{\pi}}\,\mathrm{e}^{-(s+1)\mu^2}$$
$$\times\int_{-\infty}^{\infty}\frac{\mathrm{d}n_1}{\sqrt{\pi}}\cdots\int_{-\infty}^{\infty}\frac{\mathrm{d}n_s}{\sqrt{\pi}}\,\mathrm{e}^{-\eta_1}\mathcal{M}_{as} \tag{11}$$

with

$$\eta_1 = \sum_{i=0}^{s}(n_i - n_{i+1})^2\,. \tag{12}$$

Here, we have to formally put $n_0 = n_{s+1} = 0$. The non-leading information is contained in

$$\mathcal{M}^{\mathrm{as}} = 1 + \sqrt{\epsilon}\sum_{i=0}^{s}a^{(1/2)}_{n_i,n_{i+1}} + \epsilon\left(\sum_{0\leqslant i<j\leqslant s}a^{(1/2)}_{n_i,n_{i+1}}a^{(1/2)}_{n_j,n_{j+1}} + \sum_{i=0}^{s}a^{(1)}_{n_i,n_{i+1}}\right) + \cdots,$$

where the sums result from the products of the matrix elements in (10). Now it is possible to carry out the integrations. This can be done in complete analogy to the cylindrical case. For instance, in the leading order we note

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}n_1}{\sqrt{\pi}}\cdots\int_{-\infty}^{\infty}\frac{\mathrm{d}n_s}{\sqrt{\pi}}\,\mathrm{e}^{-\eta_1} = \frac{1}{\sqrt{s+1}}. \tag{13}$$

Another square root of $(s+1)$ comes from the integration over μ and two more inverse powers of $(s+1)$ come from the integration over t. Collecting all factors together we immediately come to the expression know from the PFA, thus reconfirming that approximation independently. For the next-to-leading orders, we also use the same techniques as in the cylindrical case. Thus, the integrations over n_i are Gaussian integrations with a somehow involved combinatorics. These are completely described in appendix C in [11][3]. After that

[3] Regrettably, this appendix contains a number of misprints. These are corrected in the electronic preprint, arXiv:hep-th/0602295v2.

the integrations over the remaining variables can also be carried out. All these integrations are either Gaussian or simple exponentials with polynomial factors in front. However, the number of terms in the intermediate steps is quite large. In fact, the calculations were performed machined using to a large extent the same scripts which served in the cylindrical case. The result is the remarkably simple coefficient $1/3$ in equation (3).

Finally, we describe the changes which occur if we use Neumann boundary conditions instead of Dirichlet ones. First of all, from the Neumann condition on the plane we have a sign change in the expression for the energy which now reads

$$E = \frac{1}{2\pi}\int_0^\infty d\omega\, \mathrm{tr}_{l,m} \ln\left(\delta_{l,l'} + A^N_{l,l'}\right). \qquad (14)$$

The derivatives on the sphere result in changed matrix elements $A^N_{l,l'}$. From the derivation of the matrix elements, it follows that the radial arguments of the matrix elements r and r' are just in the arguments of the Bessel functions $I_{l'+\frac{1}{2}}(\omega r')$ and $K_{l+\frac{1}{2}}(\omega r)$ in (5) before putting them on the sphere, i.e. before putting $r = R$ and $r' = R$. The derivative in the Neumann boundary conditions acts just in these arguments. Consequently, we have to substitute $I_{l'+\frac{1}{2}}(\omega r') \to \left(r\frac{\partial}{\partial r} + u\right) I_{l'+\frac{1}{2}}(\omega r')$, where u is the parameter which appears under Robin boundary conditions. In fact, it is possible to formulate different types of Neumann conditions by multiplying the wavefunction with some power of the radius, which by means of $r\partial_r r^u \Phi = r^u (r\partial_r + u)\Phi$ is equivalent to a Robin condition. For a single sphere, one has to put $u = 1/2$ in the electromagnetic case.

Now we discuss the changes which happen in the asymptotic expansions of these two Bessel functions in the matrix element. It can be easily verified that for the asymptotic expansion of the Bessel functions, the following formulae hold:

$$\begin{aligned} I_u &\equiv (r\partial_r + u)\, I_\nu(\nu z) = \nu z I'_\nu(\nu z) + u I_\nu(\nu z), \\ K_u &\equiv (r\partial_r + u)\, K_\nu(\nu z) = \nu z K'_\nu(\nu z) + u K_\nu(\nu z). \end{aligned} \qquad (15)$$

Using the asymptotic expansions, these expressions can be rewritten in the form

$$\begin{aligned} I_u &= \nu\sqrt{1+z^2} I_\nu(\nu z)\left(\frac{u}{\nu\sqrt{1+z^2}} + \frac{\sum_{k\geqslant 0}\frac{v_k}{\nu^k}}{\sum_{k\geqslant 0}\frac{u_k}{\nu^k}}\right), \\ K_u &= -\nu\sqrt{1+z^2} K_\nu(\nu z)\left(\frac{u}{\nu\sqrt{1+z^2}} + \frac{\sum_{k\geqslant 0}(-1)^k\frac{v_k}{\nu^k}}{\sum_{k\geqslant 0}(-1)^k\frac{u_k}{\nu^k}}\right), \end{aligned} \qquad (16)$$

where u_k and v_k are the known Debye polynomials. Now, to leading order for large ν, we get for the expressions in the brackets

$$\begin{aligned} I_u &= \nu\sqrt{1+z^2} I_\nu(\nu z)\left(1 + \frac{v_1 - u_1}{\nu} + \frac{u}{\nu\sqrt{1+z^2}} + O\left(\frac{1}{\nu^2}\right)\right), \\ K_u &= -\nu\sqrt{1+z^2} K_\nu(\nu z)\left(1 - \frac{v_1 - u_1}{\nu} + \frac{u}{\nu\sqrt{1+z^2}} + O\left(\frac{1}{\nu^2}\right)\right). \end{aligned} \qquad (17)$$

These expressions have to be inserted into (5). It is clear that the factors $\nu\sqrt{1+z^2}$ cancel and the expansion in the brackets becomes

$$\frac{1 + \frac{v_1-u_1}{\nu} + \frac{u}{\nu\sqrt{1+z^2}} + O\left(\frac{1}{\nu^2}\right)}{1 - \frac{v_1-u_1}{\nu} + \frac{u}{\nu\sqrt{1+z^2}} + O\left(\frac{1}{\nu^2}\right)} = 1 + 2\frac{v_1 - u_1}{\nu} + O\left(\frac{1}{\nu^2}\right). \qquad (18)$$

The dependence on u drops out and the remaining factor is the correction factor which must be inserted into the calculation of the Dirichlet case. We note that the sign coming from the Bessel function $K_\nu(\nu z)$ in (17) compensates the changed sign in (15). These are the only changes which come in, and performing the corresponding calculation one comes to the second line in (3). In this way, the first correction beyond the PFA for Neumann boundary conditions is calculated. From the above discussion it is evident that in leading order the same result as for Dirichlet boundary conditions appears thus again reconfirming the PFA, which is insensitive to the boundary condition, and that the first correction beyond does not depend on the type of Neumann condition, i.e. it does not depend on the parameter u.

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Appendix

In this appendix, we calculate the asymptotic expansion of the matrix elements $A_{l,l'}$, (5). We start with the substitution $l'' = l + l' - 2\nu$ of the summation index:

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

We are interested in the asymptotic expansion of $A_{l+l_i,l+l_{i+1}}$ for $\epsilon \to 0$ with the variables substituted according to (8). To obtain the asymptotic expansion of $A_{l+l_i,l+l_{i+1}}$, we insert the asymptotic expansions for the Bessel functions and for the $3j$-symbols and extend the sum over ν till infinity. We face the necessity of having to derive the asymptotic expansion of the $3j$-symbols, whereas the asymptotic expansion for the Bessel functions is well known.

In general, asymptotic expansions of the $3j$-symbols, or of those related by means of

$$C^{j_3,m_3}_{j_1,m_1;j_2,m_2} = (-1)^{j_1-j_2+j_3}\sqrt{2j_3+1}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \quad (A.2)$$

Clebsch–Gordan coefficients, are well investigated. However, the main attention is usually paid to semiclassical expansions aiming for computational tools for large quantum numbers. A comprehensive and modern representation is given in [14]. Unfortunately, it does not cover our case. The point is that Mathias *et al* [14] consider the limit where all quantum numbers become large, whereas in our case the magnetic quantum number m grows more slowly than the others. Nevertheless, Mathias *et al* [14] give a very convenient integral representation which serves as the starting point in our case too. We used equation (2.11) in [14] which in our notations reads

$$C^{l'',0}_{l,m;l',-m} = \frac{(-1)^{l''}}{\pi^2}(-4)^{(l''+l+l')/2}N_{l,m;l',-m;l'',0}\int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2} \mathrm{e}^{2\mathrm{i}m(\phi-\theta)}(\cos\phi)^{l''+l-l'}(\cos\theta)^{l''-l+l'} \times (\sin(\theta-\phi))^{-l''+l+l'}\,\mathrm{d}\theta\,\mathrm{d}\phi, \quad (A.3)$$

whereby we shifted the angles θ and ϕ by $\pi/2$ which resulted in the factors $\cos\theta$ and $\cos\phi$ in place of the factors $\sin\theta$ and $\sin\phi$ in [14]. The factor $N_{l,m;l',-m;l'',0}$ is defined by

$$N_{l,m;l',-m;l'',0} = \sqrt{(4l+2n_i+2n_{i+1}-4\nu+1)} \times \left(\frac{(l+n_i+m)!(l+n_i-m)!(l+n_{i+1}+m)!(l+n_{i+1}-m)!}{(4l+2n_i+2n_{i+1}-2\nu+1)!(2\nu)!}\right)^{\frac{1}{2}} \times \frac{(2l+n_i+n_{i+1}-2\nu)!}{((2l+2n_i-2\nu)!(2l+2n_{i+1}-2\nu)!)^{\frac{1}{2}}} \tag{A.4}$$

in our notations.

The asymptotic region we are interested in is determined by equation (8). So we have to use $l''=l+l'-2\nu, l\to l+l_i$ and $l'\to l+l_{i+1}$ in equations (A.3) and (A.4), respectively, to perform calculations in the asymptotic region. First of all, we consider $N_{l,m;l',-m;l'',0}$. Its asymptotic expansion simply follows from Stirling's formula. For small ϵ, it holds

$$\left(\frac{a}{\epsilon}+\frac{b}{\sqrt{\epsilon}}+c\right)! = \frac{\sqrt{2\pi a}}{\epsilon}\exp\left[\frac{a}{\epsilon}\left(-1+\ln\frac{a}{\epsilon}\right)+\frac{b}{\sqrt{\epsilon}}\ln\frac{a}{\epsilon}+c\ln\frac{a}{\epsilon}+\frac{b^2}{2a}\right] \times\left(1+\frac{b\left(a(6c+3)-b^2\right)\sqrt{\epsilon}}{6a^2} + \frac{(b^6-12acb^4+9a^2(4c^2-1)b^2+6a^3(6c^2+6c+1))\epsilon}{72a^4}+O(\epsilon^{3/2})\right). \tag{A.5}$$

Now we make the substitutions (8) in $N_{l,m;l',-m;l'',0}$, (A.4) and obtain with (A.5)

$$N_{l,m;l',-m;l'',0} = \frac{\pi^{3/4}}{\sqrt{(2\nu)!}}2^{-4l-2(l_i+l_{i+1})+2\nu+1/4}l^{\nu+3/4}\,\mathrm{e}^{m^2/l}\tilde{N}(\epsilon), \tag{A.6}$$

where the function

$$\tilde{N}(\epsilon) = 1-\frac{((n_i+n_{i+1})(4\mu^2-4\nu-3))}{4(\sqrt{t\tau})}\sqrt{\epsilon}+\frac{1}{96t\tau^2}(3(16\mu^4-8(4\nu-5)\mu^2 +16\nu^2-24\nu-11)(n_i+n_{i+1})^2+96(1-4\mu^2+4\nu)n_in_{i+1} +(16\mu^4-48\mu^2-3(8\nu^2+4\nu-5))\tau)\epsilon+O(\epsilon^{3/2}) \tag{A.7}$$

collects the subleading contributions.

Next, we calculate the integral in (A.3) using the saddle point method. We rewrite the considered integral I in the form

$$I = \int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2}(\theta-\phi)^{2\nu}\,\mathrm{e}^{2\mathrm{i}m(\theta-\phi)}g(\theta,\phi)\,\mathrm{e}^{-(l''+l-l')h(\phi)-(l''-l+l')h(\theta)}\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{A.8}$$

with

$$h(\theta)=\ln\cos\theta, \qquad g(\theta,\phi)=\left(\frac{\sin(\theta-\phi)}{\theta-\phi}\right)^{2\nu}. \tag{A.9}$$

For small ϵ, because of $l''+l-l'=2t\tau/\epsilon+\sqrt{4t/\epsilon}(n_i-n_{i+1})-2\nu$, the dominating contributions come from the minimum of the functions h which are reached in $\theta=0$ and $\phi=0$. Therefore, we expand these functions using $h(x)=x^2/2+x^4/12+\cdots$. The leading order contribution in the exponential is then $\exp\left(-\frac{2t\tau}{\epsilon}(\theta^2+\phi^2)\right)$. Taking into account that the function g depends on the difference, $\theta-\phi$, we are motivated to make the substitution of variables

$$\theta=\sqrt{\frac{\epsilon}{2t\tau}}(\xi+\eta), \qquad \phi=\sqrt{\frac{\epsilon}{2t\tau}}(\xi-\eta). \tag{A.10}$$

After that the integral can now be rewritten in the form

$$I=\left(\frac{2\epsilon}{t\tau}\right)^{1+\nu}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}y^{2\nu}\,\mathrm{e}^{2\mathrm{i}\sqrt{2\tau}\mu\eta}\tilde{g}(\xi,\eta)\,\mathrm{e}^{-(\xi^2+\eta^2)}\,\mathrm{d}\xi\,\mathrm{d}\eta. \tag{A.11}$$

In the sense of the asymptotic expansion we are interested in, we stretched the integration until infinity. In (A.11), we defined the function

$$\tilde{g}(\xi,\eta) = g(\theta,\phi)\,\mathrm{e}^{-(l''+l-l')h(\phi)-(l''-l+l')h(\theta)+\xi^2+\eta^2}. \tag{A.12}$$

Obviously, it has an expansion in powers of $\sqrt{\epsilon}$,

$$\begin{aligned}\tilde{g}(\xi,\eta) = 1 &+ (-(n_i+n_{i+1})\eta^2 + 2(n_{i+1}-n_i)\xi\eta - (n_i+n_{i+1})\xi^2)\frac{\sqrt{\epsilon}}{\sqrt{t\tau}} + ((6(n_i+n_{i+1})^2-\tau)\eta^4 \\ &+ 24\left(n_i{}^2 - n_{i+1}{}^2\right)\xi\eta^3 + (6(6n_i{}^2 - 4n_{i+1}n_i + 6n_{i+1}{}^2 - \tau)\xi^2 + 4\nu\tau)\eta^2 \\ &+ 24\left(n_i{}^2 - n_{i+1}{}^2\right)\xi^3\eta + (6(n_i+n_{i+1})^2-\tau)\xi^4 + 12\nu\tau\xi^2)\frac{\epsilon}{12t\tau^2} + O(\epsilon^{3/2}).\end{aligned} \tag{A.13}$$

Now we carry out the integration over ξ. It is Gaussian and delivers a new function $\tilde{g}_1(\epsilon,\eta)$:

$$I = \sqrt{\pi}\left(\frac{2\epsilon}{t\tau}\right)^{1+\nu}\int_{-\infty}^{\infty} y^{2\nu}\tilde{g}_1(\epsilon,\eta)\,\mathrm{e}^{-\eta^2+2\mathrm{i}\sqrt{2\tau}\mu\eta}\,\mathrm{d}\eta \tag{A.14}$$

with the property $\tilde{g}_1(0,\eta) = 1$. Finally, we take the expansion (A.6) of the prefactor and the expansion (A.14) of the integral together and insert into equation (A.3) for the Clebsch–Gordan coefficients. This gives

$$C^{l'',0}_{l,m;l',-m} = \frac{(-1)^\nu}{\pi^{1/4}}2^{-\nu+1/4}\frac{\sqrt{(2\nu)!}}{\nu!}l^{-1/4}h(\epsilon,\mu), \tag{A.15}$$

where the new function $h(\epsilon,\mu)$ collects the sub-leading contributions:

$$h(\epsilon,\mu) = \frac{2^{2\nu}\nu!}{\sqrt{\pi}(2\nu)!}\int_{-\infty}^{\infty}\eta^{2\nu}g_2(\epsilon,\eta)\,\mathrm{e}^{2\mathrm{i}\sqrt{2}\mu\eta-\eta^2+\mu^2}\,\mathrm{d}\eta. \tag{A.16}$$

Here we defined $g_2(\epsilon,\eta) = n_1(\epsilon)\tilde{g}_1(\epsilon,\eta)$ which must be re-expanded in powers of $\sqrt{\epsilon}$ too. The function $h(\epsilon,\mu)$ has the property $h(0,\mu) = 1$. It is possible to obtain a more explicit representation of this function by carrying out the integration. However, for the application below this did not prove to be useful.

The calculation of the asymptotic expansion (A.15) of the Clebsch–Gordan coefficients was the most difficult task. It remains to insert them into the matrix elements $A_{l,l'}$, (A.1). These symbols enter twice. The second time they go with the zero magnetic quantum number m. It is possible to put $m = 0$ directly in the asymptotic formula (A.15). In (A.16) then the integration can be carried out explicitly. Putting these formulae together with the well-known asymptotic expansion of the Bessel functions (which is displayed, for instance, in equation (B.1) in [11]), we come to

$$A_{l+l_i,l+l_{i+1}} = \frac{\tau\,\mathrm{e}^{-\eta_{as}}}{\sqrt{2\pi l(1-\tau^2)}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\eta}{\sqrt{\pi}}\,\mathrm{e}^{-\eta^2+2\mathrm{i}\sqrt{2}\mu\eta+\mu^2}\sum_{\nu=0}^{\infty}\frac{\eta^{2\nu}}{\nu!}\left(\frac{1-\tau}{1+\tau}\right)^\nu C_g, \tag{A.17}$$

where C_g collects the sub-leading factors. Its dependence on ν is polynomial. Hence, the sum over ν can be carried out:

$$\sum_{\nu=0}^{\infty}\frac{\eta^{2\nu}}{\nu!}\left(\frac{1-\tau}{1+\tau}\right)^\nu C_g = \mathrm{e}^{\eta^2\frac{1-\tau}{1+\tau}}C_a, \tag{A.18}$$

where now C_a collects the non-leading contributions. The complete expression is too lengthy to be shown here. So we restrict ourselves to showing the order $\sqrt{\epsilon}$:

$$C_a = 1 + \frac{1}{2\sqrt{t}\tau(\tau+1)}\big(2\tau^2(\tau+1)n_i^3 - 2n_{i+1}\tau^2(\tau+1)n_i^2 + \left(\left(-2n_{i+1}^2 - 4t + 1\right)\tau^3 + \left(4\eta^2 - 2n_{i+1}^2 - 4t\right)\tau^2 - 8\eta^2\tau + \tau - 2\mu^2(\tau+1) + 2\right)n_i + n_{i+1}\left(\left(2n_{i+1}^2 - 4t - 3\right)\tau^3 + 2\left(2\eta^2 + n_{i+1}^2 - 2t - 2\right)\tau^2 - 8\eta^2\tau + \tau - 2\mu^2(\tau+1) + 2\right)\big)\sqrt{\epsilon}. \tag{A.19}$$

With (A.18) the integration over η in (A.17) becomes Gaussian and can be carried out. Together with the remaining factors, the result collects into the final form of the matrix elements up to the ϵ order:

$$A_{l+l_i,l+l_{i+1}} = \sqrt{\frac{\epsilon}{4\pi t}}\,\mathrm{e}^{-\eta_{as}}\,\mathrm{e}^{-\mu^2}\left(1 + a^{\frac{1}{2}}(n_i,n_{i+1})\sqrt{\epsilon} + a^1(n_i,n_{i+1})\epsilon\right), \tag{A.20}$$

where

$$\eta_{as} = -2t + (n_i - n_{i+1})^2 \tag{A.21}$$

is the same factor as in the cylindrical case [11] and the non-leading coefficients are

$$a^{\frac{1}{2}}_{n_i,n_{i+1}} = \frac{1}{2\sqrt{t}\tau^2}\big(2n_i^3\tau^3 - 2n_i^2n_{i+1}\tau^3 + n_i\left(\left(-2n_{i+1}^2 - 4t + 1\right)\tau^3 - 2\mu^2\left(\tau^2 - 2\right)\right) + n_{i+1}\left(\left(2n_{i+1}^2 - 4t - 3\right)\tau^3 - 2\mu^2\left(\tau^2 - 2\right)\right)\big)$$

$$a^1_{n_i,n_{i+1}} = \frac{1}{48t\tau^4}\big(4\left(3\tau^4 - 9\tau^2 + 6n_i^2(\tau^2-2)^2 + 6n_{i+1}^2(\tau^2-2)^2 + 12n_in_{i+1}(\tau^2-2)^2 + 4\right)\mu^4 - 12\tau\big(4\tau^2(\tau^2-2)n_i^4 - 2\left(4\left(n_{i+1}^2 + t\right)\tau^4 + \left(-8n_{i+1}^2 - 8t + 5\right)\tau^2 - 8\right)n_i^2 - 4n_{i+1}\left((4t+2)\tau^4 + (1-8t)\tau^2 - 4\right)n_i - 4t\tau^4 - \tau^4 + 2\tau^3 + 4t\tau^2 - 3\tau^2 - 4\tau + 4n_{i+1}^4\tau^2(\tau^2-2) + n_{i+1}^2(-8(t+1)\tau^4 + 2(8t+3)\tau^2 + 16) + 4\big)\mu^2 + \tau^2\big(3\big(8n_i^6 - 16n_{i+1}n_i^5 - 4\left(2n_{i+1}^2 + 8t + 5\right)n_i^4 + 16n_{i+1}\left(2n_{i+1}^2 - 1\right)n_i^3 + \left(-8n_{i+1}^4 + 8(8t+5)n_{i+1}^2 + 32t^2 - 22\right)n_i^2 + 4n_{i+1}\left(-4n_{i+1}^4 + 12n_{i+1}^2 + 16t^2 + 16t + 1\right)n_i + 8n_{i+1}^6 + 16t^2 + 8t - 4n_{i+1}^4(8t+13) + n_{i+1}^2\left(32t^2 + 64t + 58\right) - 5\big)\tau^4 + 12\left(2n_i^2 - 4n_{i+1}n_i + 2n_{i+1}^2 - 4t - 1\right)\tau^3 + \big(28n_i^4 - 16n_{i+1}n_i^3 - 12\left(2n_{i+1}^2 + 4t - 3\right)n_i^2 - 8n_{i+1}\left(2n_{i+1}^2 + 12t + 3\right)n_i + 28n_{i+1}^4 - 24t - 12n_{i+1}^2(4t+5) + 9\big)\tau^2 + 12\big)\big). \tag{A.22}$$

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