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Casimir forces beyond the proximity approximation

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Abstract – The proximity force approximation (PFA) relates the interaction between closely spaced, smoothly curved objects to the force between parallel plates. Precision experiments on Casimir forces necessitate, and spur research on, corrections to the PFA. We use a derivative expansion for gently curved surfaces to derive the leading curvature modifications to the PFA. Our methods apply to any homogeneous and isotropic materials; here we present results for Dirichlet and Neumann boundary conditions and for perfect conductors. A Padé extrapolation constrained by a multipole expansion at large distance and our improved expansion at short distances, provides an accurate expression for the sphere/plate Casimir force at all separations.

First introduced by Derjaguin [1], the proximity force approximation (PFA) relates forces between gently curved objects at close separations to the corresponding interactions between flat surfaces over an area set by the local radii of curvature. Originally developed in the context of surface adhesion and colloids, the PFA has found application as far afield as the study of internuclear forces and fission [2,3]. In particular, the PFA has long been applied to Casimir and other fluctuation forces that are short range and therefore dominated by the surface proximity. Despite its nearly universal use to parameterize Casimir forces in experimentally accessible geometries like a sphere opposite a plate [4,5], not even the first correction to the PFA in the ratio of the inter-surface separation to the scale of curvature, d/R, is known for realistic dielectric materials or even for generic perfect conductors. Casimir forces have non-trivial and sometimes counterintuitive dependence on the overall shape, increasing the interest in developing a thorough understanding of the corrections to the PFA and its range of validity. As the experimental precision of Casimir force measurements improves, they are becoming sensitive to PFA corrections, further motivating renewed interest in this subject. For example, an upper bound on the magnitude of the first-order correction to the PFA for a gold-coated sphere in front of a gold-coated plane was obtained a few years ago in an experiment by the Purdue group [6], which found that the fractional deviation from the PFA in the force gradient is less than $0.4\ d/R$.

We here provide a general expression for the first correction to the PFA for the Casimir energy of objects whose surface curvatures are large compared to their inter-surface separation. Scattering methods have provided a fertile route to computing Casimir forces for non-planar shapes [7]. While conceptual threads connected to this approach can be traced back to earlier multiple-scattering methods [8], concrete analytical [7] and numerical [9] results are relatively recent. Indeed, the experimentally most relevant set-up of a sphere and plate was only treated in 2008 [10] (see also [11] and [12,13] for related work). The scattering method is most powerful at large separation, providing analytic expressions for a multipole expansion in the ratio R/d and numerical results for $R/d \lesssim 10$, but becomes intractable at the values of $d/R \sim 10^{-3}$, needed to study the PFA. Worldline numerics have been applied to the sphere/plate set-up for a scalar field with Dirichlet

(D) boundary conditions [14]. In a feat of mathematical dexterity, Bordag and Nikolaev (BN) summed the scattering series to obtain the first correction to the PFA for the cylinder/plate and sphere/plate geometries, initially for a scalar field obeying D boundary conditions (bc) [15], and later for the electromagnetic (EM) field with ideal metallic bc [16]. Intriguingly, whereas the correction to the force in the former case for both geometries is analytic in d/R, the sphere/plate EM case was predicted to include logarithmic corrections ($\sim(d/R)\ln(d/R)$). While the BN PFA corrections for cylinders (where there are only analytic corrections), were independently verified by Teo [17], the results of refs. [15,16] for the experimentally interesting sphere/plate EM case remain unconfirmed.

A recent work by Fosco *et al.* [18] provides a quite promising perspective on Casimir PFA corrections. Reinterpreting perturbative corrections to parallel plate forces [19,20], they propose a gradient expansion in the local separation between surfaces for the force between gently curved bodies. They implement their program for scalar fields and confirm that their general approach reproduces the BN cylinder and sphere/plate correction for D bc. Inspired by this work, the current paper is organized as follows: i) We show that the extension of ref. [18] to two curved surfaces is constrained by tilt invariance of the reference plane (from which the two separations are measured). This provides a stringent test of the self-consistency of perturbative results. ii) Going beyond the scalar fields and D bc of ref. [18], we compute the form of the gradient expansion for Neumann (N), mixed D/N, and EM (perfect metal) boundaries. Interestingly, we find that the EM correction must coincide with the sum of D and N corrections. iii) We reproduce previous results for cylinders [17] with D, N, and mixed D/N conditions, and the sphere with D bc. However, we do not confirm the BN predictions for the sphere/plane geometry [16] either with N or EM bc [21]. iv) As a further test, we introduce a Padé approximant for the (sphere/plate) force at all separations, based on an asymptotic expansion at large distances and the gradient expansion at proximity. The Padé approximant agrees excellently with the existing numerical data and implies logarithmic corrections to the PFA *beyond* the gradient expansion performed here (see eq. (9)).

Consider two bodies with gently curved surfaces described by (single-valued) height profiles $z = H_1(\boldsymbol{x})$ and $z = H_2(\boldsymbol{x})$, with respect to a reference plane Σ, where $\boldsymbol{x} \equiv (x, y)$ are Cartesian coordinates on Σ and the z axis is normal to Σ. For our purposes it is not necessary to specify the precise nature of the fluctuating quantum field. Our results are valid for scalar fields, for the EM field, and indeed even for spinor fields. Similarly, the boundary conditions satisfied by the fields on the surfaces of the plates can be either ideal *e.g.*, D or N for the scalar field, or ideal metal in the EM case) or those appropriate to a real material with complex dielectric permittivity. The only restriction on the bc is that they should describe homogeneous and isotropic materials, so that the energy is invariant under simultaneous translations and rotations of the two profiles in the plane Σ.

Following ref. [18], we postulate that the Casimir energy, when generalized to two surfaces and to arbitrary fields subject to arbitrary bc, is a functional $E[H_1, H_2]$ of the heights H_1 and H_2, which has a derivative expansion,

$$\begin{aligned} E[H_1, H_2] = \int_\Sigma \mathrm{d}^2\boldsymbol{x}\, U(H)\, [1 + \beta_1(H)\boldsymbol{\nabla}H_1\cdot\boldsymbol{\nabla}H_1 \\ + \beta_2(H)\boldsymbol{\nabla}H_2\cdot\boldsymbol{\nabla}H_2 + \beta_\times(H)\boldsymbol{\nabla}H_1\cdot\boldsymbol{\nabla}H_2 \\ + \beta_-(H)\,\hat{\boldsymbol{z}}\cdot(\boldsymbol{\nabla}H_1\times\boldsymbol{\nabla}H_2) + \cdots], \end{aligned} \tag{1}$$

where $H(\boldsymbol{x}) \equiv H_2(\boldsymbol{x}) - H_1(\boldsymbol{x})$ is the height difference, and dots denote higher derivative terms. Here, $U(H)$ is the energy per unit area between parallel plates at separation H; translation and rotation symmetries in $\boldsymbol{x}$ only permit four distinct gradient coefficients, $\beta_1(H)$, $\beta_2(H)$, $\beta_\times(H)$ and $\beta_-(H)$ at lowest order. While the validity of this local expansion remains to be verified, it is supported by the existence of well-established derivative expansions of scattering amplitudes [22] from which the Casimir energy can be derived by standard methods [7].

Arbitrariness in the choice of Σ constrains the β-coefficients. Invariance of E under a displacement of Σ along the z-axis requires that all the β's depend only on the height difference H, and not on the individual heights H_1 and H_2. The β-coefficients are further constrained by the invariance of E with respect to tilting the reference plate Σ. Under a tilt of Σ by an infinitesimal angle ϵ in the (x, z)-plane, the height profiles H_i change by $\delta H_i = -\epsilon(x + H_i\frac{\partial H_i}{\partial x})$, and the invariance of E implies

$$\begin{aligned} &2\left(\beta_1(H) + \beta_2(H)\right) + 2\beta_\times(H) + H\frac{\mathrm{d}\log U}{\mathrm{d}H} - 1 = 0, \\ &\beta_-(H) = 0. \end{aligned} \tag{2}$$

Hence the non-vanishing cross-term $\beta_\times$ is determined by β_1, β_2 and U.

By exploiting eqs. (2) we see that, to second order in the gradient expansion, the two-surface problem reduces to the simpler problem of a single curved surface facing a plane, since U, β_1 and β_2 can be determined in that case and $\beta_\times$ follows from eqs. (2). Therefore in eq. (1) we set $H_1 = 0$ and define $\beta_2(H) \equiv \beta(H)$. By a simple generalization of ref. [18], where the problem is studied for a scalar field subjected to D bc on both plates, we can determine the exact functional dependence of $\beta(H)$ on H by comparing the gradient expansion, eq. (1), to a perturbative expansion of the Casimir energy around flat plates, to second order in the deformation. For this purpose, we take Σ to be a planar surface and decompose the height of the curved surface as $H(\boldsymbol{x}) = d + h(\boldsymbol{x})$, where d is chosen to be the distance of closest separation. For small deformations $|h(\boldsymbol{x})|/\mathrm{d} \ll 1$ we can expand

$E[0, d+h]$ as:

$$E[0,d+h] = A\,U(d) + \mu(d)\tilde{h}(\mathbf{0}) + \int \frac{\mathrm{d}^2\boldsymbol{k}}{(2\pi)^2} G(k;d)|\tilde{h}(\boldsymbol{k})|^2, \tag{3}$$

where A is the area, $\boldsymbol{k}$ is the in-plane wave vector and $\tilde{h}(\boldsymbol{k})$ is the Fourier transform of $h(\boldsymbol{x})$. The kernel $G(k;d)$ has been evaluated by several authors, for example in ref. [19] for a scalar field fulfilling D or N bc on both plates, as well for the EM field satisfying ideal metal bc on both plates. More recently, $G(k;d)$ was evaluated in ref. [20] for the EM field with dielectric bc. For a deformation with small slope, the Fourier transform $\tilde{h}(\boldsymbol{k})$ is peaked around zero. Since the kernel can be expanded at least through order k^2 about $k=0$ [22], we define

$$G(k;d) = \gamma(d) + \delta(d)\,k^2 + \cdots. \tag{4}$$

For small h, the coefficients in the derivative expansion can be matched with the perturbative result. By expanding eq. (1) in powers of $h(\boldsymbol{x})$ and comparing with the perturbative expansion to second order in both $\tilde{h}(\boldsymbol{k})$ and k^2, we obtain

$$U'(d) = \mu(d), \quad U''(d) = 2\gamma(d), \quad \beta(d) = \frac{\delta(d)}{U(d)}, \tag{5}$$

with prime denoting a derivative. Using the above relation, we computed the coefficient β for the following five cases: a scalar field obeying D or N bc on both surfaces, or D bc on the curved surface and N bc on the flat, or vice versa, and for the EM field with ideal metal bc. Since in all these cases the problem involves no other length apart from the separation d, β is a pure number. β_{D} was computed in [18], and found to be $\beta_{\mathrm{D}} = 2/3$. We find $\beta_{\mathrm{N}} = 2/3\,(1 - 30/\pi^2)$, $\beta_{\mathrm{DN}} = 2/3$, $\beta_{\mathrm{ND}} = 2/3 - 80/7\pi^2$ (where the double subscripts denote the curved surface and flat surface bc respectively), and $\beta_{\mathrm{EM}} = 2/3\,(1 - 15/\pi^2)$. Upon solving eqs. (2) one then finds $\beta_\times = 2 - \beta_1 - \beta_2$, where β_1 and β_2 are chosen to be both equal to either β_{D}, β_{N} or β_{EM}, for the case of identical bc on the two surfaces, or rather $\beta_1 = \beta_{\mathrm{DN}}$ and $\beta_2 = \beta_{\mathrm{ND}}$ for the case of a scalar field obeying mixed ND bc. While we obtain agreement for D conditions, our results for β in the case of N and EM conditions disagree with refs. [15,16], which finds $\beta_{\mathrm{N}} = 2/3 - 5/\pi^2$ and $\beta_{\mathrm{EM}} = -2.1$, multiplied by logarithmic terms in the latter case that we do not obtain. We note that our value of β_{EM} is equal to the average of β_{D} and β_{N}. Of course for parallel plates the EM Casimir force for perfect mirrors is the sum of Dirichlet and Neumann contributions (see, *e.g.*, ref. [23] for a calculation based on semi-classical methods); that this should hold for the first correction to PFA is noteworthy. Using the well-known results $U(d) = -\alpha\pi^2\hbar c/(1440 d^3)$, where $\alpha_{\mathrm{D}} = \alpha_{\mathrm{N}} = \alpha_{\mathrm{EM}}/2 = 1$ and $\alpha_{\mathrm{DN}} = \alpha_{\mathrm{ND}} = -7/8$ in eq. (1), it is easy to verify that to second order in the gradient expansion the ideal-metal EM Casimir energy for two arbitrary surfaces is equal to the sum of the D and N Casimir energies in the same geometry.

Using the values for β and $\beta_\times$ obtained above, it is possible to evaluate the leading correction to PFA, by explicit evaluation of eq. (1) for the desired profiles. For example, for two spheres of radii R_1 and R_2, both with the same bc for simplicity, we obtain

$$E = E_{\mathrm{PFA}}\left[1 - \frac{d}{R_1+R_2} + (2\beta - 1)\left(\frac{d}{R_1} + \frac{d}{R_2}\right)\right], \tag{6}$$

where $E_{\mathrm{PFA}} = -(\alpha\pi^3\hbar c R_1 R_2))/[1440 d^2 (R_1+R_2)]$. The corresponding formula for the sphere/plate case can be obtained by taking one of the two radii to infinity. Similarly, for two parallel circular cylinders with different radii our results, not given here for brevity, fully agree with those derived very recently by Teo [17]. Finally we consider two circular cylinders whose axes are inclined at a relative angle θ,

$$E = -\frac{\alpha\pi^3\hbar c\sqrt{R_1 R_2}}{1440 d^2 \sin\theta}\left[1 + \left(\beta - \frac{3}{8}\right)\frac{d}{R_1+R_2}\right], \tag{7}$$

again assuming the same bc on both surfaces.

Surprisingly, a hyperboloid/plate configuration, $h(r) = \sqrt{R^2 + \lambda^2 r^2} - R$ leads to a PFA correction proportional to $(2\beta + 1/\lambda^2)d/R$, which *vanishes* for the EM case if $\lambda = 1.20$. To better understand what geometric features of the surface determine the PFA corrections, we considered a general profile, expanded around the point of shortest separation, including cubic and quartic terms in addition to quadratic terms representing its curvature. The cubic terms —representing an asymmetry absent in the shapes considered above— actually result in a correction term that scales as $\sqrt{d/R}$. The more standard correction proportional to d/R depends on both cubic and quartic but no higher-order terms in the expansion of the profile. The quartic coefficients in fact have opposite signs for the sphere and hyperboloid, and it is this difference that accounts for the possibility of a vanishing PFA correction (for the hyperboloid with EM bc).

Our new understanding of Casimir forces at small separations can be combined with existing calculations at large distances to obtain a single analytic expression for the experimentally relevant sphere/plate system at all distances. Also, this analysis provides an independent comparison with the original predictions of BN [15,16], and suggests that the gradient expansion of the Casimir energy may break down at the next order. Precise numerical results based on an extrapolation of a spherical multipole expansion exist for $d/R \gtrsim 0.1$ [10]. Also, at large separations analytic asymptotic expansions (AE) of the rescaled force $f = R^2 F/(\hbar c) \sim \sum_{j=1}^{n} f_j r^{j_0+j}$ in powers of $r = R/d$ are available for sufficiently large n, where $j_0 = 2$ for D and $j_0 = 4$ for N and EM conditions, respectively. We resum the AE for f, match it with our improved PFA result using the method of Padé approximants, and compare the resulting interpolation with the numerical

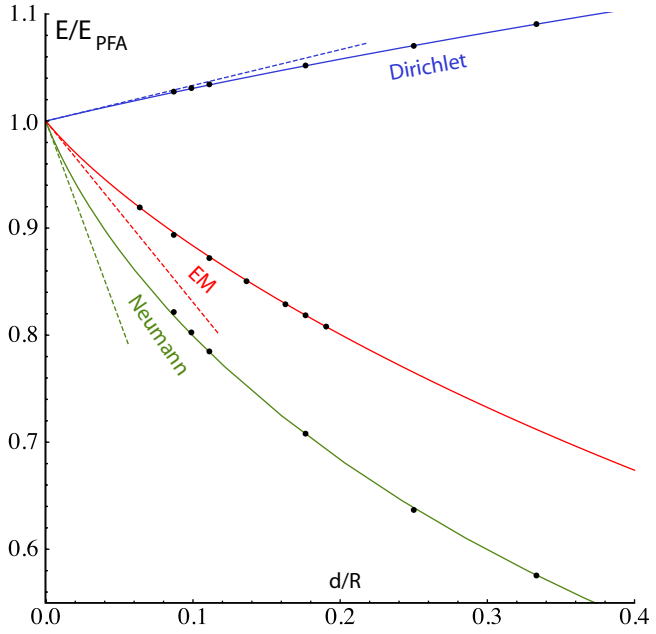

Fig. 1: (Colour on-line) Casimir energy normalized to PFA energy as a function of d/R for the sphere/plate configuration: numerical data (dots, from ref. [10]), Padé approximants (solid curves) and the first correction to the PFA (dashed lines).

results of ref. [10]. We introduce a Padé approximant $f_{[M/N]}(r)$ that agrees with n terms of the AE for small r and with the leading two terms $\sim r^3$, r^2 for large r given by eq. (6). This requires $N = M - 3$, whereas M is determined by n, so that all coefficients in

$$f_{[M/M-3]}(r) = \frac{p_0 + p_1 r + p_2 r^2 + \ldots + p_M r^M}{1 + q_1 r + q_2 r^2 + \ldots + q_{M-3} r^{M-3}} \qquad (8)$$

are uniquely determined. The energy, obtained from $f_{[M/M-3]}$ by integration over distance is shown with $n = 7$, 13 and 15 for D, N and EM bc, respectively, in fig. 1 together with our result of eq. (6) for the sphere/plate case ($R_1 = R$, $R_2 \to \infty$) and the numerical results of ref. [10]. The difference between Padé approximants and the numerical data varies between 0.009% and 0.062% (D), 0.048% and 0.42% (N), 0.009% and 0.248% (EM). This agreement is quite remarkable given that the Padé approximants are obtained independent of the numerical data. Hence, the derivative expansion in combination with a Padé approximation improves known numerical results which do not apply to very short separations [10,11]. The Padé approach may thus be valuable for Casimir interactions between slowly varying surfaces at all separations starting from expansions valid at small and large distances, respectively.

Integration of the Padé approximant for the force yields an expansion for the energy at small d/R,

$$\frac{E}{E_{\rm PFA}} = 1 + \theta_1 \frac{d}{R} + \theta_2 \left(\frac{d}{R}\right)^2 \log \frac{d}{R} + \mathcal{O}\left(\left(\frac{d}{R}\right)^3\right) \qquad (9)$$

Table 1: Coefficient θ_1 for D, N and EM boundary conditions on sphere/plate from a fit of the numerical data of ref. [10] to eq. (9) and from the gradient expansion.

Boundary condition	θ_1 from fit to numerical data [10]	θ_1 from gradient expansion
D	$+0.36$	$1/3$
N	-2.99	$1/3 - 40/\pi^2 = -3.72$
EM	-1.62	$1/3 - 20/\pi^2 = -1.69$

with $\theta_1 = 2\beta - 1$ and $\theta_2 = 0.08$ for D, $\theta_2 = -24.01$ for N and $\theta_2 = -4.52$ for EM conditions. The appearance of a logarithm at second order in eq. (9) follows from our assumption that the force can be expanded in powers of d at small d including a term $\sim 1/d$ [24]. A Padé approximation to the energy is by definition a power series with no logarithms, and would not yield a $1/d$ contribution to the force. To check that the $d^2 \log d$ term in the energy is necessary, we have tried a Padé analysis of the energy and found much poorer agreement with the numerical data (with fractional differences of the order of 100 times larger than those given above for the Padé approximant for the force and moreover a pole in the approximant). This confirms our finding that eq. (9) indeed must contain a $d^2 \log d$ term. One could perform Padé approximations to derivatives of the force which might turn out to be even more accurate but this would only change the functional form (logarithmic factors) of eq. (9) at third order in d/R. As an independent test of our result $\theta_1 = 2\beta - 1$ we fitted [25][1] the functional form of eq. (9) to the numerical data reported in ref. [10]. The corresponding values for θ_1 are summarized in table 1. When comparing numerical and analytic values for θ_1 one must consider that they are limited to $d/R \gtrsim 0.1$ with somewhat better accuracy for the D and EM case. We note that the presence of the logarithm at order $(d/R)^2$ indicates that the gradient expansion for the energy might break down at next order. Finally, we have applied both the derivative expansion and the Padé approximation to the *electrostatic* force gradient between a sphere and a plate and found excellent agreement with the exact solution (with low-order Padé approximants having an error of well below 1%.)

Based on the derivative expansion proposed by Fosco *et al.* [18], we have described a systematic treatment of the first non-trivial corrections to the PFA. While this paper focused on ideal boundary conditions, the scattering amplitudes for material with arbitrary EM response (frequency-dependent $\epsilon(\omega)$, $\mu(\omega)$, isotropic or not, local or not) have been computed in the gradient expansion [22] and can be used to compute improved PFA corrections in experimentally relevant situations

[1] We note that in refs. [10,25] numerical data have been fitted to a function that differs from eq. (9) by the absence of the log, leading to different values for θ_1.

of sphere/plate as well as corrugated plates and other set-ups.

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