Going beyond PFA: A precise formula for the sphere-plate Casimir force

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Abstract – Quantum fluctuations of the electromagnetic field in the medium surrounding two discharged macroscopic polarizable bodies induce a force between the two bodies, the so-called Casimir force. In the last two decades many experiments have accurately measured this force, and significant efforts are made to harness it in the actuation of micro- and nano-machines. The inherent many-body character of the Casimir force makes its computation very difficult in non-planar geometries, like the standard experimental sphere-plate configuration. Here we derive an approximate semi-analytic formula for the sphere-plate Casimir force, which is both easy to compute numerically and very accurate at all distances. By a comparison with the fully converged exact scattering formula, we show that the error made by the approximate formula is indeed much smaller than the uncertainty of present and foreseeable Casimir experiments.

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The Casimir effect [1] is the tiny force acting between two (or more) discharged polarizable objects, that originates from quantum and thermal fluctuations of the electromagnetic field in the medium surrounding the bodies. It represents one of the rare manifestations of the quantum at the macroscopic scale, similar to black-body radiation, superfluidity and superconductivity. Reviews can be found in refs. [2–5]. Recent years witnessed an impetuous resurgence of interest in the Casimir effect, triggered by a series of precision experiments [6,7] and by the exciting perspective of harnessing this force in the nanoworld [8]. The Casimir force is notoriously difficult to compute in non-planar geometries, like the standard sphere-plate geometry adopted in almost all experiments (see fig. 1). Recently, important progress in the understanding of the sphere-sphere and sphere-plate force has been made in the non-retarded or van der Waals regime by using transformation optics [9]. By a combination of asymptotic techniques [10–15] with a partial exact solution valid in the classical limit [16], here we derive a new semi-analytic formula for the complete retarded sphere-plate Casimir force. Comparison with high-precision numerical simulations reveals that the formula is remarkably accurate at all separations. The new formula thus provides a simple and yet fully reliable tool to interpret present and future experimental data.

In his famous 1948 paper [1], Hendrik Casimir discovered that the ground-state energy of the quantized electromagnetic (em) field is modified by the presence of material bodies that interact with the em field. By carefully adding up the zero-point energies of the em modes of a planar cavity consisting of two perfectly conducting plates of (large) area $A$ at distance $a$, he obtained his celebrated formula for the force acting on the plates at zero temperature:

$$F_C = \frac{\pi^2 hc}{240a^4} A.$$

This simple formula reveals the main features of the Casimir force: the presence of Planck’s constant indicates its quantum character, while the presence of the speed of light $c$ shows that it is a relativistic effect. The $a^{-4}$ dependence shows that the magnitude of the force increases rapidly as the distance $a$ is decreased: indeed, for typical experimental submicron separations the Casimir force is much stronger than gravity.

An important extension of Casimir’s work was made by Lifshitz in 1955 [17]: using Rytov’s theory of electromagnetic fluctuations [18], Lifshitz worked out the Casimir

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pressure between two real dielectric parallel plates described by the respective (complex) dynamical permittivities $\epsilon(\omega)$, at a finite temperature $T$. Lifshitz’ results paved the way to investigations of the Casimir effect in real physical conditions.

Even though the first observation of the Casimir force was reported just a few years after Casimir’s prediction [19], the modern era of Casimir physics began only in the late 1990s [6,7], when a series of experiments obtained the first precise measurements of the force.

Although the plane-parallel geometry studied by Casimir and Lifshitz enormously simplifies the theoretical analysis, plane-parallel plates are never used in experiments (with very few notable exceptions [20]) because it is very hard to precisely align two planar surfaces placed at a submicron distance from each other. To avoid this difficulty, almost all experimental groups [6,7,21–25] adopt the sphere-plate geometry (see fig. 1), which obviously does not suffer from the parallelism issue. In order to increase the strength of the Casimir force, as it is necessary for a precise measurement to be possible, experiments use setups with spheres of radii $R > 10 \mu m$ with large aspect ratios $R/a$ typically exceeding $10^2$–$10^3$.

Unfortunately, the sphere-plate (and more in general any non-planar) geometry presents the serious drawback that the computation of the Casimir force gets very difficult. Indeed, the Casimir force is non-additive due to its inherent many-body character and, therefore, its dependence on the system geometry is very complicated. This explains why still today the universal tool used to interpret the experiments is the old-fashioned Derjaguin [26] proximity force approximation (PFA), which expresses the Casimir force between two gently curved surfaces as the average of the force for two parallel plates, taken over the local surface-surface separation.

This state of things has not changed despite the theoretical breakthrough in the early 2000s [27–29], when by using scattering methods a mathematically exact formula for the Casimir interaction between two (or more) compact bodies of any shape has been derived in the form of a multipole expansion in terms of the respective $T$-matrices. In principle, the scattering formula allows to exactly compute the Casimir force between two objects whose $T$-matrices are either known, or can be worked out numerically. The experimental sphere-plate geometry is among these, since its $T$-matrix has been known for a very long time [30]. Notwithstanding this, in the past the scattering formula has never been used in practice, because its slow convergence makes it difficult to compute it in a reasonable computer time for the large aspect ratios $R/a$ of the experiments (more on this is given below). Only very recently a large-scale simulation of the sphere-plate scattering formula going up to multipole order $l_{\text{max}} = 2 \times 10^4$ appeared in the arXiv [31], in which the sphere-plate force and force gradient have been computed numerically for experimentally relevant aspect ratios $R/a \sim 4 \times 10^3$.

The PFA has been put on a firmer basis recently, by showing rigorously that it coincides with the leading term of the asymptotic expansion of the exact scattering formula for large $R/a$ (at fixed $a$) [10]. By the same approach, it has been also possible to estimate the $O(a/R)$ corrections to the PFA [11,12]. An alternative and equivalent method to compute curvature corrections to the PFA is based on a derivative expansion (DE) of the Casimir energy in powers of derivatives of the curved surface height profile [13–15].

Before we plunge into computations, it is useful to discuss shortly why computing precisely the Casimir force is important. There are at least two reasons for that. The first reason has to do with Casimir physics, while the second is connected with recent searches on non-Newtonian gravity in the sub-millimiter range. Let us consider the former first.

The most precise recent experiments utilizing Au-coated sphere and plate, have measured the Casimir force and its gradient with experimental errors around one percent, for separations smaller than a few hundred nm. The theoretical analysis of these experiments revealed perplexing discrepancies, at the percent level, with predictions based on the PFA. The interpretation of these discrepancies spurred a heated debate in the community. It has been argued by some authors that these discrepancies point at a fundamental flaw in Lifshitz theory, regarding the role of free charge carriers in determining the magnitude of the thermal component of the Casimir force [3]. This debate has become known in the Casimir field as the Drude vs. plasma controversy [32]: in essence the controversy is whether in Lifshitz formula one should use the familiar Drude model or rather the dissipationless plasma model of infra-red optics to describe the response of a metallic plate at low frequencies. On physical grounds one would expect that the plasma model should be used to compute the Casimir interaction between two superconducting plates [33], while for normal metals at room temperature as those used

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Fig. 1: (Colour online) The sphere-plate Casimir setup.
in the experiments the Drude model should provide the correct description. Contrary to general expectations, a series of experiments shows that the plasma model is in agreement with data, while the physically plausible Drude model is not [21,34–39]. There is, however, a single experiment which is in agreement with the Drude model [40]. On the theory side, it has been realized that the use of the Drude prescription in Lifshitz formula also leads to the violation of the Nernst heat theorem, in the idealized limit of metal test bodies with perfect lattice structures [41–43]. Since the problem has a bearing on the fundamental principles of statistical physics, many feel desirable to make sure that the PFA, which has been used to interpret the experiments, is precise enough.

The ability to compute precisely the Casimir force is also crucial in recent searches for non-Newtonian gravity in the sub-millimeter range [21,44]. Here, one measures the force of attraction between two test bodies, looking for deviations from Newton’s law. Usually the test bodies used in these experiments are Au-coated, to avoid potentially harmful forces due to stray electrostatic fields [40]. When separations in the micron and sub-micron region are probed, the measured force is indistinguishable within the errors from the Casimir force, which is much stronger than the Newtonian force, and so one can only set bounds on hypothetical non-Newtonian forces of the Yukawa type [21,44]. The strength of the obtained bounds depends crucially on the precision of the theoretical prediction of the Casimir force.

The above considerations motivated us to see if it is possible to work out a formula for the sphere-plate Casimir force that combines the precision of the scattering formula with the computational simplicity of the PFA. Our work builds up on the important progress that has been made in recent years in understanding the properties of the scattering formula.

We consider a sphere of radius $R$ placed at minimum distance $a$ from a plane (see fig. 1). For simplicity we assume that the sphere and plate are made of the same material, characterized by a common dynamical complex permittivity $\varepsilon(\omega)$. We shall specifically consider the case of Au, which is the standard material used in modern Casimir experiments. The exact scattering formula [27–29] for the Casimir free energy reads

$$\mathcal{F} = k_B T \sum_{n \geq 0} \text{Tr} \ln[1 - \hat{M}(\xi_n)],$$

(2)

where $k_B$ is Boltzmann constant, $T$ is the temperature, $\xi_n = 2\pi nk_B T/h$ are the (imaginary) Matsubara frequencies, the prime sign in the sum indicates that the $n = 0$ term is taken with weight 1/2. The trace $\text{Tr}$ in this equation is taken over the spherical multipole indices $(l,m)$ and on the polarization indices $\alpha = \text{TE,TM}$:

$$\text{Tr} = \sum_{m = -\infty}^{\infty} \sum_{l = \text{max}(1,|m|)}^{\infty} \text{tr},$$

(3)

where $\text{tr}$ denotes the trace over $\alpha$. The matrix elements $M_{lm,m',l'm'}$ of $\hat{M}$ shall not be reported here for brevity. Their explicit expressions can be found, for example, in ref. [12]. It suffices to say here that $M_{lm,m',l'm'}$ involves the Fresnel reflection coefficients of the plane, and the Mie scattering coefficients of the sphere, both evaluated for the imaginary Matsubara frequencies $\xi_n$. The Fresnel coefficients are multiplied by suitable products of the associated Legendre polynomial $P^{m}_{\ell}(\cos(\theta))$ and $P^{m}_{\ell}(\sinh(\theta))$, or their derivatives, and then integrated over the (imaginary) incidence angle $\theta$. The expressions for the Casimir force $F = -d\mathcal{F}/da$ and its gradient $F' = dF/da$ are obtained by taking derivatives of eq. (2) with respect to the separation $a$. In numerical simulations, the multipole indices $l,l',m,m'$ and the Matsubara index $n$ are truncated to $l,l' \leq l_{\text{max}}$, $m \leq m_{\text{max}}$ and $n \leq n_{\text{max}}$. The values of $l_{\text{max}},m_{\text{max}}$ and $n_{\text{max}}$ for which convergence is achieved scale with the separation $a$ as $l_{\text{max}} \sim R/a$, $m_{\text{max}} \sim \sqrt{R/a}$ and $n_{\text{max}} \sim \lambda_T/a$, where $\lambda_T = \hbar c/2\pi k_B T = 1.2\mu m$ is the thermal length [10–12]. It turns out that to estimate the Casimir force and its gradient with an accuracy of $10^{-4}$, as we seek, one needs $l_{\text{max}} \approx 6R/a$, $m_{\text{max}} \approx 6\sqrt{R/a}$, $n_{\text{max}} \approx 10\lambda_T/a$. Previous simulations [45,46] with $l_{\text{max}} = 45$ were used to compute quite precisely the force for $R/a < 20$. As we mentioned earlier, a new large simulation [31] reached $l_{\text{max}} = 2 \times 10^4$, making it possible to probe aspect ratios up to $R/a \sim 4 \times 10^4$. In our simulations we went up to $l_{\text{max}} = 120$, which allows us to compute the force with a precision of $10^{-4}$ for $R/a \leq 20$.

Below we prove that a very accurate formula for the Casimir force and its gradient can be obtained by a combined use of certain limiting exact solutions [16] and asymptotic formulae [10–12,15] that have been recently reported in the literature.

In [16] the separability of the Laplace equation in bi-spherical coordinates was exploited to derive an exact analytical formula for the classical limit, i.e., the $n = 0$ term of the complete scattering formula (2), of the Casimir energy of two metallic spheres described by the Drude model. Unfortunately, no exact solution is yet available for the $n = 0$ mode for the plasma model. Bispherical coordinates have been also used in [9] to derive a fast convergent numerical scheme and an approximate analytical formula for the van der Waals interaction of metallic plasmonic spheres. Another application of bispherical coordinates can be found in the work [47], which deals with the classical Casimir interaction of perfectly conducting sphere and plate. In the special sphere-plate case, the exact formula derived in [16] for the Drude classical Casimir energy reads

$$\mathcal{F}_{n=0}^{(\text{exact})} = \frac{k_B T}{2} \left\{ \sum_{l=1}^{\infty} (2l + 1) \ln[1 - Z^{2l+1}] + \ln \left[ 1 - (1 - Z^2) \sum_{l=1}^{\infty} Z^{2l+1} \frac{1 - Z^{2l}}{1 - Z^{2l+1}} \right] \right\},$$

(4)

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where the parameter $Z$ depends on the inverse of the aspect ratio $x = a/R$:

$$Z = [1 + x + \sqrt{x(2 + x)}]^{-1}. \quad (5)$$

By taking a derivative of the above formula with respect to $a$, the corresponding expression for the Casimir force $F_{n=0}^{(\text{exact})}$ and its derivative $F_{n=0}^{(\text{exact})}'$ are easily obtained.

Now we turn to the $n > 0$ terms of the scattering formula (2). Unfortunately, for $n > 0$ no exact solution is yet available, and we have to make recourse to approximations. It turns out that the contribution $F_{n>0}$ of the $n > 0$ terms to the Casimir force can be computed very accurately using the recently proposed DE [13–15]. To introduce the DE, we consider instead of the sphere a more general gently curved dielectric surface, described by a smooth height profile $z = H(x,y)$, where $(x,y)$ are Cartesian coordinates spanning the plate surface $\Sigma$, and the z-axis is drawn perpendicular to the plate towards the surface. The starting point of the DE is the assumption that the functional $F[H]_{n>0}$ admits a local expansion in powers of derivatives of the height profile $H$:

$$F[H]_{n>0} = F_{n>0}^{(\text{PFA})}[H] + \int_\Sigma d^2 x \alpha(H)(\nabla H)^2 + \rho^{(2)}. \quad (6)$$

The first term on the r.h.s. of the above equation coincides with the PFA (restricted to modes with $n > 0$),

$$F_{n>0}^{(\text{PFA})}[H] = \sum_{n>0} \int_\Sigma d^2 x F_n^{(pp)}(H), \quad (7)$$

where $F_n^{(pp)}(H)$ represents the contribution of the $n$-th Matsubara mode to the unit-area free-energy of two parallel plates at distance $H$, as given by Lifshitz formula [17]. The coefficient $\alpha(H)$ is a function to be determined, while the quantity $\rho^{(2)}$ represents a correction that becomes negligible as the local radius of curvature of the surface $R$ goes to infinity for fixed minimum-plate-distance $a$. The validity of the ansatz made in eq. (6) depends essentially on the locality properties of the Casimir force. The key point to notice here is that for imaginary frequencies $\omega = i\xi_n$ with $n > 0$ the photons acquire an effective mass proportional to $n$, which renders the interaction more and more local as $n$ increases, thus making the DE equation (6) more and more accurate. In previous works [14,15] the DE was used for all modes, including $n = 0$. For $n = 0$ the exact sphere-plate energy includes at the sub-sub-leading order complicated logarithmic terms [16] which render the DE less accurate for realistic values of $R/a$. Restriction of the DE to the massive $n > 0$ modes is the key ingredient to achieve a high precision. The function $\alpha(H)$ is determined by matching the DE with the perturbative expansion [48] of the Casimir force, in the common domain of validity of the two expansions (for details, see refs. [13–15]). When the integral in eq. (6) is evaluated for a sphere with $H(x,y) = a + (x^2 + y^2)/(2R) + \cdots$, and only terms up to order $a/R$ are retained, one ends up with an expression that can be recast in the form

$$F_{n>0} = F_{n>0}^{(\text{PFA})} \left(1 - \theta \frac{a}{R}\right). \quad (8)$$

In this equation $F_{n>0}^{(\text{PFA})}$ coincides with the familiar PFA formula for the sphere-plate force (restricted to modes with $n > 0$)

$$F_{n>0}^{(\text{PFA})} = 2\pi R \sum_{n>0} F_n^{(pp)}, \quad (9)$$

where $F_n^{(pp)}$ denotes the contribution of the $n$-th Matsubara mode to the unit-area free-energy of two parallel plates, as given by Lifshitz formula [17]. An analogous expression is obtained for the force gradient $F'$:

$$F'_n = F_n^{(\text{PFA})} \left(1 - \theta \frac{a}{R}\right), \quad (10)$$

where $F_n^{(\text{PFA})} = dF_{n>0}^{(\text{PFA})}/da$. The coefficients $\theta$ and $\hat{\theta}$ both depend on $a$, $\lambda_p$ and on the length parameters characterizing the materials of the sphere and plate (in the case considered here the plasma length $\lambda_p$ of Au), but are independent of the sphere radius $R$. In table 1 we list $\theta$ and $\hat{\theta}$ calculated for Au at room temperature ($T = 300K$), using tabulated optical data [49]. The weighted Kramers-Kronig dispersion relations [50] was used to compute precisely $\epsilon(\xi_n)$ starting from the real-frequency optical data given by Palik. The coefficients $\theta$ and $\hat{\theta}$ can be calculated also using the method developed by Bordag and Nikolaev [10–12], and we have verified that this alternative method gives for $\theta$ and $\hat{\theta}$ the same results as the DE.

Combining eq. (4) with eq. (8) we end up with the following approximate expression for $F$:

$$F_{\text{approx}} = F_{n=0}^{(\text{exact})} + F_{n>0}^{(\text{PFA})} \left(1 - \theta \frac{a}{R}\right). \quad (11)$$

An analogous formula can be derived for the force gradient $F'$:

$$F'_{\text{approx}} = F_{n=0}^{(\text{exact})} + F_{n>0}^{(\text{PFA})} \left(1 - \hat{\theta} \frac{a}{R}\right). \quad (12)$$

The above two equations represent the main result of this work.

We tested the precision of eqs. (11) and (12) by comparing them with high-precision numerical simulations up to $l_{\text{max}} = 120$ of the exact force and force gradient derived from the scattering formula (2). In our simulations the scattering formula was used only to estimate the modes $n > 0$, while for $n = 0$ we used the exact analytical formula (4). In fig. 2 we show the Casimir force for a Au-sphere of radius $R = 5 \mu m$. The force has been normalized by the PFA force for ideal sphere and plate $F_n^{(\text{PFA})} = \pi^3 hcR/(360a^3)$. The dots represent the numerical data computed using the fully converged exact scattering formula. The solid line shows a plot of our approximate formula for the force equation (8), while the dashed line is the standard PFA. It is evident that the
PFA performs fairly well for small separations, as expected, while it does quite poorly for moderate values of $R/a$. On the contrary, eq. (8) works remarkably well at all separations. A clear demonstration of the precision of eq. (8) is provided by fig. 3 which compares the percent errors made by the PFA (squares) and by eq. (8) (triangles). For $R = 5 \mu$m the maximum error made by eq. (8) is of 0.2 percent for $a = 1 \mu$m. The fact that the error becomes very small for separations $a$ exceeding a few microns should not come as a surprise, because for separations $a \gg \lambda_T = 1.2 \mu$m the exact classical $n = 0$ term dominates. More remarkable is the excellent performance of the formula on the small-distance side. The nature of the DE makes one expect that our formula becomes more and more accurate for smaller separations and/or larger sphere radii. Both expectations are fully confirmed by the data: when $a$ is decreased from one micron to 300 nm, keeping $R = 5 \mu$m, the error decreases from 0.2 to 0.1 percent. At the same time, when $R$ is increased from five to eight microns and $a$ is kept fixed, the error is seen to decrease for all separations. For example, for $a = 1 \mu$m, the maximum error decreases from 0.2 percent to 0.08 percent.

The dynamical experiment in [21] used a microtorsional mechanical oscillator to measure precisely the Casimir force derivative $F'$ between a Au sphere and plate for separations smaller than 700 nm, with an error of one percent for the smallest probed separation of 162 nm. The theoretical analysis in that experiment was based on the PFA, and it was concluded that the data are in disagreement with the Drude prescription, while they are in agreement with the plasma prescription [3]. It is interesting to compare the Drude-prescription values of the force-derivative $F'$ provided by our eq. (12) with the PFA. For the aspect ratios considered here, a conservative estimate of the error made by $F'_{\text{approx}}$ is smaller than 0.08 percent. In table 2 we list the respective values of $F'/2\pi R$ in mPa, computed for $R = 150 \mu$m. Within the PFA, $F'_{\text{PFA}}/2\pi R = F'_{\text{PP}}$, where $F'_{\text{PP}}$ is the plane-parallel pressure as given by Lifshitz formula [17]. As we see, $F'_{\text{approx}}$ differs from the PFA by less than 0.2 percent, confirming that the PFA is adequate for this experiment. The recent numerical simulation in [31] shows that the error made by the PFA is about two times larger if the plasma prescription is used, instead of the Drude prescription considered here.

In this letter we have derived a semi-analytic formula for the Casimir force and its gradient in the standard sphere-plate geometry used in current precision experiments. Although approximate, eqs. (8) and (10) are very accurate at all separations. Comparison with high-precision numerical simulations of the exact scattering formula demonstrates that the precision of the approximate formulae far exceeds the experimental uncertainty of present and foreseeable experiments, to the extent that the approximate formulae can be considered as experimentally

Table 1: Values of the coefficients \(\theta\) and \(\dot{\theta}\) for Au at room temperature.

| \(a (\mu m)\) | 0.10 | 0.15 | 0.2  | 0.25 | 0.3  | 0.35 | 0.4  | 0.45 | 0.5  | 0.55 | 0.6  | 0.65 |
|--------------|------|------|------|------|------|------|------|------|------|------|------|------|
| \(\theta\)   | 0.717| 0.694| 0.6645| 0.636| 0.609| 0.584| 0.561| 0.540| 0.520| 0.502| 0.485| 0.468|
| \(\dot{\theta}\) | 0.456| 0.4715| 0.470| 0.463| 0.454| 0.4445| 0.435| 0.425| 0.415| 0.4055| 0.396| 0.387|

| \(a (\mu m)\) | 0.70  | 0.75  | 0.8  | 0.85  | 0.9  | 0.95  | 1    | 1.2  | 1.4  | 1.6  | 1.8  | 2    |
|--------------|-------|-------|------|-------|------|-------|------|------|------|------|------|------|
| \(\theta\)   | 0.453 | 0.449 | 0.425| 0.413 | 0.400| 0.389 | 0.378| 0.339| 0.307| 0.279| 0.256| 0.237|
| \(\dot{\theta}\) | 0.379 | 0.370 | 0.362| 0.3545| 0.347| 0.3395| 0.332| 0.306| 0.282| 0.261| 0.242| 0.225|

Fig. 2: (Colour online) Casimir force for Au sphere ($R = 5 \mu$m) and plate at room temperature, normalized by the PFA force for ideal plates. The dots are numerical data computed using the fully converged exact scattering formula, the solid line is for the approximate formula (8), while the dashed line shows the standard PFA. All forces were computed for room temperature ($T = 300$ K) using Palik’s optical data for Au [49], extrapolated to low frequencies by the Drude model.

Fig. 3: Percent errors on the Casimir force made by the PFA (squares) and by the formula in eq. (11) (triangles).

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indistinguishable from the exact scattering formula. In this work we restricted our attention to the Drude prescription. Extension to the plasma model requires nontrivial modifications only for the \( n = 0 \) mode, since in the plasma case no exact solution is yet available for this mode. For the \( n > 0 \) modes eqs. (8)–(10) remain valid, apart from a minor change in the numerical values of the coefficients \( \theta \) and \( \tilde{\theta} \). We leave this topic for a future work.

It would be of great interest to carry out a detailed comparison between the predictions obtained by the large-scale simulation of [31] and the formulae presented here.

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Table 2: Values of \( F''/2\pi R \) (in mPa) for Au sphere plate at room temperature, computed using eq. (12) and the PFA.

| \( a \) (\( \mu m \)) | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 |
|----------------|-----|-----|-----|-----|-----|-----|
| \( F''_{\text{approx}}/2\pi R \) | 493.4 | 109.0 | 36.50 | 15.415 | 7.557 | 4.110 |
| \( F''_{\text{PFA}}/2\pi R \) | 493.7 | 109.1 | 36.53 | 15.43 | 7.568 | 4.117 |
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