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# CaPS: Casimir Effect in the Plane-Sphere Geometry

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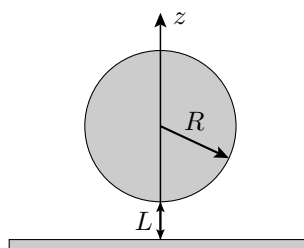
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## Summary

CaPS is a package for the analysis of the Casimir effect in the plane-sphere geometry. The Casimir force arises due to quantum and thermal fluctuations of the electromagnetic field and is closely related to the van der Waals force (Bordag, Klimchitskaya, Mohideen, & Mostepanenko, 2009). It is the dominant force between neutral non-magnetic materials in the nanometer to micrometer range and plays an important role in colloidal systems. Of technological relevance are applications to micro- and nano-electromechanical systems where the Casimir force can lead to stiction and thus constitute a failure mechanism (Buks & Roukes, 2001; Chan, Aksyuk, Kleiman, Bishop, & Capasso, 2001). On a more fundamental level, the Casimir effect is linked to the zero-point energy and the cosmological constant problem (Martin, 2012). A precise knowledge of the Casimir force is crucial for the search for possible deviations from Newton's law of gravitation that could arise from a fifth fundamental interaction (Antoniadis et al., 2011).

CaPS allows one to compute the Casimir interaction in the plane-sphere geometry as shown in Fig. 1. The plane-sphere geometry is most commonly used in precision measurements of the Casimir force. Specifically, CaPS allows one to compute the Casimir free energy and thus the Casimir force as a function of the sphere radius  $R$ , the minimal separation  $L$  between sphere and plane, the temperature  $T$ , and the material properties of plane and sphere. It is assumed that both objects are non-magnetic and placed in vacuum. In typical experiments the aspect ratio  $R/L$  is of the order of 1000. The main purpose of this package is to make aspect ratios as large as  $R/L \sim 5000$  accessible. Higher aspect ratios are usually well covered by the proximity force approximation.



**Figure 1:** Geometry of the plane-sphere setup: A sphere with radius  $R$  is separated by the distance  $L$  from an infinitely extended plate. In typical experiments, the aspect ratio  $R/L$  is about three orders of magnitude larger than shown here.

Within the scattering approach (Emig, Graham, Jaffe, & Kardar, 2007; Lambrecht, Maia Neto, & Reynaud, 2006), the Casimir free energy is given as a Matsubara sum

$$\mathcal{F} = \frac{k_{\text{B}}T}{2} \sum_{n=-\infty}^{\infty} \log \det (1 - \mathcal{M}(|\xi_n|))$$

with  $\xi_n = 2\pi n k_B T / \hbar$ .  $k_B$  and  $\hbar$  are the Boltzmann constant and Planck constant, respectively. The round-trip operator  $\mathcal{M}$  represents a complete round trip of an electromagnetic wave between the sphere and the plane. Commonly, the round-trip operator is expanded in the multipole basis. The numerical evaluation of the determinants demands a truncation of the originally infinite vector space. For a fixed accuracy, the required dimension scales linearly with the aspect ratio  $R/L$  and can become of the order of  $10^4$  or larger. Moreover, the matrices are ill-conditioned, making a numerical evaluation difficult. These problems limit the aspect ratios accessible in standard implementations to  $R/L \lesssim 100$  (Canaguier-Durand, 2011).

CaPS addresses these issues by using a symmetrized version of the round-trip operator  $\mathcal{M}$  as described in (Hartmann, 2018; Hartmann, Ingold, & Maia Neto, 2017; Hartmann et al., 2018). The matrix representation of the symmetrized round-trip operator yields hierarchical off-diagonal low-rank (HODLR) matrices that allow for a fast computation of determinants (Ambikasaran & Darve, 2013; Ambikasaran, O'Neil, & Singh, 2014). Specifically, we use HODLRLib (Ambikasaran, Singh, & Sankaran, 2019) for this purpose. Further information including explicit expressions for the matrix elements of the symmetrized round-trip operator and a run-time analysis can be found in (Hartmann, 2018; Hartmann et al., 2018).

CaPS provides the following main features:

- Computation of the free energy for aspect ratios used in typical experiments.
- Full support for perfect reflectors, metals described by the Drude and plasma model, and generic materials described by a user-defined dielectric function.
- Support for parallelization using MPI.
- Computation of the free energy in the high-temperature limit for perfect reflectors and metals described by the Drude or plasma model.

The computation of the high-temperature limit for the Drude model is based on (Bimonte & Emig, 2012).

Basic support for further geometries is provided for the special case of zero temperature and perfect reflectors:

- Computation of the free energy in the plane-cylinder geometry.
- Computation of the free energy for two spheres with equal radii.

The implementation for the plane-cylinder geometry is based on (Emig, Jaffe, Kardar, & Scardicchio, 2006).

Other packages that allow one to compute the Casimir free energy are SCUFF-EM (Reid & Johnson, 2015) and Meep (Oskooi et al., 2010). Both packages support arbitrary geometries and SCUFF-EM also has support for non-equilibrium Casimir forces. In contrast, CaPS targets the plane-sphere geometry where it allows one to cover the aspect ratios of the vast majority of existing experiments.

CaPS has been used to analyze negative Casimir entropies (Ingold et al., 2015; Umrath, Hartmann, Ingold, & Maia Neto, 2015), and to study corrections to the widely used proximity force approximation for experimentally relevant parameters (Hartmann et al., 2017). In addition, data generated using CaPS were used to analyze the experiments in Liu et al. (2019a) and Liu et al. (2019b). The package is released under the GPLv2 license.

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## References

- Ambikasaran, S., & Darve, E. (2013). An  $\mathcal{O}(N \log N)$  Fast Direct Solver for Partial Hierarchically Semi-Separable Matrices. *Journal of Scientific Computing*, 57(3), 477–501. doi:[10.1007/s10915-013-9714-z](https://doi.org/10.1007/s10915-013-9714-z)
- Ambikasaran, S., O’Neil, M., & Singh, K. R. (2014). Fast symmetric factorization of hierarchical matrices with applications. *arXiv e-prints*. Retrieved from <http://arxiv.org/abs/1405.0223>
- Ambikasaran, S., Singh, K. R., & Sankaran, S. S. (2019). HODLRlib: A Library for Hierarchical Matrices. *Journal of Open Source Software*, 4(34), 1167. doi:[10.21105/joss.01167](https://doi.org/10.21105/joss.01167)
- Antoniadis, I., Baessler, S., Büchner, M., Fedorov, V. V., Hoedl, S., Lambrecht, A., Nesvizhevsky, V. V., et al. (2011). Short-range fundamental forces. *Comptes Rendus Physique*, 12(8), 755–778. doi:[10.1016/j.crhy.2011.05.004](https://doi.org/10.1016/j.crhy.2011.05.004)
- Bimonte, G., & Emig, T. (2012). Exact Results for Classical Casimir Interactions: Dirichlet and Drude Model in the Sphere-Sphere and Sphere-Plane Geometry. *Physical Review Letters*, 109(16), 160403. doi:[10.1103/PhysRevLett.109.160403](https://doi.org/10.1103/PhysRevLett.109.160403)
- Bordag, M., Klimchitskaya, G. L., Mohideen, U., & Mostepanenko, V. M. (2009). *Advances in the Casimir Effect*. Oxford University Press. doi:[10.1093/acprof:oso/9780199238743.001.0001](https://doi.org/10.1093/acprof:oso/9780199238743.001.0001)
- Buks, E., & Roukes, M. L. (2001). Stiction, adhesion energy, and the Casimir effect in micromechanical systems. *Physical Review B*, 63(3), 033402. doi:[10.1103/PhysRevB.63.033402](https://doi.org/10.1103/PhysRevB.63.033402)
- Canaguier-Durand, A. (2011). *Multipolar scattering expansion for the Casimir effect in the sphere-plane geometry*. (PhD thesis). Université Pierre et Marie Curie – Paris VI. Retrieved from <https://tel.archives-ouvertes.fr/tel-00805047>
- Chan, H. B., Aksyuk, V. A., Kleiman, R. N., Bishop, D. J., & Capasso, F. (2001). Nonlinear Micromechanical Casimir Oscillator. *Physical Review Letters*, 87(21), 211801. doi:[10.1103/PhysRevLett.87.211801](https://doi.org/10.1103/PhysRevLett.87.211801)
- Emig, T., Graham, N., Jaffe, R. L., & Kardar, M. (2007). Casimir Forces between Arbitrary Compact Objects. *Physical Review Letters*, 99(17), 170403. doi:[10.1103/PhysRevLett.99.170403](https://doi.org/10.1103/PhysRevLett.99.170403)
- Emig, T., Jaffe, R. L., Kardar, M., & Scardicchio, A. (2006). Casimir Interaction between a Plate and a Cylinder. *Physical Review Letters*, 96(8), 080403. doi:[10.1103/PhysRevLett.96.080403](https://doi.org/10.1103/PhysRevLett.96.080403)
- Hartmann, M. (2018). *Casimir effect in the plane-sphere geometry: Beyond the proximity force approximation* (PhD thesis). Universität Augsburg. Retrieved from <https://opus.bibliothek.uni-augsburg.de/opus4/44798>
- Hartmann, M., Ingold, G.-L., & Maia Neto, P. A. (2017). Plasma versus Drude Modeling of the Casimir Force: Beyond the Proximity Force Approximation. *Physical Review Letters*, 119(4), 043901. doi:[10.1103/PhysRevLett.119.043901](https://doi.org/10.1103/PhysRevLett.119.043901)
- Hartmann, M., Ingold, G.-L., & Maia Neto, P. A. (2018). Advancing numerics for the Casimir effect to experimentally relevant aspect ratios. *Physica Scripta*, 93(11), 114003. doi:[10.1088/1402-4896/aae34e](https://doi.org/10.1088/1402-4896/aae34e)
- Ingold, G.-L., Umrath, S., Hartmann, M., Guérout, R., Lambrecht, A., Reynaud, S., & Milton, K. A. (2015). Geometric origin of negative Casimir entropies: A scattering-channel analysis. *Physical Review E*, 91(3), 033203. doi:[10.1103/PhysRevE.91.033203](https://doi.org/10.1103/PhysRevE.91.033203)

- Lambrecht, A., Maia Neto, P. A., & Reynaud, S. (2006). The Casimir effect within scattering theory. *New Journal of Physics*, 8(10), 243. doi:[10.1088/1367-2630/8/10/243](https://doi.org/10.1088/1367-2630/8/10/243)
- Liu, M., Xu, J., Klimchitskaya, G. L., Mostepanenko, V. M., & Mohideen, U. (2019a). Examining the Casimir puzzle with an upgraded AFM-based technique and advanced surface cleaning. *Physical Review B*, 100(8), 081406(R). doi:[10.1103/PhysRevB.100.081406](https://doi.org/10.1103/PhysRevB.100.081406)
- Liu, M., Xu, J., Klimchitskaya, G. L., Mostepanenko, V. M., & Mohideen, U. (2019b). Precision measurements of the gradient of the Casimir force between ultraclean metallic surfaces at larger separations. *Physical Review A*, 100(5), 052511. doi:[10.1103/PhysRevA.100.052511](https://doi.org/10.1103/PhysRevA.100.052511)
- Martin, J. (2012). Everything you always wanted to know about the cosmological constant problem (but were afraid to ask). *Comptes Rendus Physique*, 13(6), 566–665. doi:[10.1016/j.crhy.2012.04.008](https://doi.org/10.1016/j.crhy.2012.04.008)
- Oskooi, A. F., Roundy, D., Ibanescu, M., Bermel, P., Joannopoulos, J. D., & Johnson, S. G. (2010). Meep: A flexible free-software package for electromagnetic simulations by the FDTD method. *Computer Physics Communications*, 181(3), 687–702. doi:[10.1016/j.cpc.2009.11.008](https://doi.org/10.1016/j.cpc.2009.11.008)
- Reid, M. T. H., & Johnson, S. G. (2015). Efficient Computation of Power, Force, and Torque in BEM Scattering Calculations. *IEEE Transactions on Antennas and Propagation*, 63(8), 3588–3598. doi:[10.1109/TAP.2015.2438393](https://doi.org/10.1109/TAP.2015.2438393)
- Umrath, S., Hartmann, M., Ingold, G.-L., & Maia Neto, P. A. (2015). Disentangling geometric and dissipative origins of negative Casimir entropies. *Physical Review E*, 92(4), 042125. doi:[10.1103/PhysRevE.92.042125](https://doi.org/10.1103/PhysRevE.92.042125)