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CaPS: Casimir Effect in the Plane-Sphere Geometry

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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.

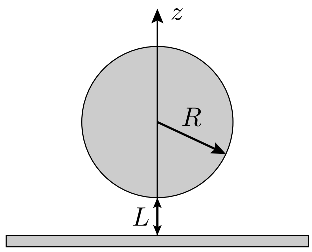

Figure 1: Geometry of the plane-sphere setup: A sphere with radius R is separated by the distance L from an infinitely extended plate. In typical experiments, the aspect ratio R/L is about three orders of magnitude larger than shown here.

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

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

with $\xi_n = 2\pi n k_\mathrm{B} T/\hbar$. 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 ration 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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