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Casimir forces for inhomogeneous planar media.

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Abstract. Casimir forces arise from vacuum fluctuations. They are fully understood only for simple models, and are important in nano- and microtechnologies. We report our experience of computer algebra calculations towards the Casimir force for models involving inhomogeneous dielectrics. We describe a methodology that greatly increases confidence in any results obtained, and use this methodology to demonstrate that the analytic derivation of scalar Green's functions is at the boundary of current computer algebra technology. We further demonstrate that Lifshitz theory of electromagnetic vacuum energy can not be directly applied to calculate the Casimir stress for models of this type, and produce results that have led to alternative regularisations. Using a combination of our new computational framework and the new theory based on our results, we provide specific calculations of Casimir forces for planar dielectrics having permittivity that declines exponentially. We discuss the relative strengths and weaknesses of computer algebra systems when applied to this type of problem, and describe a combined numerical and symbolic computational framework for calculating Casimir forces for arbitrary planar models.

1. Introduction

Casimir forces result from zero-point vacuum fluctuations confined between two dielectric materials [1]. Although these forces were predicted theoretically in the 1940s, empirical evidence confirming the theory has only been obtained in recent years [2, 3]. Lifshitz theory [4] is a theoretical approach to the calculation of Casimir forces, in which the Green's tensor for the electric field is used to derive electromagnetic stress and energy density.

The standard planar model is to have two plates, L and R , of uncharged dielectric materials separated in the x direction by a few micrometers. The materials have permittivities $\varepsilon_L(x, i\xi)$ and $\varepsilon_R(x, i\xi)$, depending on displacement and frequency ξ , which completely describe the media since we assume that there is no magnetic response (we enforce $\mu_L(x, i\xi) = 1 = \mu_R(x, i\xi)$ for the magnetic permeabilities involved). The gap between the plates, C , is either a quantum vacuum or third dielectric with $\varepsilon_C(x, i\xi)$ equal to a constant; we consider such a model to be *homogeneous*. For this model the Casimir force can be both calculated analytically and measured empirically [5].

In this paper we consider *inhomogeneous* models where the permittivity of the central region, $\varepsilon_C(x, i\xi)$, varies with x . In particular, we explore the applicability of Lifshitz theory to inhomogeneous models. The Lifshitz regularisation process described in Section 2 was derived with homogeneous media in mind, we therefore explore the possibility that this could be a confounding factor in attempts to calculate Casimir forces in the inhomogeneous case.

2. The calculation of Casimir stress in planar media

Stresses on objects in electromagnetic fields are given by Maxwell's stress tensor, in which $\hat{\mathbf{E}}$ and $\hat{\mathbf{H}}$ are respectively the electric and magnetic fields, $\hat{\mathbf{B}}$ is the magnetic induction and $\hat{\mathbf{D}}$ is the electric displacement.

$$\hat{\sigma} = \hat{\mathbf{E}} \otimes \hat{\mathbf{D}} + \hat{\mathbf{B}} \otimes \hat{\mathbf{H}} - \frac{1}{2}(\hat{\mathbf{E}} \cdot \hat{\mathbf{D}} + \hat{\mathbf{B}} \cdot \hat{\mathbf{H}})\mathbb{I}_3 \quad (1)$$

For stationary electromagnetic fields, the divergence of the Maxwell's stress tensor gives the force density $\hat{\mathbf{f}}$,

$$\hat{\mathbf{f}} = \nabla \cdot \hat{\sigma}. \quad (2)$$

The expectation values (also known as correlation functions) for the tensor products in Equation (1) are related to the retarded Green's function as follows:

$$\langle \hat{\mathbf{E}}(\mathbf{r}, t) \otimes \hat{\mathbf{D}}(\mathbf{r}', t) \rangle = -\frac{\hbar}{\pi c^2} \int_0^\infty d\xi \varepsilon(\mathbf{r}, i\xi) \xi^2 \mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi), \quad (3)$$

$$\langle \hat{\mathbf{B}}(\mathbf{r}, t) \otimes \hat{\mathbf{H}}(\mathbf{r}', t) \rangle = \frac{\hbar}{\pi} \int_0^\infty d\xi \frac{1}{\mu(\mathbf{r}, i\xi)} \nabla \times \mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi) \times \overleftarrow{\nabla}' \quad (4)$$

The notation $\times \overleftarrow{\nabla}'$ denotes a curl on \mathbf{r}' in $\mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi)$ from the right. $\mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi)$ is the retarded Green's tensor for the vector potential in a Coulomb gauge, and is defined as the solution of the following inhomogeneous electromagnetic wave equation

$$\nabla \times \frac{1}{\mu} \nabla \times \mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi) + \varepsilon \frac{\xi^2}{c^2} \mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi) = \delta(\mathbf{r} - \mathbf{r}')\mathbb{I}_3. \quad (5)$$

The Green's function should always obey the reciprocity relation:

$$\mathbf{G}(\mathbf{r}, \mathbf{r}', i\xi) = \mathbf{G}(\mathbf{r}', \mathbf{r}, -i\xi). \quad (6)$$

We are considering planar dielectrics, for which the permittivity $\varepsilon(\mathbf{r}, i\xi) = \varepsilon(x, i\xi)$ and magnetic permeability $\mu(\mathbf{r}, i\xi) = \mu(x, i\xi)$, i.e. depend only on the x-coordinate.

The Fourier-transformed Green's function $\mathbf{G}(x, x', u, v, i\xi)$ is given by the Fourier-transformed wave equation:

$$\nabla \times \frac{1}{\mu(x, i\xi)} \nabla \times \mathbf{G}(x, x', u, v, i\xi) + \varepsilon(x, i\xi) \frac{\xi^2}{c^2} \mathbf{G}(x, x', u, v, i\xi) = \delta(x - x'). \quad (7)$$

The Casimir force depends only on the xx -component of Maxwell's stress tensor because the force density is also independent of y and z. In the limit $\mathbf{r} \rightarrow \mathbf{r}'$, the result for σ_{xx} is

$$\sigma_{xx} = -\frac{\hbar c}{4\pi^2} \int_0^\infty du \int_0^\infty d\kappa u \left(\frac{1}{\mu} (w^2 - \partial_x \partial_{x'}) \tilde{g}_{Es} + \frac{1}{\varepsilon} (w^2 - \partial_x \partial_{x'}) \tilde{g}_{Ms} \right) \Big|_{v=0, \mathbf{x}'=\mathbf{x}}, \quad (8)$$

with

$$w = \sqrt{u^2 + v^2 + \varepsilon \mu \kappa^2}, \quad \kappa = \frac{\xi}{c},$$

$$\tilde{g}_{Es} = \tilde{g}_E - \mu \tilde{g}_0, \quad \text{and} \quad \tilde{g}_{Ms} = \tilde{g}_M - \varepsilon \tilde{g}_0.$$

In Lifshitz theory, \tilde{g}_{Es} and \tilde{g}_{Ms} are the regularized electric and magnetic Green's functions (where regularisation involves subtraction of the the relevant divergent part). \tilde{g}_0 is the infinite contribution from the retarded Green's function in a space with homogeneous medium:

$$\tilde{g}_0 = -\frac{1}{2w} e^{(-w|x-x'|)}. \quad (9)$$

Equation (7) reduces to

$$\frac{d^2}{dx^2} \tilde{g}(x) - (u^2 + v^2 + \varepsilon\kappa^2) \tilde{g}(x) = \delta(x - x') \quad (10)$$

where \tilde{g} denotes either the electric or magnetic Green's function, and in which none of the left-hand parameters depends on x . The general solution involves trigonometric functions and the Heaviside function; specific solutions are easily obtained from the boundary conditions.

3. Casimir forces for inhomogeneous planar media

To obtain the Casimir force for a planar dielectric model, the sequence of calculations is now :

- (i) Calculate the scalar Green's functions – Equation (7) – for the permittivity of the specific media under consideration (recalling the modelling assumption $\mu(x, i\xi) = 1$ described in Section 1). These calculations can be performed either numerically or analytically, but should incorporate two checks for internal consistency:
 - (a) The limits of the Green's functions from the left and from the right should be equal;
 - (b) The reciprocity relation – Equation 6 – should hold. Clearly, if either check fails then any further calculations will be in gross error. If both succeed, then there is no guarantee of correctness, although confidence in correctness is greatly increased.
- (ii) Perform the corrected regularisation – Equation 7 – in order to remove (most of) the infinite parts from the above scalar Green's functions. The theory behind these new results is beyond the scope of this paper, but it should be noted that, in general, infinite components remain (at the boundaries in the examples we have presented here). It may be that these discontinuities are artefacts of the new regularisation theory that do not represent physical truth, or it could be that Casimir stresses do tend to infinity at certain well-defined points. More research is needed into this intriguing possibility. In any event, the corrected regularisation is straightforward to compute as the parameters in the subtractions do not depend on x .
- (iii) Solve the double integral – Equation (8) – to obtain the stress tensor σ_{xx} . This is the hard part: we have obtained numerical solutions only for models involving exponential decay. Our approach is to make two simplifications:
 - (a) Instead of integrating from zero to ∞ , we integrate from zero to a “large” finite value which, for practical purposes, is determined by how much time we are prepared to wait for a solution;
 - (b) We search for approximations of values for the double integral at fixed points in the x region, followed by curve-fitting to obtain a smooth approximation of the stress, thereby reducing the problem to a single integration performed many times.

Even after these simplifications the resulting PDEs can not, in general, be solved using the numeric libraries of either Mathematica or Maple. Moreover, to our knowledge, no library of numeric PDE solvers (such as NAG) contains routines that solve our specific type of PDE. The main difficulties arise from the nature of the problem itself: there are, for example, three regular and one irregular singular points in the PDE of $gMs(x, x')$.
- (iv) The divergence of σ_{xx} is the theoretically predicted Casimir force per unit volume – Equation (2). This is trivial to compute given a smooth function that approximates the Casimir stress.

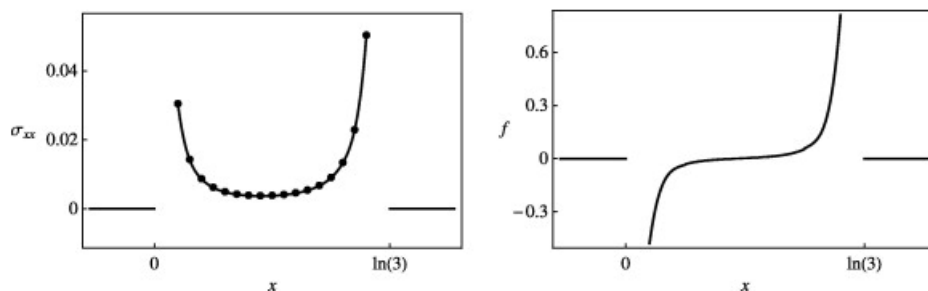


Figure 1. The Casimir stress (8) and the Casimir force per unit volume for the permittivity model $\varepsilon(x) = 3e^{-x}$ (with no magnetic response) from $x = 0$ to $x = 0.1$. In this case $\epsilon_R = \log_e(3)$.

4. Conclusions

We have reported the first (to our knowledge) calculations of Casimir forces for inhomogeneous permittivity models for planar dielectrics. Intermediate calculations suggested problems with the standard regularisation process: using these insights, new theoretical regularisation results have been derived [6], and we have incorporated and tested this new theory. We have described the computational framework used to obtain Casimir forces, and highlighted the work still needed before efficient computation for arbitrary models becomes a reality.

Our findings suggest that the calculation of scalar Green's functions for arbitrary inhomogeneous media is at the boundary of the current capabilities of Maple and Mathematica. Using Maple we can get satisfactory results for exactly one model, and believe we could increase the number of such models if the modified Heun function implementation within Maple were to be improved. Mathematica is less useful for these calculations, as no Heun function implementation is present in the current system. However, we have successfully replicated Maple results using Mathematica, indicating that the lengthy and complex Mathematica expressions produced as intermediate output are completely correct.

Future avenues of research include (i) the testing of any proposed alternative regularisation using our methodology of comparing results from two systems for both the the right and left limits, (ii) the development of a combined numeric-symbolic framework that agrees with the symbolically derived results presented here for the exponential model, and which can be used to calculate Casimir forces for those inhomogeneous model that lie beyond the current analytic capabilities of Maple and Mathematica.

Casimir forces remain difficult, both theoretically and in terms of practical computation. By predicting Casimir forces for more complicated models than simple constant-permittivity dielectrics, we can investigate the poorly-understood effects and interactions of forces at nano-scales. Moreover, our results form hypotheses for applied physics investigations: can the forces that we predict be measured in practical experiments? This multi-disciplinary approach involves investigations that are at, or beyond, the the current limits of computational mathematics, theoretical physics and applied physics.

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