Towards the calculation of Casimir forces for inhomogeneous planar media

C. Xiong[1], T.W. Kelsey[1*], S.A. Linton[1] and U. Leonhardt[2]

[1]School of Computer Science, University of St Andrews, KY16 9SX, UK
[xc,tom,sal]@cs.st-andrews.ac.uk

[2] School of Physics and Astronomy, University of St Andrews, KY16 9SS, UK
ulf@st-andrews.ac.uk

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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 boundatry 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 indicate the possibility of alternative regularisations. We discuss the relative strengths and weaknesses of computer algebra systems when applied to this type of problem, and suggest combined numerical and symbolic approaches towards a more general computational framework.

1 Introduction

Casimir forces result from zero-point vacuum fluctuations confined between two dielectric materials [4]. Although these forces were predicted theoretically in the 1940s, empirical evidence confirming the theory has only been obtained in recent years [3, 5, 7, 9, 11]. Casimir forces are important in nanotechnology and microtechnology: repulsive Casimir forces can reduce friction in nano- and micromechanical devices, whereas attractive forces can "glue" components together that are designed to be free-moving. Lifshitz theory [6] 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, and for variations of this model that include moving plates [12], the Casimir force can be both calculated analytically and measured empirically [1]. For extensions of this model involving more than two plates, numerical methods can be used to obtain the Casimir forces for specific types of plate [10].

*Correspondence to: Dr Tom Kelsey, School of Computer Science, University of St Andrews, KY16 9SX, UK; +44 (0)1334 463249 or +44 (0)1334 463253

In this paper we consider *inhomogeneous* models where the permittivity of the central region, $\varepsilon_C(x, i\xi)$, varies with x. The primary aim of the paper is to see which, if any, inhomogeneous models allow the analytic derivation of their Casimir forces from calculations performed in the widely-used computer algebra systems Maple (Waterloo Maple Inc., London, Ontario, Canada) and Mathematica (Wolfram Research Inc., Champaign, IL, USA). 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.

In Section 2 we give the standard Lifshitz theoretic approach to deriving Casimir stresses for homogeneous media, and discuss how these may be calculated using Maple and Mathematica. In Section 3 we describe our methodology for performing and checking similar calculations for inhomogeneous models, and outline the strengths and weakness of the two computer algebra systems. We present results that suggest that many, but not all, inhomogeneous models can not be dealt with analytically using current computer algebra capabilities. Section 4 contains our analysis of standard Lifshitz theory applied to the model in which the central permittivity decays exponentially ($\varepsilon_C(x, i\xi) = ae^{-bx}$), together with results that suggest that suitable alternative regularisations may be deriveable. In Section 5 we discuss computational aspects, such as the limitations of existing computer algebra systems, and the possibility of future numeric-symbolic approaches.

2 The calculation of Casimir stress in planar media

In this section we describe the mathematical and physical concepts involved in our computations, and present the sequence of calculations involved in determining the Casimir force for planar models. A more detailed exposition of the underlying physics, together with full derivation of the equations involved and descriptions of theoretic approaches other that that of Lifshitz, is given in [1]. The resulting sequence of calculations can, in principle, be done by hand, using symbolic computer algebra, via numeric techniques, or by a combined numeric-symbolic approach. We report on our experiences of the second of these options in Section 3.

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.

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

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

$$\hat{\mathbf{f}} = \nabla \cdot \hat{\sigma}. \tag{2}$$

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:

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

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

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 describe our extensive use of this as a check for correctness of our calculated scalar Green's functions in Section 3.
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 Green's function in terms of its Fourier transform in y and z is

$$\mathbf{G}(x,x',u,v,i\xi) = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \mathbf{G}(\mathbf{r},\mathbf{r}',i\xi)e^{-iu(y-y')-iv(z-z')}. \quad (7)$$

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

$$\nabla \times \frac{1}{\mu(x,i\xi)}\nabla \times \mathbf{G}(x,x',u,v,i\xi) + \varepsilon(x,i\xi)\frac{\xi^2}{c^2}\mathbf{G}(x,x',u,v,i\xi) = \delta(x-x'). \quad (8)$$

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

$$\begin{aligned}\sigma_{xx} &= -\frac{\hbar c}{8\pi^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} u\left(\frac{1}{\mu}(w^2-\partial_x\partial_{x'})\tilde{g}_{Es} + \frac{1}{\varepsilon}(w^2-\partial_x\partial_{x'})\tilde{g}_{Ms}\right) dudvd\kappa \,|_{\mathbf{x}'=\mathbf{x}} \\ &= -\frac{\hbar c}{4\pi^2}\int_{0}^{\infty} du \int_{0}^{\infty} d\kappa u\left(\frac{1}{\mu}(w^2-\partial_x\partial_{x'})\tilde{g}_{Es} + \frac{1}{\varepsilon}(w^2-\partial_x\partial_{x'})\tilde{g}_{Ms}\right) |_{v=0,\mathbf{x}'=\mathbf{x}}, \quad (9)\end{aligned}$$

with

$$\begin{aligned} w &= \sqrt{u^2+v^2+\varepsilon\mu\kappa^2}, \qquad \kappa = \frac{\xi}{c}, \\ \tilde{g}_{Es} &= \tilde{g}_E - \mu\tilde{g}_0, \quad \text{and} \quad \tilde{g}_{Ms} = \tilde{g}_M - \varepsilon\tilde{g}_0. \end{aligned}$$

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:

$$\tilde{g}_0 = -\frac{1}{2w}e^{(-w|x-x'|)}. \quad (10)$$

In summary, to obtain the Casimir force for a planar dielectric model, the sequence of calculations is:

1. calculate the scalar Green's functions – Equation (8) – for the permittivity of the specific media under consideration (recalling the modelling assumption $\mu(x,i\xi) = 1$ described in Section 1)

2. perform the regularisation that removes the infinite parts from the above scalar Green's functions

3. solve the double integral – Equation (9) – to obtain the stress tensor σ_{xx}

4. the divergence of σ_{xx} is the theoretically predicted Casimir force – Equation (2).

In the homogeneous case all the calculations can be performed analytically using either Maple or Mathematica, since $\varepsilon(x, i\xi)$ does not vary with x. Equation (8) reduces to

$$\frac{d^2}{dx^2}\tilde{g}(x) - (u^2 + v^2 + \varepsilon\kappa^2)\tilde{g}(x) = \delta(x - x') \tag{11}$$

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. The subtractions involved in stage 2 are also straightforward, again since neither μ nor ε varies with x. The double integrals with infinite ranges produce finite results, since the integrand converges to zero with increasing u and κ. Stage 4 is relatively simple. In Section 3 we commence our analysis of how the computational details are affected when homogeneity is no longer assured.

3 Specific inhomogeneous permittivity models

For a given model of the permittivity $\varepsilon(x)$ and $\mu = 1$ (no magnetic response), we first need to find the scalar Green functions,

$$\frac{d^2\tilde{g}_E}{dx^2} - \left(u^2 + \varepsilon(x)\kappa^2\right)\tilde{g}_E = \delta(x - x'), \tag{12}$$

$$\frac{d}{dx}\left(\frac{1}{\varepsilon(x)}\frac{d}{dx}\tilde{g}_M\right) - \left(\frac{u^2}{\varepsilon(x)} + \kappa^2\right)\tilde{g}_M = \delta(x - x'). \tag{13}$$

An intrinsic problem is the assessment of the validity of any results. The output from a computer algebra system will consist of symbolic expressions, which can be evaluated as real numbers for supplied values of the parameters involved. Empirical validation is not known to be possible for all models, and is expensive, time-consuming and technically demanding.

Our solution is to constrain our results to be the same when solving from the left and from the right. This is not a guarantee that any results obtained are correct, but it does increase confidence and allows us to detect models for which analytic solution is intractable using current computer algebra capabilities. Our methodology therefore is to perform the calculations using two computer algebra systems (Maple and Mathematica) and to use the reciprocity relations given in Equation (6). If the results from the two independent systems coincide, and if the results are the same from either the left 'or from the right, then we have a high level of confidence in their correctness.

For models such as $\varepsilon(x) = 1 + e^{-x}$ and $\varepsilon(x) = x^2$ using Maple we find that the reciprocity relations are violated in the magnetic case. Using Mathematica to perform the same calculations, we were unable to solve the equations analytically, and were therefore unable to perform the reciprocity check. The difference between the two systems is that recent versions of Maple contain an implementation of the use of Heun's functions [8] to solve ODEs. Heun's functions are the solutions of the Heun form of 2nd order linear ODEs;

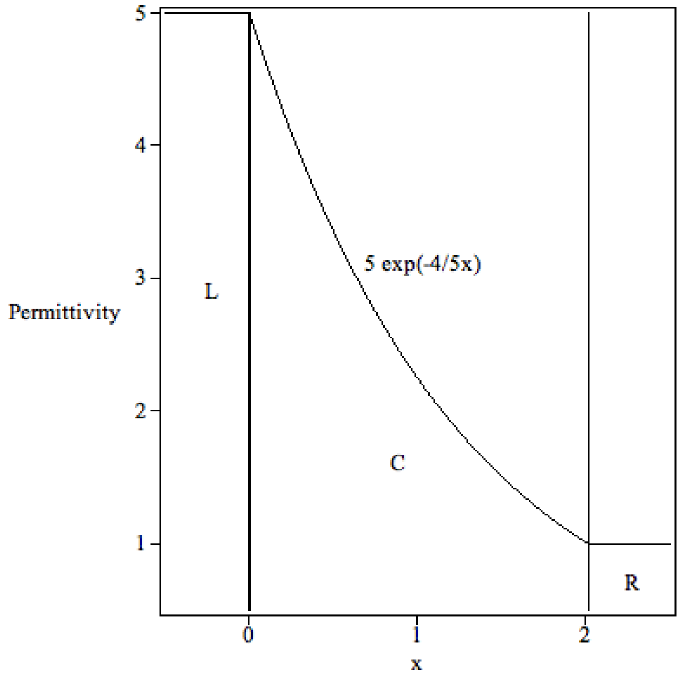

Figure 1: The inhomogeneous model given by $\varepsilon_L = 5$, $\varepsilon_C = 5\exp(-4/5x)$ and $\varepsilon_R = 1$. The central part runs from $x = 0$ to $x = log(a)/b \approx 2.0118$.

any such ODE can be converted into Heun form. Equation (12) is a linear 2nd order ODE, so, in Maple, it can be converted to Heun form and solved directly, with perfect agreement from the right and left directions. Equation (13) is non-linear, however. We can convert it into a modified Heun ODE and obtain a solution in the form of the product of a Heun C function and an exponential correction factor. There is a discrepancy between the left and right solutions, which appears to be introduced when the correction factor is computed. Unfortunately, we are never sure which, if either, of these results is correct, hence further work is needed to correct the Maple implementation. Mathematica, on the other hand, has no Heun ODE or function capabilities, and neither the linear nor nonlinear ODEs could be solved analytically.

We have found only one permittivity model for which the scalar Green's functions can be derived analytically (i.e. without using any numeric calculation options) with the reciprocity relations fully satisfied (Figure 1 is an illustrative example). This is exponentially decaying permittivity,

$$\varepsilon(x) = ae^{-bx}, \qquad \text{for positive constants } a \text{ and } b, \tag{14}$$

bounded on each side by homogeneous dielectrics.

For this case, the general solutions for $\tilde{g}_E$ and $\tilde{g}_M$ were found to be

$$\begin{aligned}\tilde{g}_E &= C_{E1}I_{\nu 1}(-\lambda) + C_{E2}K_{\nu 1}(\lambda) + \frac{2}{b}(I_{\nu 1}(-\lambda)K_{\nu 1}(\lambda') \\ &\quad -I_{\nu 1}(-\lambda')K_{\nu 1}(\lambda))\text{Heaviside}(\lambda - \lambda'),\end{aligned} \tag{15}$$

$$\begin{aligned}\tilde{g}_M &= C_{M1}\lambda I_{\nu 2}(-\lambda) + C_{M2}\lambda K_{\nu 2}(\lambda) \\ &\quad +\frac{b\lambda\lambda'}{2\kappa^2}(I_{\nu 2}(-\lambda)K_{\nu 2}(\lambda') - I_{\nu 2}(-\lambda')K_{\nu 2}(\lambda))\text{Heaviside}(\lambda - \lambda'),\end{aligned} \tag{16}$$

$$\text{where} \quad \lambda = \frac{2\kappa\sqrt{a}}{b}e^{-bx/2}, \qquad \nu 1 = 2u^2/b, \qquad \nu 2 = \sqrt{1+\nu 1^2}, \tag{17}$$

and in which the Cs are arbitrary coefficients determined by the continuity of

$$\tilde{g}_E, \qquad \tilde{g}_M, \qquad \frac{1}{\mu(x,i\kappa)}\partial_x\tilde{g}_E, \qquad \text{and } \frac{1}{\varepsilon(x,i\kappa)}\partial_x\tilde{g}_M \tag{18}$$

at the boundaries, and I and K are the modified Bessel functions.

Two interesting computational aspects were encountered. Firstly, Mathematica has no implementation of the Bessel K function; it instead uses expressions involving Gamma functions which are mathematically equivalent, but which are lengthy and hard for humans to interpret. Secondly, intermediate Maple output suggested the variable changes involving λ, $\nu 1$ and $\nu 2$ – Equations (17). These simplifying re-arrangements both (i) greatly aid the efficiency of the remaining calculations, and (ii) helped us to interpret and check the results. The calculations were therefore easier to perform in Maple than in Mathematica, but, for this model, both systems returned the same results, from the left and from the right, when evaluated as floats. We are therefore confident that our scalar Green's functions are exactly those needed for the Lifshitz regularisation process.

4 The testing of standard Lifshitz regularisation

Standard Lifshitz theory involves the subtraction the contribution to the stress that does not arise from material inhomogeneity. This is known to produce accurate (i.e. empirically verifiable) results for the standard model where the gap between the two plates is either empty or filled with a homogeneous dielectric. However, this approach is known to result in an infinite Casimir force in models involving cylinders and spheres [2]. In certain cases an alternative regularisation has been found (but not always agreed upon by the expert community), whilst for others the problem of calculating a finite stress using any theoretical approach remains unsolved. For our model (exponentially decaying permittivity for the central medium) we therefore expect to either (i) use standard Lifshitz theory to calculate a finite Casimir force, (ii) derive an infinite force, with the structure of the results indicating the possibility of alternative regularisation, or (iii) derive an infinite force, with no clues on how to proceed.

Our results, displayed for illustrative parameter choices in Figure 2, indicate that the for one of the wave parameters (κ) we obtain convergence to a finite integrand, but for the other (u) the integrand diverges. Unfortunately, we can no longer consider κ and u to be the respective x and y wave components, since we have performed a Fourier transformation.

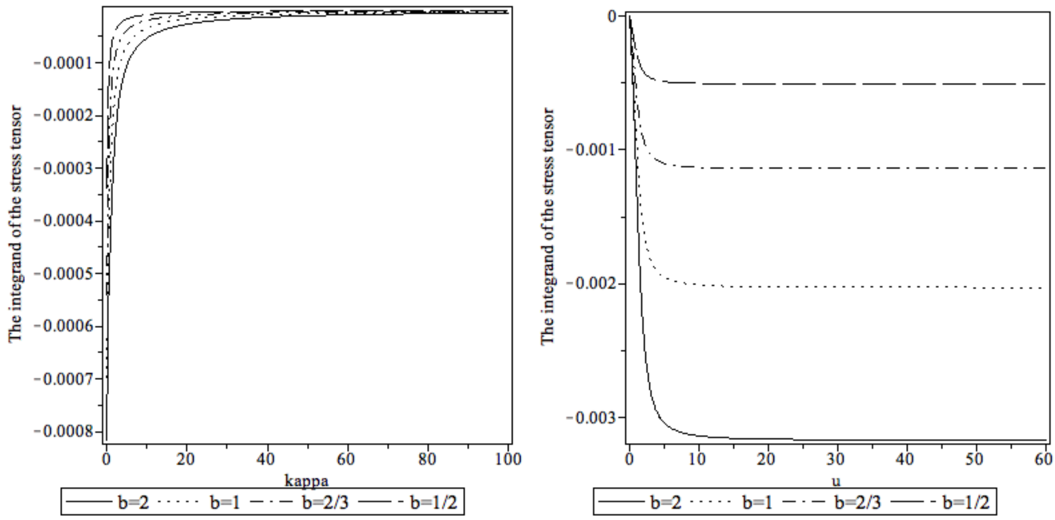

Figure 2: The integrand of the stress tensor obtained from Green's functions regularised using Lifshitz theory. We use the conventions that the physical constants $\hbar = c = 1$. The central permittivity model is $\varepsilon(x) = 5\exp(-bx)$. As κ increases, the integrand converges to zero (left plot). As u increases, the integrand converges to a nonzero constant, the value of which depends on the model parameter b but not on a (right plot).

Further investigation of the divergence shows that the constant nonzero value depends neither on a or x, but only on b (Figure 3). Routine simplification, (setting $x = x'$) gives the divergence constant DC for the stress tensor as a function of b:

$$DC = -\frac{\hbar c}{8\pi^2} b, \tag{19}$$

where $\hbar$ and c are the standard notation for the reduced Planck constant and the speed of light in a vacuum respectively. This divergent behaviour leads to the prediction of an infinite Casimir force, which is not a physically realistic outcome. However, the predictability of the amount of divergence suggests that it may be possible to modify Lifshitz theory for this model, so that a plausible finite Casimir force is predicted. Such as regularisation has recently been proposed [13], with the resulting Casimir forces calculated using the methodology presented in this paper.

5 Conclusions

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.

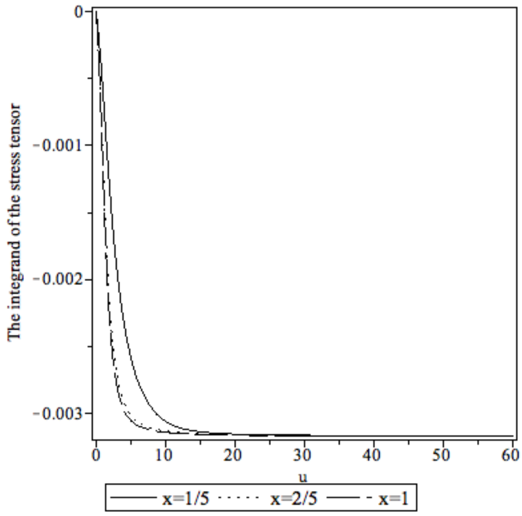

Figure 3: The integrand of the stress tensor obtained from Green's functions regularised using Lifshitz theory. We use the conventions that the physical constants $\hbar = c = 1$. The central permittivity model is $\varepsilon(x) = 5\exp(-bx)$. Model parameters have been set as $a = 5$ and $b = 4/5$. We observe that for fixed b, the nonzero convergence value is the same for all choices of x in the central region.

We are highly confident that our scalar Green's function calculations are accurate. In addition to the approach described in Section 3, we split the Green's functions into bare and scattered parts, allowing us to derive the specific solution of the bare part using initial rather than boundary conditions. The results of these calculations agree with those described in this paper for both systems, and hence also satisfy out reciprocity constraints.

In Sections 3 and 4 we discussed the first two stages of Casimir force prediction using Lifshitz theory. The third stage, a complicated double integration over infinite ranges, is, in general, not computable analytically in either Maple or Mathematica for inhomogeneous models. Instead, we substitute a realistically high finite value for the infinities and obtain numeric approximations. For example, in the model presented in Figures 2 and 3 with $u = 150$ the integrand has a magnitude of 10^{-13}, descreasing to zero with increasing u. Stage 4 is well within the capabilities of any decent computer algebra system.

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.

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