Finite difference computation of Casimir forces

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Abstract. In this Invited paper, we begin by a historical introduction to provide a motivation for the classical problems of interatomic force computation and associated challenges. This analysis will lead us from early theoretical and experimental accomplishments to the integration of these fascinating interactions into the operation of realistic, next-generation micro- and nanodevices both for the advanced metrology of fundamental physical processes and in breakthrough industrial applications. Among several powerful strategies enabling vastly enhanced performance and entirely novel technological capabilities, we shall specifically consider Casimir force time-modulation and the adoption of non-trivial geometries. As to the former, the ability to alter the magnitude and sign of the Casimir force will be recognized as a crucial principle to implement thermodynamical nano-engines. As to the latter, we shall first briefly review various reported computational approaches. We shall then discuss the game-changing discovery, in the last decade, that standard methods of numerical classical electromagnetism can be retooled to formulate the problem of Casimir force computation in arbitrary geometries. This remarkable development will be practically illustrated by showing that such an apparently elementary method as standard finite-differencing can be successfully employed to numerically recover results known from the Lifshitz theory of dispersion forces in the case of interacting parallel-plane slabs. Other geometries will be also be explored and consideration given to the potential of non-standard finite-difference methods. Finally, we shall introduce problems at the computational frontier, such as those including membranes deformed by Casimir forces and the effects of anisotropic materials. Conclusions will highlight the dramatic transition from the enduring perception of this field as an exotic application of quantum electrodynamics to the recent demonstration of a human climbing vertically on smooth glass.

1. Introduction

At the dawn of modern understanding of the existence of interatomic forces, made possible by the application of non-relativistic quantum mechanics [1], two issues became immediately central: the role played by the optical properties of interacting particles, which led to the use of the term dispersion by Eisenschitz and London [2] to characterize such forces, and the question of dispersion force additivity, quickly identified by London [3] as critical to the development of a theory of cohesion. Starting during World War II, it was suggested by Overbeek [4] and Verwey [5] that an additional element must be crucial to a satisfactory explanation of existing experimental data on the stability of lyophobic colloids: electrodynamical retardation [6].

This profound intuition was the inspiration for the work by Casimir and Polder towards a theory of interatomic forces fully consistent with quantum electrodynamics (QED) [7]. In a development fraught with immense consequences in the history of physics, Casimir continued his work in search for a deeper meaning for the result he had found with Polder and, after
an illuminating conversation with Niels Bohr [8], he reformulated the problem in terms of the zero-point energy of the electromagnetic field in the quantum vacuum [9]. An application of this approach to the problem of the force between two neutral, perfectly conducting parallel planes separated by an empty gap led Casimir, in 1948, to the famous equation for what is now referred to as the Casimir effect [10].

These momentous results successfully addressed the issue of retardation but the problem of the interaction between macroscopic bodies at very close range could only still be considered by assuming additivity and proceeding by integrations in the continuum approximation [6] as done for slabs and spherical particles by de Boer [11] and Hamaker [12], respectively. As pointed out by Milonni [13] with the benefit of hindsight, since the Clausius-Mossotti relation provides a link between atomic optical properties and the dielectric functions of the bulk material, a straightforward application of additivity to the retarded Casimir-Polder result could have shown that the Casimir effect between perfect conductors should be, in some sense, expected. However, a full generalization of the equation for the Casimir force to the simplest realistic case of two semi-infinite dielectric slabs including retardation had to wait until 1955. This remarkable achievement was contributed by Lifshitz, who employed a classical stochastic approach [14], based on solving the Maxwell equations including a noise term introduced by Rytov [15] to describe the fluctuating field within the dielectric media [16]. The final expression, reached through a very significant mathematical effort, has been confirmed by several other approaches [13] and it stands, still today, as the standard solution to the problem. Importantly, as also noticed by Lifshitz, use of the theory requires knowledge of the complex dielectric function of the bulk interacting materials over the entire frequency range [17].

Direct experimental verification of the force between two plane slabs separated by a gap is exceedingly difficult due to the challenge to accurately ensure parallelism [18] and it has been successfully reported very rarely [19]. Much more typical since the very first attempts in this field is the use of a sphere-plane system, which entirely circumvents such difficulties [13, 20, 21, 22, 23, 24, 25, 26, 27, 28]. The connection between the Lifshitz expression and experiments involving sphere-plane or sphere-sphere setups is made by the proximity force approximation [20, 29] (PFA), although challenges remain [30].

A development fueling further great interest in Casimir forces is the growing recognition that applications of such interactions are likely to lead to novel micro- and nano-technology solutions impossible or impractical to achieve by any other means [31, 32, 33, 34, 35, 36]. One of the major challenges in executing this transfer of Casimir force-enabled technologies into marketable solutions is the fact that industrial devices will not at all conform to the strict idealizations of the Lifshitz theory, including its basic plane-plane geometry. Hence the problem of the computation of dispersion forces in realistic geometries has become timely for reasons beyond even the needs of fundamental physics and not dissimilar from those motivating the development of computer-aided design (CAD) tools [37].

In the rest of this paper, rather than to discuss extreme mathematical detail, we present the key issues with a few useful references in order to provide a fish-eye view of the computational program underway at our Laboratory including fundamental motivations, status and goals in several subfields. This material is complemented by further details and references in recent mini-reviews at Refs. [38, 39, 40].

2. Dispersion force computation: Challenges and opportunities

Unlike such fundamental interactions as gravitation and electromagnetism, field equations in the form of the Einstein of Maxwell equations are not known for the general case of dispersion forces. In the limit of rarefied materials, in which the additivity approximation is held to apply, it is possible to formulate the problem in terms of central forces inversely proportional to a power $p \geq 3$ of the interatomic distance, $s$, as already done by Newton and rediscovered by de Boer
and Hamaker [41]. However, the results are completely unreliable in the general case and indeed counterexamples exist of systems in which the net force of atoms attracting each other as pairs is repulsive [42]. Under these circumstances, the natural option is to seek numerical solutions but, for quite some time, the very problem to solve could not be formulated.

The situation changed drastically in 2007 with the introduction of a numerical imaginary frequency Green’s function computation (IFGFC) method by researchers at MIT working with their collaborators [43]. Not only has the theoretical foundation provided a path to the numerical computation of dispersion forces in any geometry but it has also shown that the algorithm can be built based, with relatively little modification, on procedures largely known from classical electromagnetism. In the last few years, implementations and variations of this algorithm, initially pursued by the finite-difference frequency domain (FDFD) method, have therefore grown exponentially providing the first glimpse of interacting systems that could never before been treated [26]. Hence this is an extremely exciting time in the field of the numerical calculation of Casimir forces as the opportunity exists to explore systems for which no previous intuition can anticipate a reliable solution.

Of course, as with any numerical algorithm, the issue of computational facilities has emerged forcefully somewhat ameliorated by the fact that the intrinsic parallelization of the problem lends itself to supercomputing implementations.

3. Motivations for a finite-difference (FD) computation approach

Our program in this area has moved in a different direction than that of the mainstream [37]. Instead of pursuing development of code of increased complexity running on highly competitive machines, we have pursued the study of implementations based on the simplest possible approach, finite differencing (FD), to be run on readily available computers and a widely used computer algebra system [44] or on Fortran 90/95. Our goals with this approach are multifaceted. First, understanding the behavior of Casimir force solutions acquired by the FD method is of intrinsic interest not necessarily motivated by the need for competitiveness. Second, any solution represents a useful tool for developers working on other, possibly more effective algorithms and in need to obtain a check with results from completely different systems about problems that have never been previously solved and for which analytical solutions are probably unavailable. Third, the typical simplicity of FD algorithms translates into a relatively small code development time investment in exchange for access to problems of great importance. Finally, the FD approach is readily accessible to undergraduate students [45] thus offering opportunities for research projects that might otherwise be unaccessible at much higher levels of sophistication.

3.1. Standard FD approach

The first step into the standard FD implementation of Casimir forces was taken choosing the one-dimensional (1D) case for diagnostics [37]. In this model, both the electric and magnetic fields are assumed to fluctuate along fixed axes with respect to the two interacting slabs. In addition to demonstrating convergence to the available analytical solution, an important step forward was taken by considering dielectric boundaries not coinciding with mesh points. A second step was the generalization of this method to the case of 1D multilayers [46]. In order to carry out initial meaningful parallelization experiments, we have employed a computer algebra system capable to detect and take advantage of multiple cores on a legacy Cray CX1-LC (up to 8 cores in the present implementation) with Red Hat Enterprise Linux.

3.2. Non-standard FD schemes

Another important contribution of our initial effort was the identification of a non-standard FD scheme that exactly reproduces the necessary discrete Green’s functions (DGFs). The motivation
to pursue such an approach, beyond its intrinsic interest, is that it might shed light on more efficient FD schemes in higher dimensions.

3.3. Pedagogy
There exists a very rich literature of applications of the FD scheme in electrostatics due to its immediacy for undergraduate students [45]. Our goal is to develop FD code of Casimir force computations as part of activities for students carrying out research projects both in Fortran 90/95 and in a computer algebra system. Initial experience has already shown that students exposed to this curriculum will be well prepared to make transitions to other languages such as C and other computational methods such as FE, FDFD, BEM, etc on any platform. This process also presents unique opportunities to illustrate the role of Green functions (GF) by employing their discrete counterparts (DGF) for easier visualization.

4. Exemplary outstanding problems
Here we survey some interesting problems to be considered as both diagnostics and research by our numerical effort in dispersion forces.

4.1. Multilayers
No experiment is ever actually carried out between the two homogeneous dielectric slabs of the archetypal Lifshitz formulation since layers naturally form on any surface and also because such layers will often be part of the design. For instance, many experiments involve the interaction of substrata coated in gold (Au) or with even more complex architectures [23]. In addition, there is great interest in the use of multilayers, such as photonic crystals, as a means to engineer the Casimir force by altering its dependence as a function of the gap width between the two slabs. Although analytical solutions for such parallel plane geometry exist [17], research on multilayers in more complex geometries is relatively young.

4.2. Edge effects
In analogy to the standard capacitor problem of electrostatics, a typical assumption of the Lifshitz theory is that the gap width be much smaller than the later size of the interacting slabs. Numerical solutions can aid in developing or testing analytical expressions for Casimir force fringe effects.

4.3. Static deflection
One of the earliest considerations of the effects of Casimir forces in micro-electromechanical systems (MEMS) was as a leading cause of stiction [32]. In a later development, an effort was made to analytically determine the static deflection of microbridges and conditions for pull-in of such structures to the underlying substratum [47]. All such calculations are necessarily approximations due to the fact that, rigorously speaking, the microbridge and the substratum are no longer parallel. Numerical computations are necessary to explore the reliability of all conclusions drawn on the basis of such analytical methods specially in the case of 2D structures for which much less information is available.

As already mentioned, dispersion forces are making a rapid transition from being avoided as the cause of a failure mode – stiction – to being exploited as an enabling design component. One concept along these lines has been that of an adaptive optics system deformed not by mechanical pressure or electrostatically as typically is the case but by Casimir forces [48].
4.4. **Free and driven anharmonic Casimir vibrations**

Although the problem of a 1D anharmonic Casimir oscillator has been analyzed and also explored experimentally in MEMS [49], no generalization of such results to 2D membranes has been developed. Such systems could also serve as parametric resonators and amplifiers if the magnitude of the Casimir force between the substratum and the oscillating membrane can be modulated in time [50].

4.5. **Non-trivial topologies, anisotropic materials and Casimir torque**

A very active area for recent generalizations of the Lifshitz theory has been that of anisotropic materials both in the slabs and in the gap itself because, under specific circumstances, not only dispersion forces but also dispersion torques may appear [51, 52, 53, 54, 55, 56, 57, 58, 59, 60] and play obviously important technological roles. The behavior of such systems in more complex geometries as well as with elastic membranes is largely unexplored.

4.6. **Nanomechanical oscillators**

One of the environments in which dispersion forces completely dominate system dynamics due to the extremely small interlayer gap is that of multiwalled telescoping nanotubes with cores in oscillation or rapid ejection [35, 38]. In such structures, numerical methods would be beneficial to assess use of the proximity force approximation in very small tubes as well as the effect of illumination on the optical properties of the interacting layers [61].

4.7. **Nanomechanical engine cycles**

No realistic nanotechnological application of dispersion forces can be implemented without a means to transfer energy to and from the system. Typically, this limitation is addressed by mechanically actuating [23, 49] one of the two interacting surfaces so as to drive the other one into vibration. The problem is even more critical in nanotube applications in which it may be nearly impossible to access the oscillating shuttle [38, 62]. One of the most realistic proposals to implement nanoengines [63] is to use the dependence of dispersion forces on illumination as verified, with some open issues, by Arnold, Hunklinger and Dransfeld [64] and confirmed several years later by means of atomic force microscope (AFM) methods [65]. Numerical models are needed to create far more realistic models of the engine cycles so as to account for mutual spectral perturbations of moving interacting boundaries expected on energy conservation considerations [36] also in non-trivial geometries.

4.8. **Acoustic Casimir effect**

Although this is not often appreciated, the Casimir effect takes place not only in quantized but also in classical fields. This can be appreciated from the fact that, for instance, the radiation pressure interpretation of the Casimir force, suggested by Casimir himself [10], reiterated by Debye [66], and fully developed by Milonni, Cook, and Goggin, does not require that the radiation be quantized (Ref. [13], p. 293 and Ref. [67], p. 210). The most dramatic demonstration of such a classical effect is probably the acoustic Casimir effect, in which broadband noise is introduced by means of compression drivers according to a spectrum specifiable by the experimenter [68, 69]. Unlike the electrodynamical Casimir effect, most experimentation in this area has explored the parallel-plane case since, due to the vastly smaller value of the speed of sound with respect to the speed of light, typical gap widths will be \( s \sim 1 \text{ cm} \). For this reason, both theoretical calculations and experimentation on non-parallel plates and completely different geometries are unavailable.
5. Target applications

Let us consider the possible applications of knowledge developed, for instance, by FD schemes to evaluate Casimir forces and torques based on the assigned geometry and physics of any system possibly also under dynamical conditions.

5.1. Design tools

Dispersion forces are expected to become a key enabling technology on the micro- and nano-scales and therefore a sophisticated design tool to document the effect of such interactions in realistic market product designs is expected to be highly desirable. A possible outcome will be the evolution of dispersion force computation algorithms into an indispensable module for multiphysics analysis of such novel technologies [70]. Due to the different nature of these interactions, connected to this computing capability is also the need for enhanced visualization solutions in 3D so as to aid the designer take advantage of dispersion forces to achieve a specific technological goal.

5.2. Experiment modeling

Next generation dispersion force experimentation is poised to measure extremely small forces to unprecedented accuracy [71]. Yet, dispersion forces are now known to strongly interact with other environmental variables, such as temperature [72, 73], in possibly complex ways so that a quantitative understanding of the complex role of dispersion forces in yielding the data acquired will contribute to realistic estimates of experimental errors, still a very controversial topic [74, 75].

5.3. NOEMS and nanostructures

Beyond fundamental physics experimentation, a host of dispersion force based applications are expected to enter the marketplace in the near future [39, 40]. Perhaps the most stunning is the class of products generally referred to as “gecko glue,” which represents the most convincing demonstration that forces once characterized as weak and exotic [36] have proven themselves as potentially dominant on the macroscale. Fascinatingly, these materials have more recently evolved into novel human climbing [76] and space grappling [77] tools. Because of the drastic dependence of dispersion forces on topology, such products can only be optimized by means of accurate mathematical modeling. Such considerations extend to all nanomachines with parts actuated by dispersion force modulation, including, for instance, nanodevices for various types of medical purposes [78, 79].

5.4. Energy storage and conversion

The possibility to employ the van der Waals interaction, an important cause of cohesion and adhesion [80], as a ‘reservoir’ for energy storage was first proposed by Robert Forward in 1984 [31]. At the time, the idea, though fascinating, appeared somewhat unworkable because the surface energy density of two ordinary surfaces separated by realistic gap widths is many orders of magnitude below values of practical interest when compared, for instance, to traditional chemical batteries. However, further research into the concept has revealed that, for instance, arrays of vertical telescoping nanotubes, due to their much higher specific surface and much smaller gap width (in this case, the distance between the outer wall and the sliding inner tube) could store energy at densities even higher than those of chemical storage [35]. Far more accurate computation tools, however, could dramatically expedite the exploration of the extremely vast parameter space of various geometries and compounds and identify the best route to this new storage technology.
6. Conclusions
The computation of dispersion forces is an exponentially growing field of research with unique connections to such theories as quantum electrodynamics (QED) and acoustics, numerical techniques including, as we have seen, traditional FD methods, and extending horizontally to software design, applied physics, engineering, product analysis and business development. This field will contribute to the development of breakthrough industrial products and to next generation scientific experiments, and, as such, it offers remarkable opportunities for discovery both for professional researchers and for students just beginning to explore the practice of science.

6.1. Acknowledgments
Partial funding was made available by a Jazan University Deanship of Scientific Research grant. Nurdoğan Can (Jazan University) provided additional indispensable logistical resources. Elias C. Vagenas (Kuwait University) kindly hosted an invited talk on the subject of this paper at the 5th International Conference on Mathematical Modeling in Physical Sciences (IC-MSQUARE) held in Athens, Greece.

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