Numerical Calculation of the Force on some Generalized Casimir Pistons

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Abstract. In this talk I presented numerical calculations of the Casimir force due to a scalar field on a piston in a cylinder of radius $r$ with a spherical cap of radius $R > r$. Geometrical subtractions give a finite interaction energy. Due to reflection positivity, the vacuum force on the piston by a scalar field satisfying Dirichlet boundary conditions is attractive for these geometries, but the strength and short-distance behavior of the force depends strongly on the shape of the piston casing. For a cylindrical casing with a hemispherical head of large radius, the attractive force on the piston is inversely proportional to the square of the height of the piston.

1. Introduction
Below I define finite subtracted vacuum (interaction) energies that determine Casimir forces\cite{1} in piston geometries. A similar geometrical approach was first used by Power\cite{2} to obtain the well-known Casimir force between two parallel plates without regularizing potentially infinite zero-point energies. There has been renewed interest in such piston geometries\cite{3} because the electromagnetic vacuum self-energy of a cube (as that of a sphere\cite{4}) is positive\cite{5}. The force on a partition in a parallelepiped nevertheless is attractive\cite{6, 7, 8} at any position.

Semi-classical considerations suggest that the Casimir force on a piston depends strongly on the shape of the casing\cite{9}. I here numerically calculate the vacuum force due to a massless scalar field satisfying Dirichlet boundary conditions for some generalized Casimir pistons by generalizing the world-line approach to Casimir interaction energies of Gies et al.\cite{10} to include geometries with connected boundaries. In Casimir pistons all domains are bounded and the mathematical treatment in fact is much simpler and clear-cut than for the scattering situation with a continuous spectrum. A finite subtracted vacuum energy gives rise to the force on the piston. In the examples studied here, all domains are convex and numerical computations are vastly simplified by considering the convex hulls of Brownian bridges\cite{11}.

2. World-line approach for connected bounded domains
Consider the heat kernel operator $\mathcal{R}_D(\beta) = e^{\beta \Delta / 2}$ for the Laplacian $\Delta$ with Dirichlet boundary conditions on a bounded domain $D \subset \mathbb{R}^3$. The spectrum of eigenvalues $\{\lambda_n > 0, n \in \mathbb{N}\}$ of the negative Laplace operator in this case is discrete, real and positive. The corresponding spectral function (or trace of the heat kernel),

$$\phi_D(\beta) = \text{Tr} \mathcal{R}_D(\beta) = \sum_{n \in \mathbb{N}} e^{-\beta \lambda_n / 2}, \quad (1)$$

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is finite for $\beta > 0$. It has the well-known[12, 13, 14, 15] high-temperature (short-time) expansion,

$$\phi_\mathcal{D}(\beta \sim 0) \sim \frac{1}{(2\pi\beta)^{3/2}} \sum_{n=0}^{\infty} (2\pi\beta)^{n/2} a_n(\mathcal{D}) + \mathcal{O}(e^{-r^2/\beta}). \quad (2)$$

For smoothly bounded domains, the heat kernel coefficients $a_n(\mathcal{D})$ in this series are integrals over powers of the local curvature and reflect average geometric properties of the domain and its boundary[16, 17], such as the volume $V_\mathcal{D} = a_0(\mathcal{D})$ and the surface area $S_\mathcal{D} = -4a_1(\mathcal{D})$ of $\mathcal{D}$. Since $a_4(\mathcal{D}) \neq 0$ implies a logarithmic divergent vacuum energy, the vanishing of this coefficient is crucial for an unambiguously defined Casimir energy. Non-analytic and (for $\beta \sim 0$) exponentially suppressed contributions to the asymptotic expansion of $\phi_\mathcal{D}(\beta)$ are associated with classical periodic- and diffractive- orbits[18] of minimal length $l$.

The world-line approach to Casimir energies[10] relies on the fact[16, 19] that the spectral function for a bounded flat Euclidean domain $\mathcal{D}$ can be expressed in terms of its support of standard Brownian bridges. In three dimensions,

$$\phi_\mathcal{D}(\beta) = \int_{\mathcal{D}} \frac{dx}{(2\pi\beta)^{3/2}} P[\ell_\beta(x) \subset \mathcal{D}], \quad (3)$$

where $\ell_\beta(x) = \{B_\tau(x, \beta), 0 \leq \tau \leq \beta; B_0(x, \beta) = B_\beta(x, \beta) = x\}$ is a standard Brownian bridge from $x$ to $x$ in ”proper time” $\beta$ and $P[\ell_\beta(x) \subset \mathcal{D}]$ denotes the probability that such a bridge is entirely within the bounded domain $\mathcal{D}$. Note that $P[\ell_\beta(x) \subset \mathcal{D}]/(2\pi\beta)^{3/2}$ is the Green function from $x$ to $x$ in time $\beta$ of the associated diffusion problem with Dirichlet boundary conditions on $\partial \mathcal{D}$.

Eq.(3) implies that the spectral function for a domain of finite volume is finite. Divergences arise only in the corresponding zero-point energy. For finite vacuum energies, the leading – five, in three dimensions– heat kernel coefficients in Eq.(2) would have to vanish. Although impossible to achieve for a single domain, one can improve the asymptotic behavior by considering a (finite) linear combination of spectral functions for domains $\{\mathcal{D}_k; k = 0, 1, \ldots, M\}$

$$\tilde{\phi}(\beta) = \sum_k c_k \phi_{\mathcal{D}_k}(\beta). \quad (4)$$

When the coefficients $c_k$ are such that

$$\sum_k c_k a_i(\mathcal{D}_k) = 0 \quad \text{for} \quad i = 0, \ldots, 4, \quad (5)$$

the ”interaction” vacuum energy,

$$\mathcal{E}_{\text{int}} = -\pi \int_0^{\infty} \frac{d\beta}{(2\pi\beta)^{3/2}} \tilde{\phi}(\beta) = \sum_k c_k \mathcal{E}_{\text{vac}}(\mathcal{D}_k), \quad (6)$$

is finite because the integrand is $\mathcal{O}(\beta^{-1/2})$ for $\beta \sim 0$ when Eq.(5) holds. The $\mathcal{E}_{\text{vac}}(\mathcal{D}_k)$'s are the (divergent) formal zero-point energies of a massless scalar field satisfying Dirichlet boundary conditions on the individual bounded domains $\mathcal{D}_k$. The linear combination $\mathcal{E}_{\text{int}}$ of these vacuum energies is the difference in the zero-point energy of domains with the same total volume, total surface area, average curvature, topology,etc...

The subtraction procedure outlined above is preferable to conventional regularization procedures for numerical computations, because it can be implemented as a restriction on the set of paths. One thus avoids the numerically difficult computation of small differences in large
The overall proportionality constant in Eq.(10) is 4 times that in[10] because the unit loops here are defined by a standard Brownian bridge process rather than one of twice the variance.

3. Convex Domains and Convex Hulls

Fig. 1 depicts a suitable combination of convex domains for computing the interaction vacuum energy $E_{\text{int}}$ of a cylindrical Casimir piston of radius $r$ with a cap of radius $R \geq r$. A finite overall length $L$ ensures that the volumes of all convex domains is finite.

The main advantage of using the convex hull in numerical computations rather than the unit-loops themselves, is that the hull is a vastly reduced point-set that retains all the relevant

\[ E_{\text{int}} = -\frac{1}{8\pi^2} \int d\mathbf{x} \int_0^{\infty} d\beta \sum_k c_k \Theta[\mathbf{x} + \sqrt{\beta} \mathbf{H}[\ell_1(0)] \subset \mathcal{D}_k] \ell_1(0) \]

where the expectation $\langle \ldots \rangle_{\ell_1(0)}$ is with respect to unit loops (standard Brownian bridges over unit time). Eq.(10) is the basic formula\(^1\) used for computing Casimir interaction energies in the world-line approach[10]. Although the straightforward interpretation of an integrated interaction energy density is lost by the change in integration variables $\mathbf{x} = \mathbf{q}/\lambda, \beta = \lambda^{-2}$, the last expression for $E_{\text{int}}$ in Eq.(10) is slightly better adapted for numerical evaluation.

\(^1\) The overall proportionality constant in Eq.(10) is 4 times that in[10] because the unit loops here are defined by a standard Brownian bridge process rather than one of twice the variance.
The interaction Casimir energy $E_{\text{int}}(a)$ for a cylindrical cavity of radius $r$ with a cap of radius $R \geq r$ and a moveable planar piston at height $a$. $E_{\text{int}}(a)$ is the difference in vacuum energy of the cavity with and without piston compared to this difference for a cylinder of the same radius $r$. This difference of differences in vacuum energies is finite for all values of $a, r, L \gg 2r$ and $R \geq r$. $E_{\text{int}}$ does not require regularization and for $L \gg a$ only $E_{\alpha}$ depends on the position of the piston. Solid lines denote surfaces on which Dirichlet boundary conditions are imposed. Thick dashed lines in Figs. 1 indicate where the surface of the cylinder would be: Brownian bridges that pierce these surfaces give no contribution to $E_{\text{int}}(a)$, leading to condition (11) for large $L \gg 2r$. Note that all five different bounded domains are convex and bounded for finite $L$.

Information for the partition function on convex domains, but discards the irrelevant sequential ordering and the great number of interior points of a loop. The number of vertices of the convex hull increases only logarithmically with the number of points defining the loop. The convex hull of a loop given by a thousand points on average has $\sim 55$ vertices and that of one with a million points has about 190 vertices (see Fig. 2). The time required by efficient algorithms to compute the hull (with $v$ vertices) of $n$ points is proportional to $n \log(v)$ [24]. In evaluating the integrations in Eq.(10) for sufficiently complex convex domains $D$ like those in Fig. 1, one only requires the convex hulls.

To evaluate the spatial- and scale- integrals in Eq.(10) for a given set of vertices defining a hull, $\mathcal{F}(\ell_1(0)) = \{ \mathbf{v}_i = (x_i, y_i, z_i); i = 1, \ldots, v \}$, note that (for $L \gg r$) the only significant contribution to the interaction energy $E_{\text{int}}$ of the combination of domains shown in Fig. 1 comes from loops (hulls) that pierce the piston and the piston head, but not the cylinder. (11)

The cylindrical symmetry of the domains in Fig. 1 allows one to rotate the offset $\mathbf{q}$ of any loop (hull) to the positive $x$-axis and perform one angular integral trivially, resulting in

$E_{\text{int}}(\text{cyl}, \text{piston}) = -\frac{1}{2\pi} \int_0^\infty \rho d\rho \int_{-\infty}^\infty dz \int_0^\infty d\lambda \sum_k c_k \Theta(\rho, 0, z) + \mathcal{F}(\ell_1(0)) \subset \lambda \mathcal{D}_k) \ell_1(0)$. (12)

Further details on the numerical algorithm used to compute Eq.(12) are given in [11]. To verify the accuracy of the algorithm and estimate systematic errors, I compared (see Fig. 3) the numerical results for $R \gg r \gg d$ with the known analytic Casimir energy due to a scalar satisfying Dirichlet boundary conditions on two parallel circular plates of area $S = \pi r^2$ (half the electromagnetic Casimir energy[1] of this configuration). For $R \gg r \gg a$ the numerical results were compared with the semiclassical estimate of the asymptotic behavior in[11],

$E(a \ll r \leq R \leq 1.05r) = -\frac{hc}{96\pi a} \left( \frac{\sqrt{R^2 - r^2}}{a} + 1 + \mathcal{O}(a/r) \right)$. (13)
Figure 2. On the left is a typical triangulated hull of a Brownian bridge defined by $10^5$ points. It has 286 faces and 145 vertices and the shape of an irregularly cut rhinestone with large triangular facettes and intricate corners. The average number of vertices ($v$) of the convex hull of a Brownian bridge given by $n$ points can be read off the left axis of the graph using the upper (red) curve. Data points are from numerical simulations. The inset is the formula for the (red) trendline that best describes the data. The right axis and lower (green) line give the average CPU-time used to compute the hulls on a laptop with a 2GHz processor. Note that the left axis is linear while the right axis is logarithmic.

Including only statistical errors, the asymptotic numerical data for $r \leq R \leq 1.02r$ is best reproduced by,

$$
E_{\text{int}}(\frac{a}{R} \ll \frac{r}{R} \lesssim 1) \sim -\hbar c \left( \frac{0.00395(5) \sqrt{R^2 - r^2}}{a^2} + \frac{0.00326(4)}{a} + O(a/r) \right).
$$

The coefficients of the $\sqrt{R^2 - r^2}/a^2$ and $1/a$ terms are comparable and the leading $0.00326(4)/a^2$-behavior of the attractive force on the piston with a hemispherical head differs by less than 2% from the semiclassical estimate in Eq.(13). This 2% discrepancy is as good an estimate of the systematic errors of the numerical calculation as any I can give at this level of accuracy (the statistical error of the calculations is about 1.2%). Fig. 3 shows the difference between the numerical results and the asymptotic semiclassical energy for the hemispherical Casimir piston in a linear plot. Note that the residual force is small and repulsive.

4. Discussion

The Casimir force on a piston by a massless scalar field satisfying Dirichlet boundary conditions depends qualitatively on the shape of the casing in the systems of Fig. 1. Whereas the attractive force for small piston height $a \ll r$ is proportional to $r^2/a^4$ for a flat cylinder head, it is proportional to $\sqrt{R^2 - r^2}/a^3$ for heads with a curvature radius $r < R \ll r^2/a$ and for a hemispherical piston with $(R = r)$ is inversely proportional to $a^2$. Note that the asymptotic behavior of Eq.(13) implies that one percent deviation in radius from a hemispherical cylinder head doubles the Casimir force on the piston at a height $a \sim 0.1r$. Fig. 3 indicates that the Casimir force on the piston depends qualitatively on $R/r$ and at small piston height $a/r$ may range over several orders in magnitude.

The interaction Casimir energy defined in Eq.(10) is a priori finite (and does not require regularization) when the conditions of Eq.(5) are satisfied. Only a portion of the vacuum energy
Figure 3. The dimensionless Casimir interaction energy $r\mathcal{E}_{\text{int}}(a)/(\hbar c)$ for the cylindrical cavities of radius $r$ with caps of radius $R \geq r$ of Fig. 1 as a function of the rescaled height $a/r$ of the moveable piston. Dots indicate numerical results (dot size does not represent errors, which are too small to show on this logarithmic plot). Solid lines are piston-based Proximity Force Approximation (PFA) estimates (note that the PFA overestimates the interaction energy by an order of magnitude for $R = 1.02r$). Dashed curves correspond to the asymptotic semiclassical estimate of Eq. (13). Note the many orders of magnitude between a piston with a flat (bottom, purple) and a hemispherical (top, red) cylinder head.

is computed that includes all its dependence on the piston height $a$ and determines the force on the piston. To relate this interaction vacuum energy of a massless scalar to the spectral function of the Laplace operator, leading terms in the high-temperature expansion have to be canceled. This was here achieved by subtracting spectral functions of domains with the global characteristics represented by the first few (five in three dimensions) heat kernel coefficients. This subtraction procedure in particular implies that finite Casimir energies are differences in the vacuum energy of domains with the same topology, same volume, same average curvature etc...

The linear combination of vacuum energies for $\mathcal{E}_{\text{int}}$ in the present examples is shown in Fig. 1 – for $L \gg r$ only $\mathcal{E}_a$ depends on the height $a$ of the piston. The Casimir energy due to a massless Dirichlet scalar in this case is given by the positive probability measure for Brownian paths that satisfy Eq.(11). This implies an attractive Casimir force on the piston for any separation $a$ and cap radius $R > r$. A similar argument implies that the Casimir force by a Dirichlet scalar is attractive for a large class of piston geometries for which a condition on the Brownian bridges like Eq.(11) holds – including pistons and cylinders of arbitrary cross-section and form, with cylinder heads that are entirely contained within the cylinder. Cylinder heads that extend beyond the cylinder have also been examined[25]. Other classes of loops contribute in this case and the interaction energy can have either sign.

A semiclassical analysis of the geometries presented here reproduced[11] the numerical results for the force on the piston to better than 2% for $a/r < 0.1$, it in particular gives the correct asymptotic behavior of the force for $a/r \to 0$. By contrast, the PFA is inapplicable and overestimates the force on the piston by an order of magnitude for a hemispherical head. For a hemispherical cap the attractive Casimir force on the piston $-\hbar c/(96\pi a^2)$ does not depend on the radius $r = R \gg a$ of the cylinder and cap and mimics the electrostatic force on a metallic piston.
Figure 4. The difference $\Delta E(a) = E_{\text{int}}(a) + \hbar c/(96 \pi a)$ of the numerical- and asymptotic semiclassical-estimate for the scalar Casimir interaction energy of a hemispherical piston. The energy difference is plotted in dimensionless units against the piston height $a$ in units of the cylinder radius $r$. Only statistical errors of the numerical calculation are shown. The numerical results are those of Fig. 3 for $R = r$ and were obtained from the convex hulls of $10^5$ unit loops, each given by $10^5$ points. The (red) dot at $a/r = 0$ is the semiclassical contribution to this difference due to periodic orbits\[11\].

exerted by a charge $q^2/(\hbar c) = 1/(48\pi) \sim 1/150.8 \lesssim \alpha_{EM}$ on the axis of the cylinder at $z = 0$. This paradoxical situation arises only for the Casimir energy of a massless scalar field satisfying Dirichlet (Neumann) boundary conditions. Semiclassically the asymptotic contribution to the interaction energy due to a scalar field satisfying Neumann boundary conditions is the same in magnitude as that in Eq. (13) but of the opposite (positive) sign. This for a hemispherical piston at small $a/r$ dominant contribution to the interaction energy due to a Dirichlet scalar therefore is absent in the semiclassical approximation for metallic boundary conditions[9]. Contrary to the Dirichlet case, the reflection positivity argument fails for metallic and/or Neumann conditions, because these introduce correlations in the fluctuations on either side of the piston. The numerical (and semiclassical) attraction obtained here for all the piston configurations studied, therefore should not be taken to imply attraction for other, more realistic boundary conditions. In view of the fact that small variations in the geometry can change the Casimir force by many orders of magnitude, it remains a challenge to develop numerical methods that reliably estimate electromagnetic Casimir forces for complicated geometries.

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