Surface divergences and boundary energies in the Casimir effect

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Abstract. Although Casimir, or quantum vacuum, forces between distinct bodies, or self-stresses of individual bodies, have been calculated by a variety of different methods since 1948, they have always been plagued by divergences. Some of these divergences are associated with the volume, and so may be more or less unambiguously removed, while other divergences are associated with the surface. The interpretation of these has been quite controversial. Particularly mysterious is the contradiction between finite total self-energies and surface divergences in the local energy density. In this paper we clarify the role of surface divergences.

PACS numbers: 03.70.+k, 11.10.Gh, 03.65.Sq, 11.30.Ly

1. Introduction

The subject of local energy density associated with the confinement of quantum fields by surfaces has a rather long history. For example, Brown and Maclay [1] computed the vacuum expectation value of the electromagnetic energy-momentum tensor between two parallel perfectly conducting plates, which is twice that of a conformally coupled massless scalar field satisfying Dirichlet or Neumann boundary conditions on the plates, namely for plates separated by a distance $a$ in the $x$ direction,

$$\langle T^{\mu\nu}\rangle = \frac{\pi^2}{1440a^4} \text{diag} (-1, -3, 1, 1),$$

which corresponds precisely to the attractive energy or pressure found by Casimir [2] in the same situation. If a nonconformal scalar stress tensor is used, a position-dependent term in the stress tensor appears, which does not contribute to either the total energy or the pressure on the plates [3][4].

Local surface divergences were first discussed for arbitrary smooth boundaries by Deutsch and Candelas [5]. They found cubic divergences in the energy density as one approaches the surface; for example, outside a Dirichlet sphere (that is, for a

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conformally-coupled scalar field satisfying Dirichlet boundary conditions on the surface) the energy density diverges as

\[ u \sim \frac{1}{360\pi^2} \frac{1}{a(r-a)^3}, \]

(2)

where \( a \) is the radius of the sphere.

This raises the question: How can it be that the total Casimir energy of a Dirichlet sphere (or a perfectly conducting sphere in electrodynamics) is finite? The electromagnetic case is the well-known one first calculated by Boyer [6], \( E^E = 0.04618/a \), while the scalar case was first worked out by Bender and Milton [7], \( E^S = 0.002817/a \). In general the Casimir energy of a region bounded by a perfect hyperspherical surface depends in a complicated way upon the number of spatial dimension \( D \), as shown in Figure 1.

Thus there has been a suspicion since the time of Deutsch and Candelas that there was something incomplete in the calculations of Casimir self energies of ideal closed boundaries. (We note that there is now a proof that any smooth perfectly conducting boundary possesses a finite electromagnetic Casimir energy [9]. Whether such an idealized limit is physical is, of course, another question.) This suspicion has been recently intensified by a series of talks and papers by Graham et al [10]. The essential outcome of their analysis is that for a \( \delta \)-function sphere, described by the following Lagrangian for a massless scalar field,

\[ L = -\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} \frac{\lambda}{a^2} \delta(r-a)\phi^2, \]

(3)

a divergence occurs in third order in \( \lambda \). (They claimed a divergence in second order, but that was spurious, arising from the omission of a surface term in the integration by parts [3, 11, 12]. See (30) below.) This divergence in \( O(\lambda^3) \) in fact was discovered much earlier by Bordag, Kirsten, and Vassilevich [13], and possible ways of dealing with it have been suggested [14, 15]. Objections complementary to those of Graham et al
have also been voiced by Barton [16, 17], all of which raise doubts as to the physical relevance of results such as those of Boyer.

2. Green’s function for λ sphere

We consider the potential
\[ \mathcal{L}_{\text{int}} = -\frac{\lambda}{2a^2} \phi^2 \sigma(r), \]  
where \( \sigma(r) = \begin{cases} 
0, & r < a_-, \\
\hbar, & a_- < r < a_+, \\
0, & a_+ < r. 
\end{cases} \]  
(4)

Here \( a_\pm = a \pm \delta/2 \), and we set \( \hbar \Delta = 1 \). We have chosen the dimensions of \( \lambda \) so that the total energy of interaction does not explicitly refer to the radius \( a \). In the limit as \( \delta \to 0 \) (or \( \hbar \to \infty \)) we recover the \( \delta \)-function sphere.

The Green’s function equation, with \( \kappa^2 = -\omega^2 \),
\[ \left( -\nabla^2 + \kappa^2 + \frac{\lambda}{a^2} \sigma \right) \mathcal{G}(r, r') = \delta(r - r'), \]  
(5)

may be straightforwardly solved. We introduce the reduced Green’s function
\[ \mathcal{G}(r, r') = \sum_{lm} g_l(r, r') Y_{l}(\theta, \phi) Y^*_{lm}(\theta', \phi'), \]  
(6)

which in turn may be expressed in terms of the modified Riccati-Bessel functions,
\[ s_l(x) = \sqrt{\frac{\pi x}{2}} I_{l+1/2}(x), \quad e_l(x) = \sqrt{\frac{2x}{\pi}} K_{l+1/2}(x). \]  
(7)

The reduced Green’s function is, outside of the shell:
\[ r, r' < a_- : \quad g_l = \frac{1}{k' r} \left[ s_l(k'r_<) e_l(k'r_> - s_l(k'r_<) e_l(k'r_>) \right], \]  
(8a)
\[ r, r' > a_+ : \quad g_l = \frac{1}{k' r} \left[ s_l(k'r_<) e_l(k'r_> - \hat{\Xi} e_l(k'r_<) e_l(k'r_>) \right]. \]  
(8b)

Here the denominator is
\[ \Xi = [k s_l(k'a_-) e_l(k'a_+) - k' s_l(k'a_-) e_l(k'a_-)][k' e_l(k'a_-) s_l(k'a_+) - k e_l(k'a_-) s_l(k'a_-)] \]  
\[ - [k s_l(k'a_-) s_l(k'a_-) - k' s_l(k'a_-) s_l(k'a_-)][k' e_l(k'a_-) e_l(k'a_-) - k e_l(k'a_-) e_l(k'a_-)] - [k s_l(k'a_-) e_l(k'a_-) - k' s_l(k'a_-) e_l(k'a_-)][k' e_l(k'a_-) s_l(k'a_-) - k e_l(k'a_-) s_l(k'a_-)], \]  
(9)

while the numerator \( \hat{\Xi} \) is obtained from \( \Xi \) by replacing \( s_l(k'a_-) \to e_l(k'a_-) \), and \( \hat{\Xi} \) is obtained from \( \Xi \) by replacing \( e_l(k'a_-) \to s_l(k'a_-) \). Here \( k' = \sqrt{\kappa^2 + \lambda \hbar} \). Green’s function within the shell, \( a_- < r < a_+ \), is given by
\[ g_l = \frac{1}{k' r} \left\{ s_l(k'r_<) e_l(k'r_>) - \frac{1}{\Xi} \left[ s_l(k'r_<) e_l(k'r_') + s_l(k'r_<) e_l(k'r') \right] \right\} \]  
\[ \times [k e_l(k'a_-) e_l(k'a_+) - k' e_l(k'a_-) e_l(k'a_+)] \left[ k s_l(k'a_-) s_l(k'a_-) - k' s_l(k'a_-) s_l(k'a_-) \right] \]  
\[ - s_l(k'r_<) s_l(k'r_') [k e_l(k'a_-) e_l(k'a_+) - k' e_l(k'a_-) e_l(k'a_+)] \]  
\[ \times [k s_l(k'a_-) e_l(k'a_-) - k' s_l(k'a_-) e_l(k'a_-)] \]  
\[ - e_l(k'r_<) e_l(k'r_') [k e_l(k'a_-) s_l(k'a_-) - k' e_l(k'a_-) s_l(k'a_-)] \]  
\[ \times [k s_l(k'a_-) s_l(k'a_-) - k' s_l(k'a_-) s_l(k'a_-)] \right\}, \]  
(10)
3. Energy density

We can calculate the local energy density from the stress tensor:

\[ T^\mu\nu = \partial^\mu \phi \partial^\nu \phi - g^\mu\nu \mathcal{L} - \xi (\partial^\mu \partial^\nu - g^\mu\nu \partial^2) \phi^2, \]  

from which the energy density follows:

\[ T^{00} = \frac{1}{2} \left[ \partial^0 \phi \partial^0 \phi + \nabla \cdot \nabla \phi + \frac{\lambda}{a^2} \sigma \phi^2 \right] - \xi \nabla^2 \phi^2, \]  

where the conformal value is given by \( \xi = 1/6 \). To obtain the one-loop vacuum expectation values, we use the connection to the Green's function

\[ \langle \phi(x)\phi(x') \rangle = \frac{1}{i} G(x, x'). \]  

The energy density thus is, within or outside the shell,

\[ \langle T^{00} \rangle = \frac{1}{2i} \left[ \frac{\partial^0 \phi \partial^0 \phi + \nabla \cdot \nabla \phi + \frac{\lambda}{a^2} \sigma \phi^2}{\xi} \right] - \xi \nabla^2 \phi^2. \]  

When we insert the partial wave decomposition of the Green’s function [6], the expression for the energy density is immediately reduced to (inside or outside the shell, but not within it)

\[ \langle T^{00} \rangle = \int_0^\infty \frac{dk}{2\pi} \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \left\{ \frac{1}{\kappa^2 + \partial_r \partial_{r'} + \frac{l(l+1)}{r^2}} \right\} g_l(r, r') \bigg|_{r'=r} - 2 \frac{1}{r^2} \frac{\partial}{\partial r} \frac{1}{r^2} \frac{\partial}{\partial r} g_l(r, r) \right\}. \]  

We insert the Green’s function in the exterior region, but delete the free part, the first term in (8a), (8b), (10), which corresponds to the bulk energy which would be present if either medium filled all of space, leaving us with for \( r > a_+ \) (for \( r < a_- \), \( e_l \to s_l \) and \( \hat{\Xi} \to \tilde{\Xi} \))

\[ u(r) = -(1 - 4\xi) \int_0^\infty \frac{dk}{2\pi} \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \left\{ \frac{\hat{e}_l^2(\kappa r)}{\kappa r^2} \left[ -\kappa^2 \frac{1 + 4\xi}{1 - 4\xi} + \frac{l(l+1)}{r^2} + \frac{1}{r^2} \right] \right\} \]

\[ - 2 \frac{1}{r^3} e_l(\kappa r)e'_l(\kappa r) + \frac{\kappa}{r^2} e_l^2(\kappa r) \right\}. \]  

4. Surface divergences

We want to examine the singularity structure as \( r \to a_+ \). For this purpose we use the leading uniform asymptotic expansion, \( l \to \infty \),

\[ e_l(x) \sim \sqrt{zt} e^{-\nu z}, \quad s_l(x) \sim \frac{1}{2} \sqrt{zt} e^{\nu z}, \quad e'_l(x) \sim -\frac{1}{\sqrt{zt}} e^{-\nu z}, \quad s'_l(x) \sim \frac{1}{2} \frac{1}{\sqrt{zt}} e^{\nu z}; \]  

where \( \nu = l + 1/2, \ x = \nu z, \ t = (1 + z^2)^{-1/2}, \ d\eta/dz = 1/zt. \)

Let us consider the thin shell limit, \( \delta \to 0, \ h\delta = 1 \), where it is easy to check that

\[ \frac{\hat{\Xi}}{\tilde{\Xi}} \to \frac{\lambda}{\kappa a^2 e_l(\kappa a) s_l(\kappa a)} \]  

\[ 1 + \frac{\lambda}{\kappa a^2 e_l(\kappa a) s_l(\kappa a)}, \]  

\[ \]
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which is exactly the coefficient occurring in the δ-function potential. There are two simple limits of this, strong and weak coupling: \((\kappa a \sim 1)\)

\[
\frac{\lambda}{a} \to \infty : \quad \hat{\Xi} \left( \frac{a}{\kappa a} \right) \to \frac{s_i(\kappa a)}{e_i(\kappa a)}, \quad \frac{\lambda}{a} \to 0 : \quad \hat{\Xi} \left( \frac{a}{\kappa a} \right) \to \frac{\lambda}{\kappa a^2} s_i^2(\kappa a). \tag{19}
\]

In either case, we carry out the asymptotic sum over angular momentum using the uniform asymptotic expansion and

\[
\sum_{l=0}^{\infty} e^{-\nu x} = \frac{1}{2 \sinh \frac{x}{2}}, \quad \chi = 2 \left[ \eta(z) - \eta \left( \frac{a}{r} \right) \right] \approx 2 \nu \eta(z) \frac{r-a}{r} = \frac{2r-a}{t}. \tag{20}
\]

The remaining integrals over \(z\) are elementary, and in this way we find that the leading divergences are as \(r \to a+\),

\[
\frac{\lambda}{a} \to \infty : \quad u \sim -\frac{1}{16\pi^2} \frac{1 - 6\xi}{(r-a)^4}, \tag{21a}
\]

\[
\frac{\lambda}{a} \to 0 : \quad u^{(n)} \sim \left( -\frac{\lambda}{a} \right)^n \frac{\Gamma(4-n)}{96\pi^2a^4} \left( 1 - 6\xi \right) \left( \frac{a}{r-a} \right)^{4-n}, \quad n < 4, \tag{21b}
\]

the latter being the leading divergence in order \(n\), which clearly seems to demonstrate the virtue of the conformal value of \(\xi = 1/6\). (The value for the Dirichlet sphere first appeared in Deutsch and Candelas [5].) Thus, for \(\xi = 1/6\) we must keep subleading terms. This includes keeping the subdominant term in \(\chi\), and the distinction between \(t(z)\) and \(\tilde{t} = t(\tilde{z} = za/r)\),

\[
\chi \approx \frac{2r-a}{t}, \quad \tilde{t} \approx zt - t^3 \frac{r-a}{r}, \quad \tilde{z} \approx zt - t^3 \frac{r-a}{r}, \tag{22}
\]

as well as the next term in the uniform asymptotic expansion of the Bessel functions,

\[
s_i(x) \sim \frac{1}{2\sqrt{zt}} e^\nu (1 + u_1(t)/\nu + \ldots), \quad e_i(x) \sim \sqrt{zt} e^{-\nu} (1 - u_1(t)/\nu + \ldots), \tag{23a}
\]

\[
s_i'(x) \sim \frac{1}{2\sqrt{zt}} e^\nu (1 + v_1(t)/\nu + \ldots), \quad e_i'(x) \sim -\frac{1}{\sqrt{zt}} e^{-\nu} (1 - v_1(t)/\nu + \ldots), \tag{23b}
\]

where \(u_1(t) = (3t - 5t^3)/24\), \(v_1(t) = (3t + 7t^3)/24\), as \(l \to \infty\). Including all this, it is straightforward to recover the well-known result \([2]\) of Deutsch and Candelas for strong coupling (Dirichlet BC). Following the same process for weak coupling, we find that the leading divergence in order \(n\), \(1 \leq n < 3\), is \((r \to a+)\)

\[
u^{(n)} \sim \left( \frac{\lambda}{a^2} \right)^n \frac{1}{144\pi^2} \frac{1}{a^3 - \lambda^2} (n-1)(n+2)\Gamma(3-n). \tag{24}
\]

Note that the subleading \(O(\lambda)\) term again vanishes. Both of these results apply for the conformal value \(\xi = 1/6\).

The above results for the conformally coupled scalar show that the inverse linear divergences which occur in either order \(\lambda\) or \(\lambda^2\) cancel between inside and outside, when one computes the total energy, while the divergence encountered at \(n = 3\) is logarithmic:

\[
u^{(3)} \sim \frac{\lambda^3}{a^7} \frac{1}{144\pi^2} \Gamma(0) \to -\frac{\lambda^3}{144\pi^2a^7} \ln \frac{r-a}{a}, \tag{25}
\]

where the latter form is shown by explicit calculation, rather than continuing in \(n\). The integral of this, however, is finite, so this does not signal any difficulty.
5. Surface and shell energy

However, as discussed first by Dowker, Kennedy and Critchley \[18, 19\], and later elaborated by Saharian and Romeo \[20, 21\], and put in a broader context by Fulling \[22\], for situations when other than Neumann or Dirichlet boundary conditions apply, an additional term must be supplied in calculating the energy, a term which resides entirely on the surface. For the case of the general stress tensor, that extra term is \[12\]

\[
\mathcal{E} = -\frac{1 - 4\xi}{2i} \int dS \cdot \nabla G(x, x') \bigg|_{x=x'},
\]

(26)

where the direction of the normal is out of the region in question, which arises from the \(T^{00}\) component of the stress tensor. The total energy in a given region is not, therefore, just the integral of the local energy density, but has this extra contribution \[12\]

\[
\mathcal{E} = \int (dr) \langle T^{00} \rangle + \mathcal{E} = \frac{1}{2i} \int (dr) \int \frac{d\omega}{2\pi} 2\omega^2 \mathcal{G}(r, r) e^{-i\omega\tau},
\]

(27)

which is independent of \(\xi\). (\(\tau\) is a point-splitting regulator \[23\].) The latter expression has a rather evident interpretation in terms of summing zero-point energies. The surface energy cancels for a nonsingular potential when computing the total energy in all space.

In the limit of \(\hbar \to \infty\) for the region in the shell, \(a_- < r, r' < a_+\), the reduced Green’s function becomes (for further details about this limit see \[24\])

\[
g_l \to \frac{1}{2\kappa r r'} \frac{\epsilon_l(\kappa a) s_l(\kappa a)}{1 + \frac{\lambda}{\kappa a} \epsilon_l(\kappa a) s_l(\kappa a)} \left[ \cosh \frac{\sqrt{\lambda h}}{a} (r - r') + \cosh \frac{\sqrt{\lambda h}}{a} (r + r' - a_+ - a_-) \right].
\]

(28)

In the thin shell limit (\(\delta \to 0\)) this leads to an energy density in the shell nearly independent of \(r\), leading to the energy \((\epsilon = \tau E / a, y = |x|)\)

\[
E_s = \frac{\lambda}{4\pi a^2} (1 - 4\xi) \sum_{l=0}^{\infty} (2l + 1) \int_{-\infty}^\infty dx \frac{I_\nu(y) K_\nu(y)}{1 + \frac{\sqrt{\lambda h}}{a} I_\nu(y) K_\nu(y)} e^{ix\tau}.
\]

(29)

However, we have to include the surface term \[20\] in the shell at \(r = a_\pm\), which exactly cancels this: \(E_s = E_s + \mathcal{E}_s = 0\), because the total energy of the shell is given by \[27\] integrated over the volume of the shell, which clearly vanishes as the thickness of the shell \(\delta \to 0\). However, we shall see shortly that \(E_s\) plays a special role.

6. Total energy of \(\lambda\) sphere (\(\delta = 0\))

Likewise, if one integrates the interior and exterior energy density, and includes the surface energy, one gets, for arbitrary \(\xi\), the total energy as found by Bordag et al \[13\],

\[
\mathcal{E} = E_{in} + E_{out} + \mathcal{E} = -\frac{1}{4\pi a} \sum_{l=0}^{\infty} (2l + 1) \int_{-\infty}^\infty dx \frac{y dx}{dy} \ln \left[ 1 + \frac{\lambda}{a} I_\nu(y) K_\nu(y) \right] e^{ix\tau},
\]

(30)

exactly that obtained from the integral \[27\] of the Green’s function.

However, there is more to say here. As noted above, the integral of the local energy, inside and outside the sphere, is finite perturbatively, because of cancellations between inside and outside, for the conformally coupled scalar. But it is well known
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that divergences occur in the total energy at order $\lambda^3$. These evidently must arise from the surface term. So let us consider the latter, which is given in the outside region by

$$e = a^2(1 - 4\xi) \sum_{l=0}^{\infty} 2\nu \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\xi}{2\pi} \frac{\partial}{\partial r} g_l(r, r') \bigg|_{r=r'=a} e^{i\xi r}, \quad |\xi| = \kappa.$$  (31)

In the strong coupling limit, there is, of course, no surface term. This is because then $r, r' > a$:

$$g_l(r, r') = 1 - \kappa r r' \left[ s_l(\kappa r_<) e_l(\kappa r_) - s_l(\kappa a) e_l(\kappa r_<) e_l(\kappa r_') \right],$$  (32)

which vanishes on the surface, and has a derivative proportional to the Wronskian.

In general, in the thin-shell limit, the sum of the inside and outside surface terms is given by

$$e = \frac{\lambda^4}{4\pi a^2} (1 - 4\xi) \int_{-\infty}^{\infty} dx \sum_{l=0}^{\infty} (2l + 1) \frac{I_{\nu}(y) K_{\nu}(y)}{1 + \frac{\lambda a}{I_{\nu}(y) K_{\nu}(y)}} e^{ix\epsilon}. \quad \text{(33)}$$

Perhaps not remarkably, this is precisely the same as the integrated local shell energy $E_s$ [29]. Thus the surface energies within and outside the shell regions cancel. (This is generally true, as follows from the continuity requirements on the Green’s function.)

For weak coupling, we expand this in powers of $\lambda$. Perhaps the easiest way to isolate the asymptotic behavior is to use the leading uniform asymptotic expansion, $I_{\nu}(x) K_{\nu}(x) \sim t/2\nu$. This yields the following expression for the $n$th term in the total surface energy, ($\epsilon = 0$, analytically continued in $n$ from $\Re n > 3$)

$$e^{(n)} = -\frac{(-1)^n}{2\sqrt{\pi a}} (1 - 4\xi) \left( \frac{\lambda}{2a} \right)^n \frac{\Gamma \left( \frac{n-1}{2} \right)}{\Gamma \left( \frac{n}{2} \right)} (2^{n-2} - 1) \zeta(n-2).$$  (34)

Note that this expression vanishes for $n = 2$; in this approximation the order $\lambda^2$ term in the energy arises only from the local energy density. However, for $n = 3$ we obtain for the conformal value, $\xi = 1/6$,

$$e^{(3)} \sim \frac{\lambda^3}{24\pi a^4} \zeta(1),$$  (35)

precisely the divergent term in the energy first found by the heat kernel calculation of Bordag, Kirsten, and Vassilevich [13]. The universality of these results supports the hypothesis of analyticity in the order $n$. Alternatively, if we keep $\epsilon \neq 0$:

$$e^{(2)} \sim -\frac{i\lambda^2}{24\pi a^4} \int_{-\infty}^{\infty} \frac{dz}{z^2 + 1} = 0, \quad e^{(3)} \sim \frac{\lambda^3}{12\pi a^4} \ln \epsilon.$$  (36)

The former integral vanishes by oddness, while the $O(\lambda^3)$ term is logarithmically divergent as $\epsilon \to 0$. Thus, by expanding [30] in powers of $\lambda$, $E^{(2)} = \lambda^2/32\pi a^3$, is unambiguously finite, while $E^{(3)}$ is unambiguously divergent.

7. Conclusions

For the case of a massless scalar field in a spherically symmetric step-function shell potential, we have shown that there is a net effective surface energy in the thin shell limit,
to be added to the integrated local energy density for the inside and outside regions, which is exactly the integrated local energy density of the shell. This shell energy, for the conformally coupled theory, is finite in second order in the coupling, but diverges in third order. We show that the latter precisely corresponds to the known divergence of the total energy in this order. Thus we have established the suspected correspondence between surface divergences and divergences in the total energy, which has nothing to do with divergences in the local energy density as the surface is approached. This precise correspondence should enable us to absorb such global divergences in a renormalization of the surface energy, and should lead to further advances of our understanding of quantum vacuum effects. Further details are given in [24].

Acknowledgments

This work was supported by grants from the U.S. Department of Energy. We thank Steve Fulling, Noah Graham, Klaus Kirsten, and Prachi Parashar for helpful conversations. We are grateful to Emilio Elizalde for his superb organization of the QFEXT05 workshop, and all the participants of that meeting for making that event such a success. KAM thanks the Physics Department of Washington University for its hospitality.

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