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Boundary conditions at spatial infinity for fields in Casimir calculations

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Abstract
The importance of imposing proper boundary conditions for fields at spatial infinity in the Casimir calculations is elucidated.

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1. Introduction

The starting formula in calculations of the Casimir energy $E_0 = (1/2)\sum \omega_n$ requires knowledge of the spectrum of the quantum field model under consideration [1]. For this aim the boundary conditions at the spatial infinity should be imposed on the field in the case of an unbounded configuration space. Making here use of the *radiation condition* leads, as a rule, to a *complex discrete energy spectrum* (open systems with energy losses due to the outgoing waves). In this situation more admissible is the condition utilized in formulation of the scattering problem, i.e., at the spatial infinity the field should be *a sum of incoming and outgoing waves*. The spectrum of the same Hamiltonian with scattering conditions is nonnegative but continuous, and the respective natural modes are not squared integrable. In order to define a correct integration over such a spectrum one has to introduce *the spectral density*, which is expressed in terms of the Jost function of the relevant scattering problem. The frequency equation, which is derived by making use of the radiation condition, is related, in a direct way, to the Jost function. As a result the final formulae for the spectral sums and spectral integrals turn out to be identical in the end. Thus a rigorous justification of the results of Casimir calculations obtained by employment of the radiation condition and frequency equations with a discrete set of complex roots is proposed.

2. Complex frequencies and quasi-normal modes in unbounded oscillating regions

Here we show in the general case in what way complex frequencies and quasi-normal modes appear when considering harmonic oscillations in unbounded regions. Let a closed smooth surface S divide the d-dimensional Euclidean space $\mathbb{R}^d$ into a compact internal region $D_{\rm in}$ and a noncompact external region $D_{\rm ex}$. We consider here a simple scalar wave equation

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)u(t,\mathbf{x}) = 0, \tag{1}$$

where c is the velocity of the oscillation propagation and Δ is the Laplace operator in $\mathbb{R}^d$. For harmonic oscillations

$$u(t,\mathbf{x}) = \mathrm{e}^{-\mathrm{i}\omega t}u(\mathbf{x}) \tag{2}$$

the wave equation (1) is reduced to the Helmholtz equation

$$(\Delta + k^2)u(\mathbf{x}) = 0, \qquad k = \frac{\omega}{c}. \tag{3}$$

The oscillations in the internal region $D_{\rm in}$ are described by an infinite countable set of normal modes

$$u_n(t,\mathbf{x}) = \mathrm{e}^{-\mathrm{i}\omega_n t}u_n(\mathbf{x}), \qquad n = 1, 2, \ldots. \tag{4}$$

The spatial form of the normal modes (the functions $u_n(\mathbf{x})$) is determined by the boundary conditions which are imposed upon the function $u(\mathbf{x})$ on the internal side of the surface S. These conditions should fit the physical content of the problem under study. The set of normal modes is a complete one. Hence any solution of (3) obeying relevant boundary conditions can be expanded in terms of the normal modes $u_n(\mathbf{x})$.

When considering the oscillations in the external domain $D_{\rm ex}$ one imposes, in addition to the conditions on the compact surface S, a special requirement concerning the behaviour of the function $u(\mathbf{x})$ at large $r \equiv |\mathbf{x}|$. Usually for this purpose the radiation boundary conditions, proposed by Sommerfeld [2, 3], are used

$$\lim_{r\to\infty} r^{\frac{d-1}{2}}u(r) = \text{const}, \qquad \lim_{r\to\infty} r^{\frac{d-1}{2}}\left(\frac{\partial u}{\partial r} - \mathrm{i}ku\right) = 0. \tag{5}$$

For real values of the wave vector k (for real frequencies ω) the solution to (3), which obeys the radiation conditions (5) and reasonable boundary condition on a compact surface S, identically vanishes.

If we remove the requirement of reality of the wave vector k, then the statement, formulated above, does not hold. Namely, the wave equation (1) and the Helmholtz equation (3) have nonzero solutions with complex frequencies, these solutions obeying the radiation boundary conditions (5) and a common condition on a closed compact surface S (for instance, Dirichlet or Neumann conditions).

As a very simple and clear example we consider the oscillations of electromagnetic field outside a perfectly conducting sphere of radius a. In this case the electric and magnetic fields are expressed in terms of two scalar functions $f_{kl}^{\rm TE}(r)$ and $f_{kl}^{TM}(r)$ (Debye potentials) which are the radial parts of the solutions to the scalar wave equation (1). Outside the perfectly conducting sphere placed in vacuum the solution to the Helmholtz equation (3) obeying the radiation conditions (5) has the form ($d = 3$)

$$f_{kl}(r) = Ch_l^{(1)}\left(\frac{\omega}{c}r\right), \qquad r > a, \tag{6}$$

where $h_l^{(1)}(z)$ is the spherical Hankel function of the first kind [4]. At the surface of perfectly conducting sphere the tangential component of the electric field should vanish. This leads to the following frequency equation for TE modes,

$$h_l^{(1)}\left(\frac{\omega}{c}a\right) = 0, \qquad l \geqslant 1 \tag{7}$$

and for TM modes

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r h_l^{(1)}\left(\frac{\omega}{c}r\right)\right) = 0, \qquad r = a, \quad l \geqslant 1. \tag{8}$$

The spherical Hankel function $h_l^{(1)}(z)$ is $\mathrm{e}^{\mathrm{i}z}$ multiplied by the polynomial in $1/z$ of a finite order. Hence the frequency equations (7) and (8) have a finite number of roots, which are in the general case complex numbers. For $l = 1$ (the lowest oscillations) equations (7) and (8) assume the form ($z = a\omega/c$)

$$h_l^{(1)}(z) = -\frac{1}{z}\,\mathrm{e}^{\mathrm{i}z}\left(1 + \frac{\mathrm{i}}{z}\right) = 0 \quad \text{(TE modes)}, \tag{9}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(z h_l^{(1)}(z)\right) = -\frac{\mathrm{i}}{z^2}\,\mathrm{e}^{\mathrm{i}z}(z^2 + \mathrm{i}z - 1) = 0 \quad \text{(TM modes)}. \tag{10}$$

Thus the lowest eigenfrequencies are

$$\frac{\omega}{c} = -\frac{\mathrm{i}}{a} \quad \text{(TE modes)}, \tag{11}$$

$$\frac{\omega}{c} = -\frac{1}{2a}(\mathrm{i} \pm \sqrt{3}) \quad \text{(TM modes)}. \tag{12}$$

The complex eigenfrequencies lead to a specific time and spatial dependence of the respective natural modes and ultimately of the electromagnetic fields. So, with allowance of (11), we obtain

$$\mathrm{e}^{-\mathrm{i}\omega t} f_{k1}^{\mathrm{TE}}(r) = -\mathrm{i}C\frac{a}{r}\,\mathrm{e}^{(r-ct)/a}\left(1 - \frac{a}{r}\right), \qquad r \geqslant a. \tag{13}$$

Thus, the eigenfunctions are exponentially going down in time and exponentially going up when r increases. Such time and spatial behaviour is typical for eigenfunctions describing oscillations in external unbounded regions, the physical content and details of oscillation process being irrelevant. The eigenfunctions corresponding to complex eigenvalues are called *quasi-normal modes* keeping in mind their unusual properties [5]. The physical origin of such features is obvious; in fact, we are dealing here with *open systems* in which the energy can be radiated to infinity. Therefore in open systems field cannot be in the stationary state.

Quasi-normal modes do not obey the standard completeness condition and the notion of norm cannot be defined for them [5]. Therefore these eigenfunctions cannot be used for expansion of the classical field with the aim at quantizing it and at introducing the relevant Fock operators. Thus the radiation conditions are not appropriate for the Casimir calculations.

The same situation, with regard to quasi-normal modes, takes place when we consider the oscillations of compound media. In this case in both the regions D_{in} and D_{ex} the wave equations are defined,

$$\left(\Delta - \frac{1}{c_{\mathrm{in}}^2}\frac{\partial}{\partial t^2}\right)u_{\mathrm{in}}(t, \mathbf{x}) = 0, \qquad \mathbf{x} \in D_{\mathrm{in}}, \tag{14}$$

$$\left(\Delta - \frac{1}{c_{\mathrm{ex}}^2}\frac{\partial}{\partial t^2}\right)u_{\mathrm{ex}}(t, \mathbf{x}) = 0, \qquad \mathbf{x} \in D_{\mathrm{ex}} \tag{15}$$

with the matching conditions at the interface S, for example, of the following kind,

$$u_{\rm in}(t,\mathbf{x}) = u_{\rm ex}(t,\mathbf{x}), \tag{16}$$

$$\lambda_{\rm in}\frac{\partial u_{\rm in}(t,\mathbf{x})}{\partial n_{\rm in}(\mathbf{x})} = \lambda_{\rm ex}\frac{\partial u_{\rm ex}(t,\mathbf{x})}{\partial n_{\rm ex}(\mathbf{x})}, \qquad \mathbf{x}\in S, \tag{17}$$

where $n_{\rm in}(\mathbf{x})$ and $n_{\rm ex}(\mathbf{x})$ are normals to the surface S at the point $\mathbf{x}$ for the regions $D_{\rm in}$ and $D_{\rm ex}$, respectively. The parameters $c_{\rm in}$, $c_{\rm ex}$, $\lambda_{\rm in}$ and $\lambda_{\rm ex}$ specify the material characteristics of the media. At the spatial infinity the solution $u_{\rm ex}(t,\mathbf{x})$ should satisfy the radiation conditions (5). For real k we again have only a zero solution in this problem; both functions $u_{\rm in}(t,\mathbf{x})$ and $u_{\rm ex}(t,\mathbf{x})$ vanish. However, the wave equations (14) and (15) have nonzero solutions with complex frequencies, i.e. quasi-normal modes, which satisfy the matching conditions (16) and (17) at the interface S and radiation conditions (5) at spatial infinity. It is important that the frequencies of oscillations in internal ($D_{\rm in}$) and external ($D_{\rm ex}$) regions are the same. A typical example here is the complex eigenfrequencies of a dielectric ball. This problem has been investigated by Debye in his PhD thesis concerned with the light pressure on a material ball [6].

The physical content of the radiation conditions is very clear. They select only the oscillations with real frequencies caused by external sources, which are situated in a compact spatial area. From the mathematical point of view, these conditions ensure the uniqueness of the solution of the nonhomogeneous boundary problems in the external region $D_{\rm ex}$ or in the whole space ($D_{\rm in} + D_{\rm ex}$) in the case of compound media.

When formulating the radiation conditions in the text books, only the real wave vector k is considered. The possibility of existence of quasi-normal modes with complex frequencies satisfying the radiation conditions at spatial infinity with complex wave vector k is not mentioned usually. I am aware only of one literature source where the eigenfunctions with complex frequencies are noted in this context. It is the article written by Sommerfeld in the book [3].

The standard physical method to escape appearance of complex frequencies and quasi-normal modes is the following: the system under study is placed in a sphere of a large radius R and the field is subjected to an additional boundary condition on this sphere. The initial differential operator has now a real discrete spectrum, and the respective eigenfunctions are normalized in L_2. Upon conducting the calculations the limit $R\to\infty$ should be taken.

However, in order to justify this approach one has to prove that the final result does not depend on the explicit form of auxiliary boundary conditions imposed on the large sphere $r = R$. Obviously, it is a nontrivial task. Furthermore, in this approach always the feeling remains that something is lost because the region $r > R$ is actually ignored. Fortuitously, there is a rigorous way of considering the open systems by making use of the formalism of the scattering problem without introducing a large auxiliary sphere.

3. Description of open systems by scattering method

In the scattering problem the same differential operator (for example, the Laplace operator (3)) is considered, but instead of the radiation conditions (5) it is required that the eigenfunctions $\phi_l(k,r)$ at spatial infinity $r\to\infty$ are reduced to the sum of incoming and outgoing waves

$$\phi_l(k,r) \simeq -\frac{1}{2\mathrm{i}k}[F_l(-k)\,\mathrm{e}^{-\mathrm{i}kr} - F_l(k)\,\mathrm{e}^{\mathrm{i}kr}], \qquad r\to\infty. \tag{18}$$

Here $F_l(k)$ is the Jost function, and spherical symmetry in the problem under consideration is expected. The operators of the type

$$-\Delta + V(r) \tag{19}$$

have real continuous spectrum

$$0 \leqslant k^2 < \infty, \tag{20}$$

when the potential $V(r)$ obeys known conditions at $r = 0$ and at infinity $r \to \infty$.

Due to the continuity of the spectrum the corresponding eigenfunctions are not normalized in L_2. Making here use of the normalization on the Dirack δ-function proves to be useful in many physical applications; however it does not allow one to define, in a correct way, the integration over a continuous spectrum. Indeed, let $\psi_{\mathbf{k}}(\mathbf{x})$ be the eigenfunctions corresponding to the spectrum (20) normalized on the Dirack δ-function

$$\int \psi_{\mathbf{k}}^*(\mathbf{x})\psi_{\mathbf{k}'}(\mathbf{x})\,\mathrm{d}^3\mathbf{x} = \delta^{(3)}(\mathbf{k}-\mathbf{k}'), \tag{21}$$

for example, those can be plane waves

$$\psi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\,\mathrm{e}^{\mathrm{i}\mathbf{kx}}. \tag{22}$$

Due to its meaning, the spectral density $\rho(k)$ should be defined in the following way,

$$\rho(k) = \int \psi_{\mathbf{k}}^*(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{x})\,\mathrm{d}^3\mathbf{x} = \delta^{(3)}(0) = \frac{V}{(2\pi)^3}, \tag{23}$$

where V is the volume of the space $\mathbb{R}^3$ and obviously $V \to \infty$. It is worth noting that the spectral density (23), considered just on the formal footing, does not depend on the details of the dynamics, i.e. on the potential $V(r)$ and corresponding boundary conditions; therefore it cannot be used in physical calculations.

In the rigorous mathematical theory of scattering processes this problem has been solved. In the most simple way the spectral density for scattering states can be derived as a consequence of a *spectral property* [7]. Let $r(z) = (h - z)^{-1}$ and $r_0(z) = (h_0 - z)^{-1}$ be the resolvents of a complete (h) and free (h_0) Hamiltonians. When the potential meets the relevant conditions, then the relation, known as the spectral property, holds

$$2\,\mathrm{Im}\,\mathrm{Tr}\,[r(E+\mathrm{i}0) - r_0(E+\mathrm{i}0)] = \mathrm{tr}[q(E)], \tag{24}$$

where

$$q(E) = -\mathrm{i}S^\dagger(E)\frac{\mathrm{d}}{\mathrm{dE}}S(E) \tag{25}$$

is the two-body time delay operator and S is the scattering matrix

$$S(k) = \mathrm{e}^{2\mathrm{i}\delta(k)} = \frac{F(k)}{F(-k)}. \tag{26}$$

Here $\delta(k)$ is the phase shift and $F(k)$ is the Jost function.

By making use of the spectral representation for the resolvents and definition (23) one obtains immediately

$$\begin{aligned}\Delta\rho(k) \equiv \rho(k) - \rho_0(k) &= \frac{1}{2\pi\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}k}\ln S(k) \\ &= \frac{1}{2\pi\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}k}\ln\frac{F(k)}{F(-k)} = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}k}\delta(k).\end{aligned} \tag{27}$$

It is worth noting that in this formula the contribution of a free unbounded space is already subtracted. The finite expression for $\Delta\rho(k)$ is a direct consequence of considering complex values of the wave vector k and respective energy k^2.

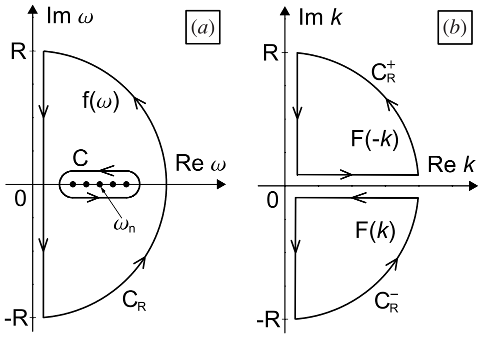

Figure 1. The contours on the complex k plane which are used when going on to the integration over the imaginary frequencies in the case of bounded (a) and unbounded (b) configuration spaces.

4. Correct transition to imaginary frequencies in the case of unbounded domains

In the Casimir calculations the spectrum of quantum field systems is not known explicitly. As a rule, it is given by the roots (ω_n) of a frequency equation

$$f(\omega) = 0 \tag{28}$$

with the known function f. For summing these roots the counter integration can be used,

$$\frac{1}{2}\sum_n \omega_n = \frac{1}{2\pi \mathrm{i}}\oint_C \frac{z}{2}\frac{\mathrm{d}}{\mathrm{d}z}\ln f(z)\,\mathrm{d}z, \tag{29}$$

where the counter C encloses, counterclockwise, all the roots of (28).

For a compact configuration space without dissipation the roots of (28) are real and positive. The counter C can be deformed continuously into the counter C_R with $R \to \infty$ (see figure 1(a)). Usually $f(x) = f(\sqrt{x^2})$, therefore $f(x) = f(-x)$. The integral along the semicircle of radius R vanishes when $R \to \infty$ or it is cancelled by the subtraction of the free space contribution. As a result we obtain

$$\frac{1}{2}\sum_n \omega_n = -\frac{1}{\pi}\int_0^\infty \frac{y}{2}\frac{\mathrm{d}}{\mathrm{d}y}\ln f(\mathrm{i}y)\,\mathrm{d}y. \tag{30}$$

Let us derive the analogue of (30) for the open systems. According to the inferences of the previous section we have to consider the following integral along the continuous spectrum,

$$\frac{1}{2}\int_0^\infty k\,\Delta\rho(k)\,\mathrm{d}k = \frac{1}{2\pi \mathrm{i}}\int_0^\infty \frac{k}{2}\frac{\mathrm{d}}{\mathrm{d}k}\ln\frac{F(k)}{F(-k)}\,\mathrm{d}k, \tag{31}$$

where $F(k)$ is the Jost function in the pertinent scattering problem. This function is analytic in the lower half-plane of the complex variable k. We assume that there are no bound states in the system in question. Under this assumption the zeros of the Jost function $F(k)$ can lay only in the upper half-plane k [8, 9]. In view of this we infer that the counter integrals (see figure 1(b))

$$\frac{1}{2\pi \mathrm{i}}\oint_{C_R^\mp} \frac{k}{2}\frac{\mathrm{d}}{\mathrm{d}k}\ln F(\pm k)\,\mathrm{d}k = 0 \tag{32}$$

vanish because inside the counter $C_R^+(C_R^-)$ there are no zeros and singularities of the function $F(-k)(F(k))$. Now we can transform in (31) the integration along the real positive axes k to the integration along the imaginary frequencies $k = \mathrm{i}y$, $y > 0$:

$$\frac{1}{2}\int_0^\infty k\Delta\rho(k)\,\mathrm{d}k = -\frac{1}{\pi}\int_0^\infty \frac{y}{2}\frac{\mathrm{d}}{\mathrm{d}y}\ln F(-\mathrm{i}y)\,\mathrm{d}y. \tag{33}$$

Now we take into account the following. The function $f(\omega)$ in the frequency equation (28), which is derived by making use of the radiation conditions at spatial infinity, is actually the Jost function up to irrelevant multiplier. Indeed, the solution (18) will contain only outgoing waves when

$$F(-k) = 0. \tag{34}$$

For simplicity we have dropped here the index l. Thus we have

$$f(\omega) = F(-k), \qquad k^2 = \omega^2/c^2. \tag{35}$$

Now we can infer that the right-hand sides of (30) and (33) coincide. Hence, the formula (30) with the function f defining the frequency equation is applicable also to unbounded configuration spaces.

All this removes the objections [10, 11] against using (30) for unbounded regions and explains why it gives correct results there [1] (in this connection, see also [12]).

5. Conclusion

The Casimir studies, which allow for the material properties of the boundaries, show the importance of the evanescent waves, or more precisely, of surface plasmon contributions [13] at least at short separations between the material bodies (regime without retardation). When formulating the scattering problem in the direction normal to the interface between two material media the evanescent waves are treated as the bound states which exist at any given value of the wave number parallel to the interface. Obviously such bound states should be added to the spectral density (27). In order to determine whether there are evanescent waves in the problem at hand one has to impose explicitly the condition that the electric and magnetic fields evanesce in the direction normal to the interface and only after that to solve the matching conditions at the interface. In this connection it is worth elucidating [14] in what way the evanescent waves are taken into account in the Casimir calculations dealing with a circular infinite dielectric cylinder [15, 16]. It is these field configurations (surface waves with a discrete spectrum) that are used in dielectric wave guides [17].

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