QED Quantum Fluctuations in the Presence of Half-Spaces Filled with Dirac Materials

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From the Dirac model of graphene to half spaces

The first example where the Casimir calculations go the beyond Hamiltonian quadratic in the fields is the Dirac model of graphene. Here, the coupling is the usual electrodynamic one, $\bar{\psi}\gamma^{\mu}\psi A_{\mu}$, and the corresponding Hamiltonian is no longer quadratic.

The EM field (D=3+1) interacts with fermions living in (2+1) dimensions

$$
\begin{aligned}
S &= -\frac{1}{4}\int d^4x\, F_{\mu\nu}^2 + \int d^3x\, \overline{\psi}(i\tilde{\gamma}^{\mu}\partial_{\mu} - m)\psi, \quad \textit{free part} \\
&\quad + \int d^3x\, \overline{\psi}(i\tilde{\gamma}^{\mu} A_{\mu}{}_{|_{z=0}})\psi, \quad \textit{interaction part}.
\end{aligned}
$$

Since the spinor field describing the electrons in graphene is confined to a 2D surface in 3D space, the reflection coefficients could be expressed explicitly in terms of the polarization tensor of the electrons calculated within unconstrained $D = 2 + 1$ QFT of the spinor field representing the electrons. [E. V. Gorbar, V. P. Gusynin, V. A. Miransky, and I. A. Shovkovy. Phys. Rev. B, 66:045108, 2002; V. P. Gusynin and S. G. Sharapov. Phys. Rev. B, 73(24):245411, 2006; Bordag et all, Phys. Rev. B 80 245406, 2009]

Talk by G. Klimchitskaya tomorrow

The generalization

- to confine electrons in half spaces and to consider a field theory in D=3+1 restricted to two half spaces.
- to use more sophisticated model instead of conventional QED in order to describe unusual properties of new materials.

For example, to consider Chern-Simons action, which accounts for Hall conductivity.

$$\sim \int d^3r\, dt\, \theta(\mathbf{r}, t)\varepsilon^{\mu\nu\alpha\beta} F_{\mu\nu} F_{\alpha\beta}, \quad \theta(\mathbf{r}, t) = 2\mathbf{b} \cdot \mathbf{r} - 2b_0 t$$

$2b$ is the distance between Weyl nodes in k space, $2b_0$ is their energy offset.

J. H. Wilson, A. A. Allocca, and V. Galitski, PHYSICAL REVIEW B 91, 235115 (2015), Repulsive Casimir force between Weyl semimetals
A. G. Grushin, ”Consequences of a condensed matter realization of Lorentz-violating QED in Weyl semi-metals”, Phys. Rev. D 86, 045001 (2012)

M. Belén Farias, A. A. Zyuzin, T.L. Schmidt, Casimir force between Weyl semimetals in a chiral medium, Phys.Rev.B 101 (2020) 23, 235446 (2020)

Talk by M. Belén Farias, today

The objectives

- to describe peculiar properties of new materials such as time-reversal symmetry breaking using effective quantum field theory approach.
- to develop such a QFT description of a material which can be naturally implanted into the Casimir force calculation (into scattering approach), including finite temperature.
- to check whether effective QFT (PolTensor) description properly accounts for internal dynamical properties of the interacting bodies and gives predictions compartible with experiment.

Previous developments:

I. Fialkovsky, M. Kurkov, and D. Vassilevich, Quantum Dirac fermions in a half-space and their interaction with an electromagnetic field, PRD 100, 045026 (2019)
Computed the renormalized polarization tensor in coordinate representation, discussed the induced Chern-Simons type action, and studied the Hall conductivity near the boundary of the material.

M. Bordag, I. Fialkovsky, N. Khusnutdinov , D. Vassilevich, Bulk contributions to the Casimir interaction of Dirac materials, PRB 104, 195431 (2021)
Computed the bulk dielectric functions for Dirac materials at imaginary frequencies and studied their effect on the Casimir interaction.

QED in half spaces with bag boundary conditions

We are going to calculate the Casimir effect between two parallel half-spaces filled with Dirac materials. These are modeled by spinor fields with bag boundary condition on their surfaces. To evaluate the Casimir force we need the dielectric functions or reflection coefficients of the half-spaces.

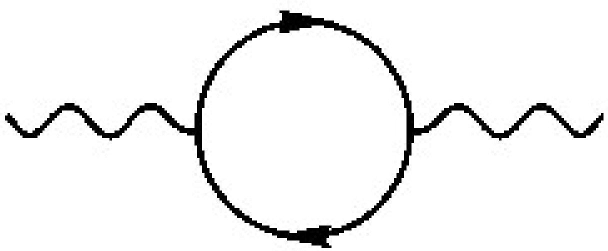
The frequency dependent electrical conductivity of a Dirac material may be obtained by the Kubo formula

$$\sigma_{ij} = \frac{\mathrm{Im}\Pi^R_{ij}(\Omega + i\mathcal{O})}{\Omega}$$

Here $\Pi^R_{ij}(\Omega)$ is the retarded current-current correlation function. It is obtained from the imaginary time expression

$$\Pi_{ij}(i\Omega_m) = \frac{1}{V}\int_0^\beta d\tau e^{i\Omega_m\tau}\langle T_\tau J_i(\tau)J_j(0)\rangle$$

by analytical continuation, $\Pi^R_{ij}(\Omega) = \Pi_{ij}(i\Omega_m \to \Omega + i\mathcal{O})$. In QFT $\Pi_{ij}(i\Omega)$ is called the polarization tensor and corresponds to a one-loop diagram.



QED in half spaces with bag boundary conditions

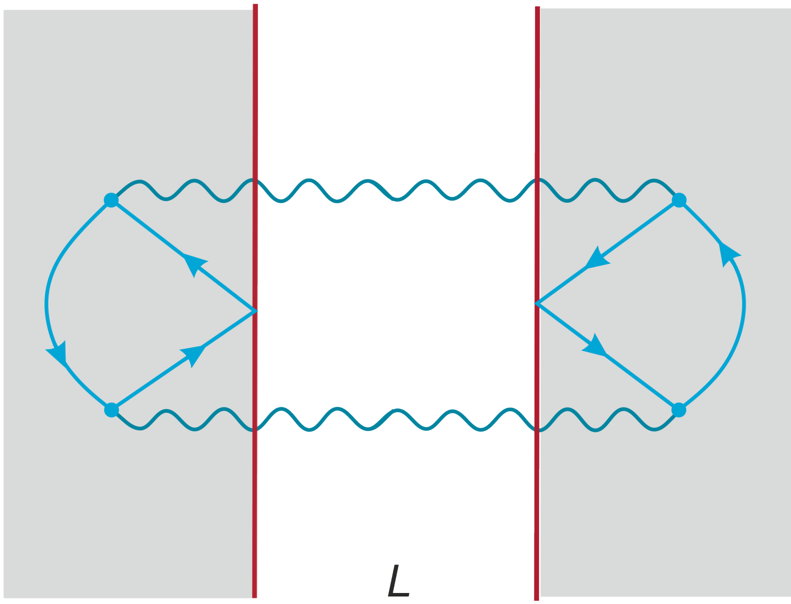
It is important to note that very often in the Casimir effect calculations the explicit expression for the conductivity is not used, as the reflection coefficients in the Lifshitz formula can be obtained in terms of the polarization tensor, entering the Cubo formula.

Since we are interested in the response of a material to an applied electromagnetic field, we can derive an effective theory by integrating out the spinor field. This results in an effective action,

$$S_{eff} = \frac{1}{2} \int d^4x\, d^4y\, A_\mu(x)(g^{\mu\nu}\partial^2 - \partial^\mu\partial^\nu\delta(x-y) + \hat{\Pi}^{\mu\nu}(x-y))A_\nu$$

After that we may investigate the modes of the electromagnetic field considered as a classical field, following from the effective action.

QED in half spaces with bag boundary conditions



$$S = -\frac{1}{4}\int d^4x\, F_{\mu\nu}^2 + \int d^3x \left[\int_{-\infty}^{0} + \int_{L}^{\infty}\right] dx_3\, \overline{\psi}(i\tilde{\gamma}^{\mu}\partial_{\mu} - m)\psi, \quad \textit{free part}$$

$$+ \int d^3x \left[\int_{-\infty}^{0} + \int_{L}^{\infty}\right] dx_3\, \overline{\psi}(i\tilde{\gamma}^{\mu}A_{\mu})\psi, \quad \textit{interaction part}.$$

Bag boundary conditions:

$$(1 + i\gamma^3)\psi(x)|_{x_3=0,L} = 0, \quad \bar{\psi}(x)(1 - i\gamma^3)|_{x_3=0,L} = 0,$$

where $\bar{\psi}$ is the conjugated spinor $\bar{\psi}(x) \equiv \psi^{+}(x)\gamma^{0}$.

PolTensor with bag boundary conditions (eucledian version)

Because of the boundary conditions we use mixed three and one dimensional notations: $\alpha, \beta = 4, 1, 2$ denote the directions parallel to the interface, with momenta k^α, q^α; perpendicular momenta are denoted by p and p'.

The free spinor propagator after partial Fourier transform,

$$S(k_\alpha; z) = -\int \frac{dp}{2\pi} \frac{\hat{k} + \gamma p - m}{k^2 + p^2 + m^2} e^{ipz}.$$

The spinor propagator with boundary condition

$$S(k; z, z') = -\int \frac{dp}{2\pi} \frac{\hat{k} + \gamma^3 p - m}{k^2 + p^2 + m^2} \left\{ e^{ip(z-z')} - \frac{m + \gamma p}{m + ip} e^{ip(z+z')} \right\}, \quad \hat{k} = \gamma^\alpha k_\alpha$$

The polarization tensor in coordinate representation

$$\Pi^{\mu\nu}(x_\alpha; z, z') = e^2 \operatorname{tr} \gamma^\mu S(x_\alpha; z, z') \gamma^\nu S(-x_\alpha; z', z)$$

After partial Fourier transform reads

$$\Pi^{\mu\nu}(q_\alpha; z, z') = \int d^3 x_\alpha \, e^{-iq_\alpha x_\alpha} \Pi^{\mu\nu}(x_\alpha; z, z')$$

$$\Pi^{\mu\nu}(q_\alpha; z, z') = e^2 \int \frac{d^3k}{(2\pi)^3} \int \frac{dp}{2\pi} \int \frac{dp'}{2\pi} \frac{Z^{\mu\nu}(k, p, p', z, z')}{(k^2 + p^2 + m^2)((k-q)^2 + p'^2 + m^2)}$$

where

$$Z^{\mu\nu}(k, p, p', z, z') = \operatorname{tr} \gamma^\mu (\hat{k} + \gamma p - m) \left[e^{ip(z-z')} - \frac{m + \gamma p}{m + ip} e^{ip(z+z')} \right]$$
$$\cdot \gamma^\nu (\hat{k} - \hat{q} + \gamma p' - m) \left[e^{ip'(z'-z)} - \frac{m + \gamma p'}{m + ip'} e^{ip'(z'+z)} \right].$$

We number the four contributions consecutively from 1 to 4 and introduce factors $\sigma, \sigma' = \pm 1$,

$$Z^{\mu\nu}(k, p, p', z, z') = \sum_{i=1}^{4} Z_i^{\mu\nu}(k, p, p') \exp[ip(z - \sigma z') + ip'(z' - \sigma' z)],$$

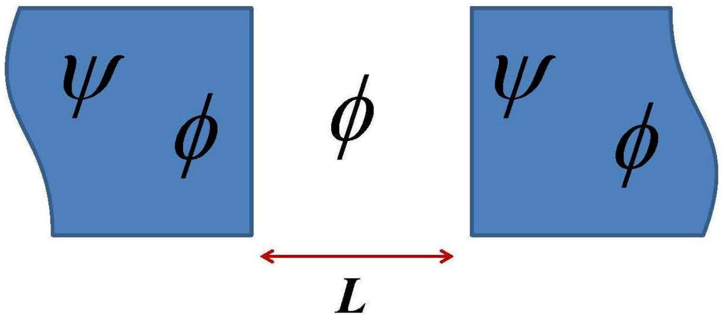
For $Z_i^{\mu\nu}(k, p, p')$ the traces should be calculated.

We divide the polarization tensor according to the subdivision of $Z^{\mu\nu}$. The first part is the free space contribution. It carries the ultraviolet divergence, etc.

I omit the details, but we encountered technical difficulties, therefore I present a simplified example of such a calculation.

Scalar Field Confined to Half Spaces

In *M. Bordag, I.P., Symmetry 10(3), 74 (2018)* we considered a simplified model with a massive scalar field $\psi(x)$ confined in two half spaces $z < 0$ and $z > L$ with Dirichlet boundary conditions on $z = 0$ and $z = L$ and another massless scalar field $\phi(x)$, defined in the whole space. This field mimics EM field.



$$S_{int}(x) = \lambda \int d^3 x_\alpha \Big(\int_{-\infty}^{0} dz\, \phi(x)\psi^2(x) + \int_{L}^{\infty} dz\, \phi(x)\psi^2(x) \Big), \quad \alpha = 0, 1, 2.$$

λ is a coupling constant with a dimension of inverse length

Objective: to develop a convenient formalism for the calculation of the vacuum energy in this configuration $\longrightarrow$ Casimir Effect

Hardships to overcome: UV-divergence in the loop and broken translational invariance in the z-direction.

Basic formulas

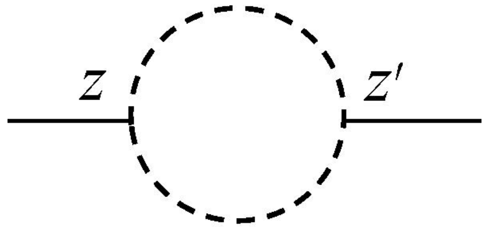
The propagator of the field $\phi(x)$ defined in the whole space in one-loop approximation

$$\Delta^{-1} = \Delta_0^{-1} + \Pi,$$

where $\Delta_0 \equiv \partial_\mu \partial^\mu$ is the wave operator and Π is the polarization operator induced by the interaction with the field $\psi(x)$ in half spaces.

In the lowest order perturbation theory, the polarization operator $\Pi(x, x')$ is

$$\Pi(x_\alpha; z, z') = -i\lambda^2 D_{\mathcal{D}}(x_\alpha; z, z')^2 = -i\lambda^2$$



Notations:
$x = (x^0, x_{||}, z)$, $x_{||} = (x, y)$, $\Gamma = \sqrt{k_\alpha k^\alpha + i0}$, $\Pi(x, x') \equiv \Pi(x_\alpha - x'_\alpha; z, z')$.

The Fourier transforms in translation invariant directions are denoted by
$\phi(z) = \int d^3 x_\alpha e^{ik_\alpha x_\alpha} \phi(x)$, $\Pi_\Gamma(z, z') = \int d^3 x_\alpha e^{ik_\alpha x_\alpha} \Pi(x_\alpha; z, z')$, $\alpha = 0, 1, 2$

Basic formulas

In $\Pi(x, x')$ the propagator $D_{\mathcal{D}}$ corresponds to the field ψ obeying Dirichlet boundary conditions. Its Fourier transform in the translational invariant directions is as follows:

$$\Pi_{\Gamma}(z, z') = \lambda^2 \int d^3 x_\alpha e^{ik_\alpha x_\alpha} D_{\mathcal{D}}(x_\alpha; z, z')^2$$

where

$$D_{\mathcal{D}}(x, x') \equiv D_{\mathcal{D}}(x_\alpha - x'_\alpha; z, z').$$

Then, for the field ψ obeying Dirichlet boundary conditions the propagator is

$$D_{\mathcal{D}}(x, x') = \sum_{\sigma=\pm 1} \sigma D(x_\alpha - x'_\alpha; z - \sigma z'),$$

and

$$D(x) = D(x_\alpha; z) = \int \frac{d^4 q}{(2\pi)^4} \frac{e^{-iqx}}{q^2 - m^2 + i0}$$

is the usual propagator of the scalar field ψ.

Transition to *TGTG* formula

Understanding $\Pi(x, x')$ as a potential, $V(x, x')$ one can use the *TGTG* formula where T and G stand for T-matrix and Green's function.

The vacuum energy of the field ϕ in the presence of the half spaces is

$$E = -\frac{i}{2}\int \frac{d^3 k_\alpha}{(2\pi)^2} \mathrm{T}r \ln(1 - \mathcal{M}),$$

where

$$\mathcal{M}(y, y') = \Pi_1(y, y_1)G_0(y_1 - z_1)\Pi_2(z_1, z_2)G_0(z_2 - y').$$

Integrations $\int_{-\infty}^{0} dy$ and $\int_{L}^{\infty} dz$ are assumed, and y's belong to the left half space and z's belong to the right one;

$$\Pi_1(y, y') = 0 \text{ for } y > 0 \text{ or } y' > 0, \quad \Pi_2(z, z') = 0 \text{ for } z < L \text{ or } z' < L$$

$G_0(z)$ is the free space Green's function of the field ϕ, where the Fourier transform in the α-directions ($\alpha = 0, 1, 2$) is taken,

$$G_0(z) = \int \frac{dk_3}{2\pi} \frac{e^{ik_3 z}}{\Gamma^2 - k_3^2 + i0} = \frac{e^{i\Gamma|z|}}{-2i\Gamma}, \quad \Gamma = \sqrt{k_\alpha k^\alpha + i0}.$$

Let $D_{\mathcal{D}_L}$ denote the propagator with boundary conditions on $z = L$ entering Π_1, and $D_{\mathcal{D}}$ denote the propagator with boundary conditions at $z = 0$ in Π_2, then

$$\Pi_1(y, y') = \Pi_\Gamma(y, y') = \Pi_\Gamma(-y, -y'), \quad \Pi_2(z, z') = \Pi_\Gamma(z - L, z' - L).$$

The relation between $D_{\mathcal{D}}$ and D_{D_L} is given by

$$D_{\mathcal{D}_L}(x_\alpha - x'_\alpha; z, z') = \sum_{\sigma=\pm 1} \sigma D(x_\alpha - x'_\alpha; z - L - \sigma(z' - L)) = D_{\mathcal{D}}(x_\alpha - x'_\alpha; z - L, z' - L).$$

Then after taking the trace $\mathcal{M}$ can be rewritten as

$$\mathcal{M} = \mathcal{N}_1 \cdot \mathcal{N}_2$$

$$\mathcal{N}_1 = \int_{-\infty}^{0} dy \int_{-\infty}^{0} dy' \, \frac{e^{-i\Gamma(y+y')}}{-2i\Gamma} \, \Pi_1(y, y') = \int_{0}^{\infty} dy \int_{0}^{\infty} dy' \, \frac{e^{i\Gamma(y+y')}}{-2i\Gamma} \, \Pi_\Gamma(y, y')$$

$$\mathcal{N}_2 = \int_{L}^{\infty} dz \int_{L}^{\infty} dz' \, \frac{e^{i\Gamma(z+z')}}{-2i\Gamma} \, \Pi_2(z, z') = \int_{L}^{\infty} dz \int_{L}^{\infty} dz' \, \frac{e^{i\Gamma(z+z')}}{-2i\Gamma} \, \Pi_\Gamma(z - L, z' - L).$$

Doing the substitutions, $z \to z + L$, $z' \to z' + L$ thus gives

$$\mathcal{N}_2 = e^{2i\Gamma L} \int_0^\infty dz \int_0^\infty dz' \, \frac{e^{i\Gamma(z+z')}}{-2i\Gamma} \Pi_\Gamma(z, z').$$

This way, we can define

$$\mathcal{N} = \int_0^\infty dz \int_0^\infty dz' \, \frac{e^{i\Gamma(z+z')}}{-2i\Gamma} \Pi_\Gamma(z, z')$$

and $\mathcal{N}_1 = \mathcal{N}$ and $\mathcal{N}_2 = e^{2i\Gamma L}\mathcal{N}$ hold. As a result,

$$E = -\frac{i}{2} \int \frac{d^3 k_\alpha}{(2\pi)^2} \mathrm{T}r \ln(1 - \mathcal{N}^2 e^{2i\Gamma L}),$$

and $\mathcal{M} = \mathcal{N}^2 e^{2i\Gamma L}$. Comparing this equation with the Lifshitz formula at zero temperature, one can define the reflection coefficient of the half spaces in terms of the factors $\mathcal{N}$:

$$r(\omega, k_{||}; \lambda, m) = \mathcal{N}\left(\sqrt{\omega^2 - k_{||}^2}; \lambda, m\right).$$

Polarization Operator in a Half Space

To obtain the factors $\mathcal{N}$ (reflection coefficients) we first calculate the polarization operator Π. We substitute into Π the propagator of the field ψ obeying the Dirichlet boundary conditions at $z = 0$,

$$\Pi(z_\alpha; z, z') = -i\lambda^2 \int \frac{d^4q}{(2\pi)^4} \int \frac{d^4q'}{(2\pi)^4} \sum_{\sigma,\sigma'} \sigma\sigma' \frac{e^{-i(q_\alpha+q'_\alpha)z_\alpha + iq_3(z-\sigma z') + iq'_3(z-\sigma' z')}}{(-q^2+m^2-i0)(-q'^2+m^2-i0)},$$

where σ and σ' take values ± 1. With the integral representation of the δ-function,

$$\int d^3z_\alpha e^{i(k_\alpha - q_\alpha - q'_\alpha)z_\alpha} = (2\pi)^3\delta^3(k_\alpha - q_\alpha - q'_\alpha),$$

we can integrate with respect to q'_α and arrive at

$$\Pi_\Gamma(z, z') = -i\lambda^2 \sum_{\sigma,\sigma'} \sigma\sigma' \int \frac{d^3q_\alpha}{(2\pi)^3} \int \frac{dq_3}{2\pi} \int \frac{dq'_3}{2\pi} \frac{e^{iq_3(z-\sigma z') + iq'_3(z-\sigma' z')}}{(-q_\alpha^2+q_3^2+m^2-i0)(-(k_\alpha-q_\alpha)^2+q_3'^2+m^2-i0)}$$

where $\Gamma = \sqrt{k_\alpha k^\alpha + i0}$.

To proceed, we divide $\Pi_\Gamma(z, z')$ into the translationally invariant part, $\Pi_\Gamma^{(t)}(z, z')$, arising from $\sigma = \sigma' = +1$, and the remaining part, $\Pi_\Gamma^{(nt)}(z, z')$:

$$\Pi_\Gamma(z, z') = \Pi_\Gamma^{(t)}(z, z') + \Pi_\Gamma^{(nt)}(z, z').$$

Taking all contributions together we obtain for the overall factor $\mathcal{N}$,

$$\mathcal{N}|_{\gamma\to 0} = \frac{\lambda^2}{128\pi^2\gamma}\left\{-\frac{\pi}{m}+\frac{4\gamma}{3m}+\mathcal{O}(\gamma^2)\right\}$$

$$\mathcal{N}|_{\gamma\to\infty} = \frac{\lambda^2}{128\pi^2\gamma}\left\{-4\frac{\ln(\gamma/m)}{\gamma}-\frac{0.0624567}{\gamma}+\mathcal{O}(1/\gamma^2)\right\}.$$

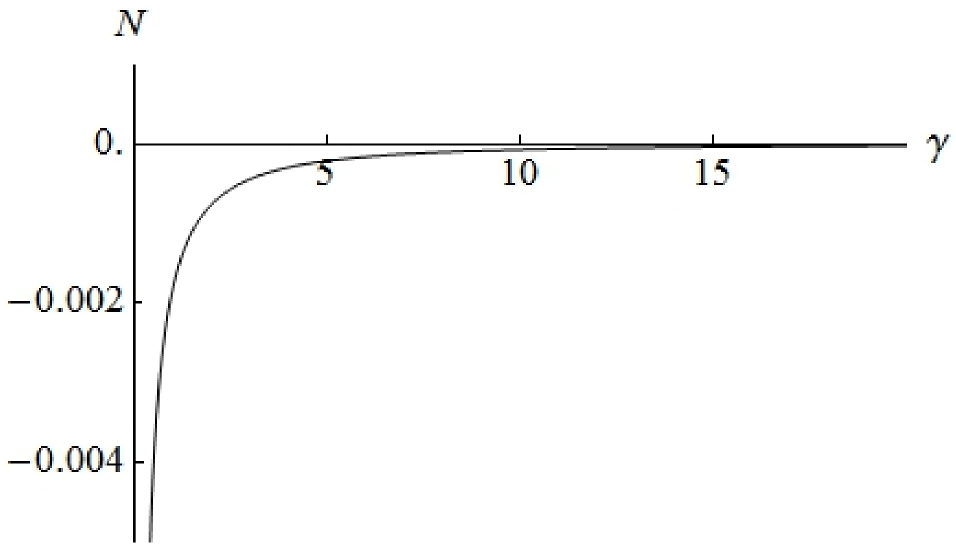


Figure: The factor $\mathcal{N}$ playing the role of the reflection coefficient of the half space as a function of momenta $\gamma = \sqrt{q_1^2+q_2^2+q_4^2}$, $m = 1, \lambda = 1$.

Vacuum energy

$$E = \frac{1}{4\pi}\int_0^\infty d\gamma\gamma^2 \ln(1 - \mathcal{N}^2 e^{-2\gamma L}).$$

For $\gamma \to 0$, $\mathcal{N}^2 \sim 1/\gamma^2$, and the argument of the logarithm becomes negative. This yields a complex vacuum energy of the field ϕ for any finite width of the gap between the half spaces.

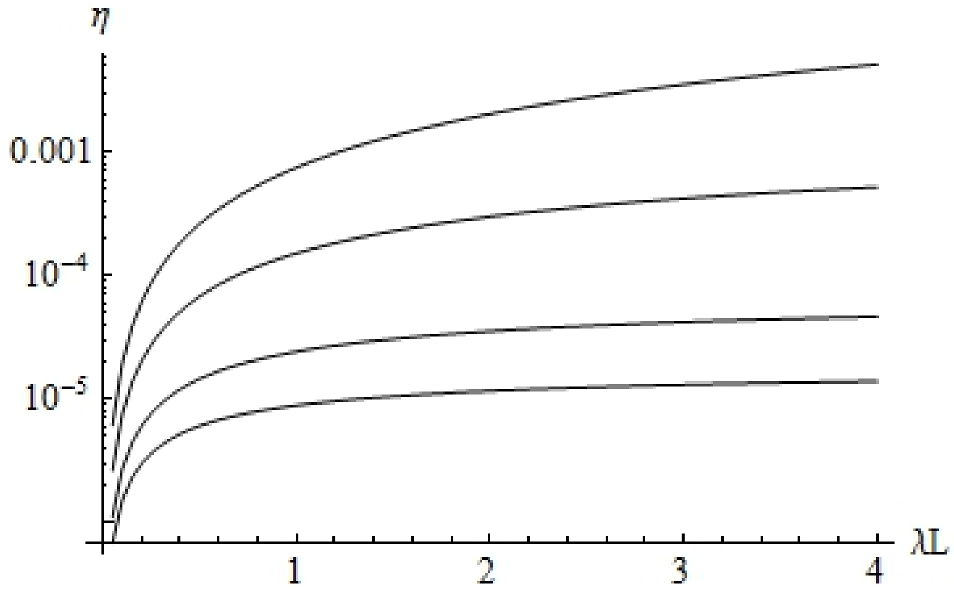
Our model was aimed to mimic the interaction of the photon field with the electron and phonon fields in a solid. The Coulomb interaction between the electrons and the phonons is screened, and the electron charge density interacts with the gradient of the phonon displacement field. It corresponds to the gradient in the interaction vertex, which turns into a momentum after Fourier transform. To account for this gradient in some way, we made the coupling momentum dependent:

$$\lambda \to \lambda(\gamma) = \lambda_0\sqrt{\gamma}, \quad \text{such that} \quad \mathcal{N}|_{\gamma\to 0} \sim C, \quad \mathcal{N}|_{\gamma\to\infty} \sim \frac{\ln(\gamma)}{\gamma}.$$

The behavior of the Casimir (vacuum) energy for large separation can be obtained by scaling $\gamma \to \gamma/L$.

$$E|_{L\to\infty} = \frac{1}{4\pi L^3}\int_0^\infty d\gamma\gamma^2 \ln(1 - \lambda^2 C_1 e^{-2\gamma}) = -\frac{1}{16\pi L^3}\mathrm{Li}_4(\lambda^2 C_1).$$

Numerical results



The ratio $\eta = E/E_D$, where $E_D = -\pi^2/(1440L^3)$ of the Casimir energy the massless scalar field with Dirichlet boundary conditions on the plates in the units $\hbar = c = 1$, drawn in logarithmic scale as a function of dimensionless separation λL. From top to bottom, $\mu = m/\lambda = 0.001, 0.01, 0.5, 1$.

At large separations, the ratio tends to a constant determined by the equation

$$E|_{L\to\infty} = -\frac{1}{16\pi L^3}\mathrm{Li}_4(\lambda^2 C_1).$$

Outlook

1. We considered the Casimir effect between two slabs in the framework of quantum field theory. A scalar field ϕ mimics the electromagnetic field, and another scalar field ψ, which is confined by Dirichlet boundary conditions, mimics the matter inside the slabs. Both fields interact by a Yukawa coupling.
2. For the calculation of the vacuum interaction energy, we used the TGTG formula and calculated the reflection coefficient for the field ϕ from the one-loop polarization operator Π of the field ψ. The polarization operator divides into a translationally non-invariant part, $\Pi^{(nt)}$, and an invariant part, $\Pi^{(t)}$. The invariant part $\Pi^{(t)}$ has an ultraviolet divergence, which can be removed by standard methods of coupling renormalization. Together, the polarization operator, and with it the reflection coefficient, can be calculated numerically, and their asymptotics for large and small momenta can be obtained. Finally, the Casimir energy can be calculated.
3. The considered model has an instability that can be avoided by a more realistic model with a momentum dependent coupling.
4. We demonstrated in principle how the Casimir energy can be calculated for a $(3+1)$-dimensional matter field in the slabs within the framework of QFT quantum field theory beyond cases with graphene where the matter field is in $D = 2 + 1$.
5. We have not yet succeeded to calculate the Casimir energy for "true QED" in half spaces with bag boundary conditions. The reason is in the divergences that we uncounted.