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On the Inner Topological Pressure within the Topological Insulators

*Daniel Faílde and Daniel Baldomir**

Topological insulators (TIs) have axion electrodynamics instead of the usual Maxwell. Then, there is an additional energy density, whose origin is topological, generating a pressure that is found analytically. It is shown that the topological electric and magnetic fields act only on the surface, while the scalar axion does as a real Klein–Gordon field in all the TI, giving rise to a behavior quite similar to the Casimir effect without the intervention of the virtual photons of the vacuum. This opens the possibility to experimentally test the electrodynamics of axions for the TIs.

1. Introduction

The quantum field theory tells us that the vacuum is not empty, but it is formed by virtual particles which are created and destroyed within fluctuating fields having a zero-point energy.[1,2] One paradigmatic example is given by the vacuum of quantum electrodynamics, where the virtual photons transform into pairs of electron-positron. Those photons have high energy, high frequency, or short wavelength. Thus, two near parallel conductor plates can cut such photons selecting the ones of short wavelength and even create a region of negative energy in their inner part. This means that it must appear an attractive force between those plates or one equivalent pressure on them, which is known as the Casimir effect.[3–6] That is to say, this assumes that the photons of high frequency go in by the surfaces where there are not conductors, which do not apply to the topological insulators (TIs) where all its surface is metallic. Later on, this calculation was generalized to dielectrics, showing that the condition of having good metallic boundary conditions for the plates was not necessary for obtaining such effect.[7–9] Although there are differences, for instance, the Casimir employing the van der Waals interaction shows that the pressure depends on the magnitude of the fine structure constant α.[10] This is also a straightforward dependence that is present in this paper for the TIs employing its associated axion electromagnetic fields and without needing to use van der Waals fluctuations. The special dynamics and features of these materials, which present both conductor and insulating behaviors, made them very interesting for introducing different fields and boundary conditions to measure experimentally singular Casimir effects.[11–13]

For taking into account all these physics, we need to enlarge the usual Maxwell electrodynamics action, which only uses the scalar Lorentz invariant associated with the fields for obtaining all Maxwell electrodynamics in the vacuum because classically the pseudoscalar invariant does not contribute to the motion equations more than with a surface term. In fact, the Lorentz pseudoscalar can only be implemented physically within an action working on a phase of an exponential expression, that is, in a quantum formalism.[14] Besides that, it is also necessary to introduce a scalar field $\theta(\boldsymbol{r}, t)$, named axion field to take into account the non-trivial topology. This field might be interpreted as an angle between the electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ fields because it keeps invariant the action under a shift of 2π. In the non-trivial zone of the TIs, that is, in the surfaces, where the bands are crossed, this field takes a constant value equal to π for conserving the time invariance $\hat{T}$ and having Kramers currents. Hence, the axion electrodynamics employs the two Lorentz invariants associated with the fields and a new scalar field.[15–19]

Furthermore, the non-trivial topology of TIs is simultaneously found within the band structure through their Berry curvature besides in the axion electrodynamics. In one case, the $\boldsymbol{E}$ and $\boldsymbol{B}$ fields can also be determined by constraining it into a Brillouin zone torus $S^1 \times S^1$ employing the Gauss–Bonnet formula, whereas the Chern number is used for the bands through the Berry curvature only.[19,20] The crossing band singularities in the k−space are in correspondence with the genus of the torus in the Brillouin zone. More accurately, in the TIs, where the topology is non-trivial, taking the energy $\xi(\boldsymbol{r}_n, \boldsymbol{k}) = \xi(\boldsymbol{k}) + e\boldsymbol{E} \cdot \boldsymbol{r}_n - \boldsymbol{m}_n(\boldsymbol{k}) \cdot \boldsymbol{B}$ under electric and magnetic fields, the equations of motion for an electron in a single band n would be [21, 22]

$$\frac{\partial}{\partial t}\boldsymbol{k} = -\frac{1}{\hbar}\nabla_r \xi_n - \frac{e}{\hbar}\frac{\partial}{\partial t}\boldsymbol{r}_n \times \boldsymbol{B} \tag{1}$$

$$\frac{\partial}{\partial t}\boldsymbol{r}_n = \frac{1}{\hbar}\nabla_k \xi_n - \frac{\partial}{\partial t}\boldsymbol{k} \times \boldsymbol{\Omega}_n \tag{2}$$

where $\boldsymbol{m}_n = -\frac{e}{2}\langle n|\boldsymbol{r} \times (\boldsymbol{v} - \langle \boldsymbol{v}\rangle)|n\rangle = \frac{e}{\hbar}\xi_n \boldsymbol{\Omega}_n$ is the orbital magnetic moment of the electrons in the band n, $\langle \boldsymbol{v}\rangle$ their average

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velocity, Ω_n the Berry curvature, $\hbar$ the Planck bar constant, and $-e$ the charge of the electron. This shows clearly a relationship between the transport in the bands or in the lattice, where the electric and magnetic fields produce anomalous contributions to the particle's velocity in the presence of non-zero Berry curvatures. Thus, it is straightforward to obtain the quantized electric conductivity $\sigma_{xy} = \frac{e^2}{h} C_n$ for a filled band, $C_n = \frac{1}{2\pi} \int_{S^1 \times S^1} d^2k\, \Omega_n$ being the integer Chern number of the n-band, just using $\boldsymbol{j_n} = -\frac{e}{(2\pi)^2} \int_{S^1 \times S^1} d^2k \frac{\partial}{\partial t} \boldsymbol{r_n}$.[20] This is one of the main results for the topological transport, but we are interested to focus on the pressure made by the electromagnetic fields. For such an aim, we are going to enlarge the axion electrodynamics action allowing it to propagate the scalar field $\theta(\boldsymbol{r}, t)$ within the bulk, while in the surface taking the constant value $\theta(\boldsymbol{r}, t) = \pi$.

2. Results and Discussion

The action in the axion electrodynamics contains the two Lorentz invariants associated with the fields. That is to say, the pseudoscalar quantity $\frac{1}{2}\epsilon_{\mu\nu\alpha\beta} F^{\mu\nu} F^{\alpha\beta} = -\frac{4}{c} \boldsymbol{E} \times \boldsymbol{B}$ is added, besides the usual scalar $F_{\alpha\beta}F^{\alpha\beta} = -2(E^2/c^2 - B^2)$ which is enough to provide Maxwell electrodynamics in the trivial topological vacuum, without taking into account finite local boundaries for the fields or their global properties. Hence, we have the Lagrangian density[17,23]

$$\mathcal{L} = -\frac{1}{4\mu_0} F_{\alpha\beta} F^{\alpha\beta} - A_\mu J^\mu + \frac{e^2 c}{32\pi^2 \hbar} \theta(r, t) \epsilon_{\mu\nu\alpha\beta} F^{\mu\nu} F^{\alpha\beta} \tag{3}$$

where the first two terms are associated with the usual Maxwell's electrodynamics and the last term gives the axion electromagnetism contribution through the $\theta(r, t)$ scalar field. This leads directly to the equivalent Maxwell equations in TIs considering the variation of the electromagnetic potential A_μ

$$\nabla \cdot \boldsymbol{D} = \rho_f - \frac{e^2}{4\pi\hbar} \nabla\left(\frac{\theta}{\pi}\right) \cdot \boldsymbol{B} \tag{4}$$

$$\nabla \times \boldsymbol{H} = J_f + \frac{\partial \boldsymbol{D}}{\partial t} + \frac{e^2}{4\pi\hbar} \left[\frac{\partial}{\partial t}\left(\frac{\theta}{\pi}\right)\boldsymbol{B} + \nabla\left(\frac{\theta}{\pi}\right) \times \boldsymbol{E}\right] \tag{5}$$

The first equation substitutes the Gauss expression, while the second does it for the Ampere–Maxwell. The other two equations, Faraday and non-existence of isolated magnetic poles, maintain the same form allowing to define locally the usual electromagnetic potentials.[24,25] It is necessary to observe in the previous equations that $\theta(r, t)$ must be a scalar field of modulo 2π for the action. That is to say, it needs to be a function of the space and time if the new electrodynamics wants to take into account the topological background. In fact, the axions can be thought as excitations of the $\theta(\boldsymbol{r}, t)$ scalar field coupled to the electromagnetic field as the phonons, magnons, or plasmons do for obtaining polaritons.[26,27] Their coupling with the photons is quite weak and we are going to neglect their mass m_θ in this paper where these axions are going to play a fundamental role under thermal changes in the TIs.

To have the same non-trivial topology for the bands and for the lattice, in the surface, where $\theta = \pi$, we can determine the magnetic and electric fields living on torus on each Brillouin zone. This can be done through the magnetic and static electric flux quantization over the torus[19,28,29]

$$|\boldsymbol{B}_\theta| = n \frac{h}{ea^2} \tag{6}$$

$$|\boldsymbol{E}_\theta| = n' \frac{hv_F}{ea^2} \tag{7}$$

Here, $n, n' \in \mathcal{N}$ are natural numbers that determine the topological sector and v_F the Fermi velocity that share the relativistic Dirac electrons and photons due to having both rest mass zero; that is, the relativistic Minkowski spacetime is taken with v_F instead of c for assuming the diffusion equation $\xi = pv_F$ for low energies. It is worthy to observe that we can choose a common gauge function $\Lambda(x, t) = \frac{xh}{ea}$ for the electromagnetic potential and the Berry's connection, x being the position of one point of the torus and a the lattice constant.[30] This means that we can synchronize the change of the phase $\theta(x, t)$ on the Bloch bands and the electromagnetic potential for each topological sector where the function is continuous, keeping control of the gauge freedom parameter. This allows to define simultaneously Equations (1) and (2) on the surface, where the singularities exist, for the electromagnetic fields associated with the axion electrodynamics as pieces of the same topological manifold. Mathematically, we are using the common gauge $U(1)$ Abelian group, which is not trivial topologically, for the bands and the lattice symmetries in the case of TIs; that is, $\pi_1(S^1) = Z$ can have homotopies with values different than zero and define them out of each singularity.[30]

It is immediate to find the density of energy of these topological axion electromagnetic fields $\xi_\theta = \frac{1}{2}(\boldsymbol{E}_\theta \boldsymbol{D}_\theta + \boldsymbol{H}_\theta \boldsymbol{B}_\theta)$ given by

$$\xi_\theta = \frac{\pi\hbar v_F}{\alpha a^4} \tag{8}$$

α being the fine structure constant in this medium with the Fermi velocity v_F instead of c.[31,32] This term corresponds only to the fields because the density of energy due to the electric polarization $\boldsymbol{P}$ and magnetization $\boldsymbol{M}$ cancel each other. $\boldsymbol{M}$ is negative while $\boldsymbol{P}$ is positive as can be seen from the above generalized Maxwell equations. Explicitly, the values are given by $\boldsymbol{M} = -\frac{e^2}{4\pi\hbar}\boldsymbol{E}$ and $\boldsymbol{P} = \frac{e^2}{4\pi\hbar}\boldsymbol{B}$, taking that the fields have π radians between them.[15] Actually, this expression was calculated in a Brillouin zone, but it must be the same in all these zones for the surfaces. Interpreting the energy density as a classical conductor is very easy since $\boldsymbol{E} = \sigma/\epsilon_0\, \hat{\boldsymbol{n}}$, where σ is the surface density of charge, and the density of energy is $\xi = \sigma^2/(2\epsilon_0)$. Notice that here $\hat{\boldsymbol{n}}$ stands for the unit vector normal to the surface. That is, the energy density in the surface is associated with the square of the charge density and reasoning in parallel; we could also think that we have a growth of the density of charges due to the topological fields that exert an orthogonal force to the metallic surface and outward in the direction $\hat{n}$, but going to the generalized Gauss equation, we obtain that $\rho = \alpha v_F \epsilon B \partial_{\boldsymbol{n}}(\frac{\theta}{\pi})$, where the $\frac{\theta}{\pi}$ is a step Heaviside function, going from 1 to 0 outside the TI, whose derivative gives a Dirac delta function. Thus, the density of charge in the surface gives $\sigma = \alpha\epsilon v_F B$ which grows with these fields. Hence, although we can observe that the above density of energy, Equation (8), might be interpreted as a pressure and only

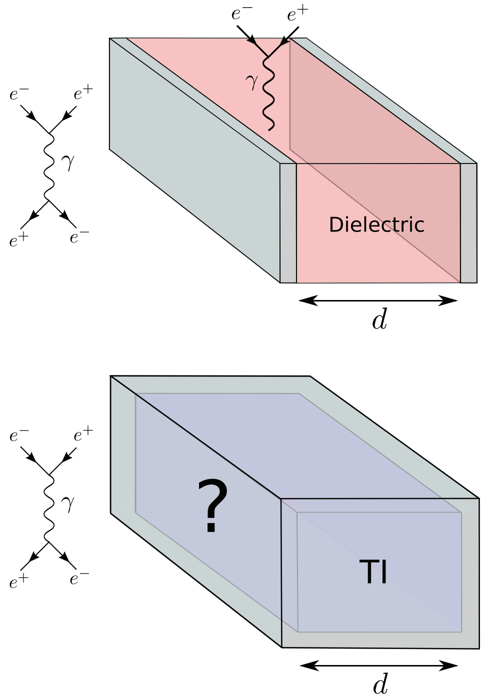

Figure 1. Representation of the Casimir effect (upper panel) between two conductor plates placed at a distance d and its counterpart effect produced by the axions within the topological insulators. Due to all the surfaces in the TI being metallic no virtual photons are expected to penetrate leading to a measurable pressure different from the Casimir between opposite plates.

differs on some constants from the Casimir pressure between two conductor plates placed at a distance d instead of the lattice constant a, nevertheless its source is absolutely different (**Figure 1**). Remember that the Casimir pressure at $T = 0$ is given by

$$P = -\frac{\pi^2 \hbar c}{240 d^4} \tag{9}$$

and its dependence at low temperatures can be written as

$$P = -\frac{\pi^2 \hbar c}{240 d^4}\left[1 + \frac{1}{3}\left(\frac{T}{T_e}\right)^4\right] \tag{10}$$

where $T_e = \frac{\hbar c}{2dk_B}$ is the effective temperature, whose pressure is important at distances higher than the thermal wavelength $\frac{\hbar c}{k_B T}$.[7,8,33] Unlike what happens for the electric and magnetic fields, the scalar axion field $\theta(\boldsymbol{r}, t)$ is defined in all the material and it can evolve naturally with the temperature changes as we show in what follows.

Following with the TI, in a layer with width d where the x and y lengths are much higher than d, the scalar axion $\theta(\boldsymbol{r}, t)$ field has good Dirichlet conditions in the z-direction orthogonal to the plates. That is to say, we have a normalized field $\bar{\theta} = \theta/\pi$ which satisfies that $\bar{\theta}(z = 0) = \bar{\theta}(z = d) = 1$, knowing that $\theta(\boldsymbol{r}, t) = \pi$ must be the constant value that this field takes on the surface. Hence, we have a discrete quantized linear moment $p_z = n_z \hbar \frac{2\pi}{d}$ as the translator generator. In fact, it is a Klein–Gordon field with rest mass zero and Lagrangian density $\mathcal{L} = \frac{1}{2}\partial_\mu \bar{\theta} \partial^\mu \bar{\theta}$,[34] which allows to quantize it via the mode expansion

$$\bar{\theta}(\boldsymbol{r}, t) = \frac{1}{(2\pi)^3} \int \frac{d^3\boldsymbol{p}}{\sqrt{2p_0}} \left[a_p exp\left(-\frac{i}{\hbar}\boldsymbol{p}.\boldsymbol{r}\right) + a_p^\dagger exp\left(+\frac{i}{\hbar}\boldsymbol{p}.\boldsymbol{r}\right)\right] \tag{11}$$

where the Lorentz invariant measure is given by $\int \frac{d^3\boldsymbol{p}}{2p_0}$, being $p_0 = \xi v_F^{-1}$, making to define the creation–annihilation operators by $a_p = \sqrt{\frac{\hbar}{2p_0}} f(p_0, p)$ and $a_p^\dagger = \sqrt{\frac{\hbar}{2p_0}} f(-p_0, -p)$ being $f(p_0, p)$ and $f(-p_0, -p)$ relativistic normalized annihilation and creation operators to obtain the only nonvanishing commutators

$$[a_p, a_{p'}^\dagger] = (2\pi)^3 2\hbar\omega\delta^3(\boldsymbol{p} - \boldsymbol{p'}) \tag{12}$$

which keep the form of the Heisenberg's indeterminacy within the canonical quantization for this real scalar field. Thus, the dispersion energy $\xi_n = v_F\sqrt{p_s^2 + (\hbar\frac{2\pi n}{d})^2}$, where $p_s^2 = p_x^2 + p_y^2$ are the momenta on the surfaces determined by x and y coordinates, allows us to write the density of energy

$$\xi_{0A} = \sum_{n=0}^{\infty} \frac{1}{2\hbar^2(2\pi)^2} \int \xi_n d^2 p_s \tag{13}$$

This leads us to an infinite value which needs regularization as usually is made for the Casimir effect with the difference of having one polarization for the axions instead of the two arising for photons.[35] For doing this regularization, we use the factor $e^{-\epsilon d \xi_n / 2\pi\hbar v_F}$ whose limit is one when ϵ tends to zero. Making this straightforward calculation, we have the result $\frac{4\pi}{v_F^2}(\frac{2\pi\hbar v_F}{\epsilon d})^3 e^{-n\epsilon}(1 + n\epsilon + \frac{n^2\epsilon^2}{2})$ for the integral. In this way, the sum on n is made by considering it as a geometric progression with ratio $e^{-\epsilon}$ for obtaining the density of energy

$$\xi_{0A} = \frac{12\pi^2\hbar v_F}{\epsilon^4 d^3} - \frac{\pi^2\hbar v_F}{180 d^3} + \frac{\pi^2\epsilon^2}{1260 d^3} \tag{14}$$

where we have developed the approximation till quadratic terms in ϵ and subtracted the zero-point energy $\frac{1}{2}\hbar\omega$ in Equation (13).[3] In contrast with the third term that tends to zero, the first term diverges as ϵ becomes smaller. Nevertheless, this term is well-known as the one associated with the vacuum contribution in non-periodicity conditions or long distances $\frac{1}{2(2\pi)^2\hbar^2}\int_0^\infty dn \int \xi_n d^2 p_s$ whose contribution, making use of the same regulator, must be subtracted for obtaining the equivalent Casimir pressure

$$P = -\frac{\pi^2\hbar v_F}{60 d^4} \tag{15}$$

for the axion field $\theta(\boldsymbol{r}, t)$. This expression differs from the one exerted by the photons in some constants that are associated with the change in the field periodicity, number of wave polarizations, and velocity propagation of the fields in the medium. However, its dependence on the distance and sign remains invariant, and hence, it tends to decrease the distance between the surfaces giving an attractive force between them, as it happens with the Casimir force.

Furthermore, we can see the dependence on the temperature of the above pressure considering that the partition function of this gas of bosons is given by

$$Z = \prod_p \left(\sum_{N=0}^{\infty} exp\left[-N \frac{\xi_n - \mu}{k_B T} \right] \right) = \prod_p \frac{1}{1 - exp\left[-\frac{\xi_n - \mu}{k_B T} \right]} \tag{16}$$

where the sum was taken as a geometric series with N the number of particles and μ the chemical potential. This is possible if and only if $\xi_n - \mu \geq 0$ or when the chemical potential is negative or zero because we can reach the fundamental state. Notice that this condition cannot be filled by a fermion system where the chemical potential is always positive. From a physical point of view, it seems natural to think that the axions are special photons in the TIs or at least that both are directly related. Now we can calculate the density of free energy F of our system for a finite temperature T

$$F = \frac{k_B T}{(2\pi)^2 \hbar^2} \sum_{n=(0)1}^{\infty} \int d^2 p_s ln\left(1 - exp\left[-\frac{\xi_n - \mu}{k_B T} \right] \right) \tag{17}$$

where we used that $ln\, Z = -\sum_p ln[1 - exp(-(\frac{\xi_n - \mu}{k_B T}))]$ and where the sum in n has a factor of 1/2 for the term $n = 0$ for taking into account properly the zero-energy point energy as before.[3] Setting $\mu = 0$ and making the change of variable $x = \frac{\xi_n}{k_B T}$ with $d^2 p_s = 2\pi (k_B T)^2 v_F^{-2} x dx$, we have

$$F = \frac{(k_B T)^3}{2\pi \hbar^2 v_F^2} \sum_{n=(0)1}^{\infty} \int_{\frac{2\pi n \hbar v_F}{k_B T d}}^{\infty} ln(1 - e^{-x}) x dx \tag{18}$$

Thus, for $n = 0$, we can do an integration by parts and employ the result $\frac{1}{(s-1)!} \int \frac{x^{s-1} dx}{e^x - 1} = \zeta(s)$ for obtaining

$$F = -\frac{(k_B T)^3}{4\pi \hbar^2 v_F^2} \zeta(3) + \frac{(k_B T)^3}{2\pi \hbar^2 v_F^2} \sum_{n=1}^{\infty} \int_{\frac{2\pi n \hbar v_F}{k_B T d}}^{\infty} ln(1 - e^{-x}) x dx \tag{19}$$

where $\zeta(s)$ is the Riemann zeta function. On the other hand, the second integral has no analytical expression, but for low temperatures (or distances) with $\frac{2\pi \hbar v_F}{k_B T d}$ much higher than one, the logarithm can be expanded in powers of e^{-x} and the dominant term is for $n = 1$. Thus, we have for this integral term the approximation $-\frac{(k_B T)^3}{2\pi \hbar^2 v_F^2} [1 + \frac{2\pi \hbar v_F}{k_B T d}] exp(-\frac{2\pi \hbar v_F}{k_B T d})$. Therefore, we find the density of free energy of the axions associated with the topological fields at low-temperatures

$$F = -\frac{\pi^2 \hbar v_F}{180 d^3} - \frac{(k_B T)^3}{4\pi \hbar^2 v_F^2} \zeta(3) - \frac{(k_B T)^3}{2\pi \hbar^2 v_F^2} \left[1 + \frac{2\pi \hbar v_F}{k_B T d} \right] exp\left(-\frac{2\pi \hbar v_F}{k_B T d} \right) + \frac{(k_B T)^4 d}{2\pi^2 (\hbar v_F)^3} \zeta(4) \tag{20}$$

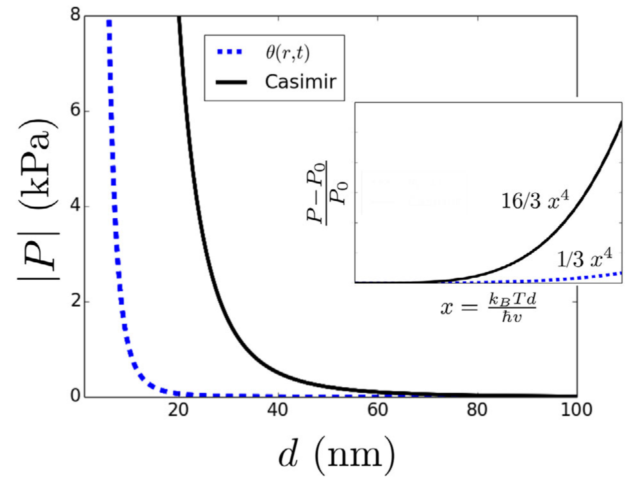

Figure 2. Distance dependency of the pressure associated with the axions in a topological insulator (dashed line) compared with the pressure exerted by the photons in the Casimir effect (solid line) taking $T = 10$ K and $v_F = 6\ 10^5$ m s^{-1}. The inset shows the normalized pressure with respect to the dimensionless parameter $x \equiv T/T^* = k_B T d/(\hbar v) << 1$ for both cases.

and the pressure exerted by them on the surfaces

$$P = -\frac{\pi^2 \hbar v_F}{60 d^4} + \frac{2\pi k_B T}{d^3} exp\left(-\frac{2\pi \hbar v_F}{k_B T d} \right) - \frac{(k_B T)^4}{2\pi^2 (\hbar v_F)^3} \zeta(4) \tag{21}$$

Again, the last term corresponds to the temperature dependence of the free energy without taking into account the axion field periodicity which is subtracted following the same procedure as before. Notice that for photons this latter factor, known as the black body free energy of a photon gas $2(k_B T)^4 d/(\pi^2 \hbar^3 c^3) \zeta(4)$, is proportional to four times the given value due to the change in the number of possible polarization and periodicity of the fields. It is worthy to observe that for low temperatures or distances, the second term in Equation (21) is negligible when compared with the other two. Thus, we can write the force or pressure exerted on the surfaces as $P = P_0(1 + \frac{1}{3}(\frac{T}{T^*})^4)$. This follows the same dependence as the Casimir force Equation (10) but redefining its principal variables $P_0 = -\frac{\pi^2 \hbar v_F}{60 d^4}$ and the effective temperature $T^* = \hbar v_F/(k_B d)$ (**Figure 2**). In this context, it seems obvious that it is possible to get a technological advantage when making thin-film based devices due to having an effective pressure for the axions substantially smaller than the one of Casimir. This latter fact about its magnitude constitutes a differentiating signature when testing experimentally the physics of the axions in these systems.

3. Conclusion

In summary, we examined the topological magneto-electric effect of the TIs and obtained a behavior quite similar to that of Casimir, although with very different origins. The electric and magnetic fields have a very high density in the surface, and inside the TIs, it is the axionic scalar field that acts as the temperature-dependent Casimir. Thus, we can obtain a distribution of the topological energy associated with the electric, magnetic, and axion fields within the TIs. All these results are suitable for being measured and therefore help to understand both the topological behavior of the TIs and the electrodynamics of axions.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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