TOPOLOGICAL CASIMIR EFFECT IN
NANOTUBES AND NANOLOOPES

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The Casimir effect is investigated in cylindrical and toroidal carbon nanotubes within the framework of the Dirac-like model for the electronic states. The topological Casimir energy is positive for metallic cylindrical nanotubes and is negative for semiconducting ones. The toroidal compactification of a cylindrical nanotube along its axis increases the Casimir energy for metallic-type (periodic) boundary conditions along its axis and decreases the Casimir energy for the semiconducting-type compactifications. For finite length metallic nanotubes the Casimir forces acting on the tube edges are always attractive, whereas for semiconducting-type ones they are attractive for small lengths of the nanotube and repulsive for large lengths.

Keywords: Casimir effect; Carbon nanotubes.

1. Introduction

An interesting application of the quantum field theoretical models with non-trivial topology recently appeared in nanophysics. The long-wavelength description of the electronic states in graphene can be formulated in terms of the Dirac-like theory with the Fermi velocity playing the role of speed of light (see, e.g., Ref.1). Single-walled carbon nanotubes are generated by rolling up a graphene sheet to form a cylinder and the background spacetime for the corresponding Dirac-like theory has topology $R^2 \times S^1$. Compactifying the direction along the cylinder axis we obtain another class of graphene made structures called toroidal carbon nanotubes with the background topology $R^1 \times (S^1)^2$.

The boundary conditions imposed on the fermionic field in these nanostructures give rise to the modification of the spectrum for vacuum fluctuations and, as a result, to the Casimir-type contributions in vacuum expectation value (VEV) of the energy-momentum tensor (for the topological
Casimir effect see\(^2\)). In the present paper, based on Refs.,\(^3,4\) we investigate the fermionic Casimir effect in nanotubes. The paper is organized as follows. In the next section the topological Casimir effect is considered in cylindrical nanotubes. The VEV of the energy-momentum tensor for a fermionic field in toroidal nanotubes is discussed in Sec. 3. The Casimir forces acting on the edges of finite-length carbon nanotubes are investigated in Sec. 4. The main results are summarized in Sec. 5.

2. Cylindrical nanotubes

A single wall cylindrical nanotube is a graphene sheet rolled into a cylindrical shape. For this case we have spatial topology \(R^1 \times S^1\) with the compactified dimension of the length \(L\). The carbon nanotube is characterized by its chiral vector \(C_h = n_w a_1 + m_w a_2\), with \(n_w, m_w\) being integers, and \(L = |C_h| = a \sqrt{n_w^2 + m_w^2 + n_w m_w}\), \(a = |a_1| = |a_2| = 2.46\) A. A zigzag nanotube corresponds to the special case \(C_h = (n_w, 0)\), and an armchair nanotube corresponds to the case \(C_h = (n_w, n_w)\). All other cases correspond to chiral nanotubes. In the case \(n_w - m_w = 3q_w, q_w \in \mathbb{Z}\), the nanotube will be metallic and in the case \(n_w - m_w \neq 3q_w\) the nanotube will be semiconductor with an energy gap inversely proportional to the diameter.

The electronic band structure of a graphene sheet close to the Dirac points shows a conical dispersion \(E(k) = v_F |k|\), where \(k\) is the momentum measured relatively to the Dirac points and \(v_F\) represents the Fermi velocity. The corresponding low-energy excitations can be described by a pair of two-component Weyl spinors. By taking into account that in the presence of an external magnetic field an effective mass term is generated for the fermionic excitations, we consider the general case of massive spinor field \(\psi\) on background of 3-dimensional flat spacetime with spatial topology \(R^1 \times S^1\). The corresponding line element has the form \(ds^2 = dt^2 - (dz^1)^2 - (dz^2)^2\), where \(-\infty < z^1 < \infty\) and \(0 \leq z^2 \leq L\).

We assume that the field obeys the boundary condition

\[
\psi(t, z^1, z^2 + L) = e^{i\beta} \psi(t, z^1, z^2),
\]

with a constant phase \(\beta\). For metallic nanotubes \(\beta = 0\) and for semiconductor nanotubes, depending on the chiral vector, we have two classes of inequivalent boundary conditions corresponding to \(\beta = \pm 2\pi/3\). In the expression for the Casimir densities the phase \(\beta\) appears in the form \(\cos(n\beta)\) and, hence, the Casimir energy density and stresses are the same for these two cases. The VEV of the energy-momentum tensor for a cylindrical nan-
tube has the form (no summation over $l$)
\[ \langle T_k \rangle_{(cyl)} = \delta_k^l \sum_{n=1}^{\infty} \cos(n\beta) G^{(l)}(nmL) \frac{e^{-nmL}}{nL^3 n^3}, \] (2)
with the notations $G^{(0)}(z) = G^{(1)}(z) = 1 + z, G^{(2)}(z) = -(2 + 2z + z^2)$.
In particular, the Casimir energy density is positive for metallic nanotubes and negative for semiconducting ones.

In the massless case we have $\langle T_0 \rangle_{(cyl)} = -\langle T_2 \rangle_{(cyl)} = S_{1\beta}/(\pi L^3)$, with the notation $S_{1\beta} = \sum_{n=1}^{\infty} \cos(n\beta)/n^3$. In particular, $S_0 = 1.202$ and $S_{2\pi/3} = -0.534$. In carbon nanotubes we have two sublattices and each of them gives the contribution to the Casimir densities given by (2). So, for the Casimir energy density on a carbon nanotube with radius $L$ one has $\langle T_0 \rangle_{1,1} = 2\hbar v_F S_{1\beta}/(\pi L^3)$, where the standard units are restored.

3. Toroidal nanotubes

For the geometry of a toroidal nanotube we have the spatial topology $(S^1)^2$. The boundary conditions have the form
\[ \psi(t, z^1 + L_1, z^2) = e^{i\beta_1} \psi(t, z^1, z^2), \psi(t, z^1, z^2 + L_2) = e^{i\beta_2} \psi(t, z^1, z^2). \] (3)
The corresponding energy density and the vacuum stresses are given by the expressions (no summation over $l$)
\[ \langle T_0 \rangle_{(tor)} = \sum_{j=1,2} \langle T_0 \rangle_{(cyl)}(L_j) + \frac{2}{\pi} \sum_{m_1=1}^{\infty} \sum_{m_2=1}^{+\infty} \frac{1 + mg(L_2, m_2)}{g^5(L_2, m_2)} \times \frac{\cos(m_1\beta_1) \cos(m_2\beta_2)}{\exp(mg(L_2, m_2))}, \] (4)
\[ \langle T_1 \rangle_{(tor)} = \langle T_0 \rangle_{(tor)} - \frac{m_5^5}{\pi} \sum_{j=1,2} \sum_{m_1=1}^{+\infty} \cos(m_j\beta_j)L_j^2 m_2^2 G(mL_j m_j) \]
\[ - \frac{2m_5^5}{\pi} \sum_{m_1=1}^{+\infty} \cos(m_1\beta_1) \cos(m_2\beta_2)L_1^2 m_2^2 G(mg(L_2, m_2)), \] (5)
with $G(x) = (3 + 3x + x^2)e^{-x}/x^5$, $l = 1, 2$, and $g(L_2, m_2) = \sqrt{m_1^2 L_1^2 + m_2^2 L_2^2}$. The corresponding formulae for the Casimir densities in toroidal nanotubes are obtained with an additional factor 2. In standard units the factor $\hbar v_F$ appears as well. From the formulae given above it follows that the toroidal compactification of a cylindrical nanotube along its axis increases the Casimir energy for periodic conditions ($\beta_1 = 0$) and decreases the Casimir energy for the semiconducting-type compactifications.
4. Finite-length nanotubes

In this section we will assume that the nanotube has finite length $a$. We assume the periodicity condition (1) along the compact dimension. As the Dirac field lives on the cylinder surface it is natural to impose bag boundary conditions
\[ (1 + i \gamma^l m_l) \psi = 0, \quad z^1 = 0, a, \]
on the cylinder edges, with $\gamma^l$ being the Dirac matrices and $n_l$ is the normal to the boundaries. The additional confinement of the electrons along the tube axis leads to the change of the ground state energy. The corresponding Casimir energy is decomposed as
\[ E = aL \langle T^0_0 \rangle_{\text{(cyl)}} + 2E^{(1)} - \frac{1}{\pi} \sum_{l=-\infty}^{+\infty} \int_{m_l}^{\infty} \frac{dx}{\sqrt{x^2 - m_l^2}} \ln \left( 1 + \frac{x - m}{x + m} e^{-2ax} \right), \]
with $m_l^2 = [(2\pi l + \beta)/L]^2 + m^2$. The part $E^{(1)}$ is the Casimir energy for a single edge (when the other edge is absent) in the half-space. The last term in Eq. (6) is the interaction part. The single edge part of the Casimir energy does not depend on the length of the tube and will not contribute to the Casimir force.

For the Casimir force acting on the edges of the tube we have
\[ P = -\langle T^0_0 \rangle_{\text{(cyl)}} - \frac{2}{\pi L} \sum_{l=-\infty}^{+\infty} \int_{m_l}^{\infty} dx \frac{x}{x^2 - m^2} e^{2ax} + 1. \]
The corresponding expressions for the Casimir energy and force in finite length cylindrical nanotubes are obtained with an additional factor 2. So, for the Casimir force acting per unit length of the edge of a carbon nanotube one has: $P^{(CN)} = 2\hbar v_F P$. For long tubes, $a/L \gg 1$, the first term on the right of (7) is dominant and we have $P^{(CN)} \approx -0.765 \hbar v_F / L^3$ for metallic nanotubes and $P^{(CN)} \approx 0.34 \hbar v_F / L^3$ for semiconducting ones. In the limit $a/L \ll 1$ the Casimir force do not depend on the chirality and one has $P^{(CN)} \approx -0.144 \hbar v_F / a^3$. In Fig. 1 we have plotted the Casimir forces acting on the edges of metallic (full curves) and semiconducting-type (dashed curves) carbon nanotube as functions of the tube length for different values of the fermion mass. As it is seen, for metallic nanotubes these forces are always attractive, whereas for semiconducting-type ones they are attractive for small lengths and repulsive for large lengths.

5. Conclusion

We have investigated the Casimir effect for cylindrical and toroidal nanotubes within the framework of the Dirac-like model for electrons. The VEV
Fig. 1. The fermionic Casimir forces acting on the edges of the metallic (full curves) and semiconducting-type (dashed curves) nanotubes as functions of the tube length.

of the energy-momentum tensor is given by formula (2) for cylindrical nanotubes and by (4) and (5) (with an additional factor 2 which takes into account the presence of two sublattices) for toroidal nanotubes. The topological Casimir energy is positive for metallic cylindrical nanotubes and is negative for semiconducting ones. We have shown that the toroidal compactification of a cylindrical nanotube along its axis increases the Casimir energy for periodic boundary conditions and decreases the Casimir energy for the semiconducting-type compactifications. For finite-length carbon nanotubes the Casimir forces acting on the tube edges are always attractive for metallic nanotubes, whereas for semiconducting-type ones they are attractive for small lengths and repulsive for large lengths.

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