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VAN DER WAALS AND CASIMIR INTERACTIONS OF SOME GRAPHENE, MATERIAL PLATE AND CNTs SYSTEMS

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Abstract. *The Van der Waals and Casimir interactions between graphene and a material plate are studied by using the Lifshitz theory and approximate expressions for the free energy and force. The reflection properties of electromagnetic oscillations on graphene are governed by specific boundary conditions imposed on the infinitely thin positively charged plasma sheet, carrying a continuous fluid with some mass and charge density. The obtained formulas are applied to the cases of a graphene interacting with Au plate. We calculated also the Casimir interaction between carbon nanotube single wall and Au plate. The comparision with other recently obtained theoretical results are made and the generalizations to more complicated carbon nanostructures are discussed.*

I. INTRODUCTION

The van der Waals and Casimir interactions which are generally called are a dispersion interaction investigated in technology. When the characteristic size of micro devices shrinks below a micrometer, collective quantum phenomena caused by the existence of zero point oscillations of the electromagnetic field come into play.At separations below 100 nm, the role of physical phenomena originating from vacuum oscillations, the dispersion interaction can become dominant. There are several experiments on measurement of the Casimir effect between two bodies performed [1, 2, 3, 8]. Thereafter, the precision of measurements of Casimir force was significantly increased and different methods controlling the force magnitude were elaborated opening possible applications to nanomachines.

It is much crucial to understand dispersion interaction between macroscopic bodies (a material plate with carbon nanostructures). A unified theory of dispersion interaction between parallel material plates in thermal equilibrium separated by a vaccum gap was developed by Lifshitz (1956). In Ref.[1, 4] the Lifshitz formulas were obtained for the dispersion interaction between graphene and a material plate. The Lifshitz theory presents an considerable opportunity for extensive studies of Casimir force. The use of approximations such as the proximity force theorem [9] permitted one to achieve rather acurate results for CNTs near a plane plate, basing on a configuration frequently used in recent experiments on measuring the Casimir force . In most cases, the macrobodies with plane boundaries were supposed to be isotropic.

In the present paper, we use the description of graphene in terms of the two dimensional free electron gas [1, 4] in order to extend the Lifshitz theory of the dispersion interaction to the case of carbon systems. Graphene is considered as an infinitely thin

positively charged flat sheet, carrying a contunuous fluid with some mass and negative charge densities. The sheet is characterized by some typical wave number Ω determined by the parameters of the hexagonal structure of graphite. In Refs [1, 2, 3, 4, 10] the interaction of the electromagnetic oscillations with such sheet was condidered and the normal modes and reflection coefficients were found. The Lifshitz formula for interaction of Au plate and graphene is obtained. The fit function associating with Proximity Force Approximation (PFA) method for interaction of CNTs with Au plate are used to calculate when the nanotube is in close the plate.

This paper is organized as follows: In section 2, we present the Lifshitz formula for the van der Waals and Casimir interactions between bodies. In section 3, calculation results are presented not only for the Casimir interaction between Au plate and graphene but also for that between Au plate and CNTs. Finally, section 4 shows our discussions and conclusions.

II. LIFSHITZ FORMULA OF CASIMIR INTERACTION BETWEEN GRAPHENE AND AU PLATE

We consider the van der Waals and Casimir interaction of a graphene occupying the xy-plane, $z = 0$, with a material semispace or a plate. The separation distance between the boundary plane of the semispace (plate) and graphene is a. The dispersion interaction of the two plane parallel bodies (plates or semispaces) labeled by the upper indices 1 and 2 with the electromagnetic oscillations can be described in terms of the reflection coefficients $r^{(1)}_{TM,TE}$ and $r^{(2)}_{TM,TE}$ for two independent polarizations of electromagnetic field (transverse magnetic and transverse electric). In so doing the van der Waals and Casimir interaction (the dispersion ineraction) free energy per unit area is given by the Lifshitz formula [1]

$$E(a) = \frac{\hbar}{4\pi^2}\int_0^\infty k_\perp dk_\perp \int_0^\infty d\xi \left[ln\left(1 - r^{(1)}_{TM} r^{(2)}_{TM} e^{-2aq}\right) + ln\left(1 - r^{(1)}_{TE} r^{(2)}_{TE} e^{-2aq}\right)\right]. \quad (1)$$

Here $k_\perp$ is the magnitude of the wave vector component perpendicular to the z-axis, ξ is the frequency variable along the imaginary axis (ω=$i\xi$) and

$$q = \sqrt{k_\perp^2 + \frac{\xi^2}{c^2}}. \quad (2)$$

Equation (1) is applicable at very low temperatures. If the temperature is higher Eq.(1) is simply generalized by changing the integration with respect to ξ for the summation over the discrete Matsubara frequencies. The general derivation of Eq.(1) for arbitrary reflection coefficients can be found in Ref.[1, 10]. From Eq.(1) the Van der Waals and Casimir forces acting between two bodies are :

$$F(a,T) = -\frac{\hbar}{2\pi^2}\int_0^\infty qk_\perp dk_\perp \int_0^\infty d\xi \left(\frac{r^{(1)}_{TM} r^{(2)}_{TM}}{e^{2aq} - r^{(1)}_{TM} r^{(2)}_{TM}} + \frac{r^{(1)}_{TE} r^{(2)}_{TE}}{e^{2aq} - r^{(1)}_{TE} r^{(2)}_{TE}}\right). \quad (3)$$

Equations (1) and (3) can be used to obtain the interaction energy and the force between a graphene and an atom (molecule), graphene and graphene sheet, graphene and carbon nanotube, between two carbon nanotubes, and a single wall carbon nanotube with Au plate. Now we specify the reflection coefficients. Let a semispace made of isotropic material

(labeled by upper index 2) and be describled by the dielectric by the dielectric permittivity $\varepsilon(\omega)$.In this case the reflection coefficients are [1, 4, 10]

$$r_{TM}^{(2)}(\varepsilon, k_\perp) = \frac{\varepsilon(i\xi)q - k}{\varepsilon(i\xi)q + k}, r_{TE}^{(2)}(\varepsilon, k_\perp) = \frac{k-q}{k+q}, \tag{4}$$

where

$$k = \sqrt{k_\perp^2 + \varepsilon(i\xi)\frac{\xi^2}{c^2}}, \tag{5}$$

In our computations, the reflection coefficients for an Au semispace are peresented in Eq.(4). As to Eq.(4), it depends on the dielectric permittivity of Au which can be approximated by means of the plasma model [5, 7]

$$\varepsilon(i\xi) = 1 + \frac{\omega_p^2}{\xi^2}, \tag{6}$$

where ω_p is the plasma frequency (in gold, $\omega_p = 1.37 \times 10^{16}$ rad/s).

If the first body is graphene, the idealization of the frequency-dependent dielectric permittivity cannot be used. In this case the reflection coefficients can be found [1, 4] by modeling graphene as a two-dimensional plasma sheet carring a negatively charged fluid of π-electrons.For the hexagonal structure of carbon layers, there is one π-electrons per atom resulting in two π-electrons per one hexagonal cell. This leads to the following values for the density of π-electrons and the wave number of the sheet

$$n = \frac{4}{3\sqrt{3}l^2}, \Omega = 2\pi\frac{ne^2}{mc^2} = 6.75 \times 10^5 m^{-1}, \tag{7}$$

where $l = 1.421A^0$ is the side length of a hexagon. This result leads to the following reflection coefficients on the graphene plasma sheet taken at the imaginary frequency axis [1, 2, 3]

$$r_{TM}^{(1)}(\xi, k_\perp) = \frac{c^2 q\Omega}{c^2 q\Omega + \xi^2}, r_{TE}^{(2)}(\xi, k_\perp) = \frac{\Omega}{\Omega + q}. \tag{8}$$

III. CALCULATION OF THE CASIMIR INTERACTION BETWEEN AU PLATE AND GRAPHENE

We apply Eqs.(1) and (3) to calculate the Casimir interaction energy and force acting per area between Au plate and graphene per unit area. The computational results for Caimir energy and force density $E(a)$, $F(a)$ between Au plate and graphene normalized to the Casimir energy and force density in the configuration of an ideal metal plate are calculated with the range of a from 2 nm to 80 nm. These results absolutely match with those presented in Ref.[1]. From these data above, we are likely to design a programme to find the fit function $E_{fit}(a)$ and $F_{fit}(a)$ describing the dependence of free energy and force per unit area on a distance, respectively.

Let the single-wall nanotube of radius R lie along the y axis at a separation a from the boundary surface of the material semispace. For sufficiently small a, the interaction free energy and force in such configuration can be approximately obtained by using the proximity force theorem , $E_{fit}(a)$ and $F_{fit}(a)$. According to the proximity force theorem,

we replace the cylindrical surface by a set of infinitely long plane strips of width dx and the nanotube is modeled by a cylindrical graphene sheet. The interaction between each strip, substituting a part of the cylindrical surface, and the opposite strip belonging to the boundary plane of Au semispace is calculated by both fit functions. The separation distance between the two opposite strips with coordinate x is

$$z = z(x) = a + R - \sqrt{R^2 - x^2}. \tag{9}$$

The computational results are represented in Figures 1 and 2

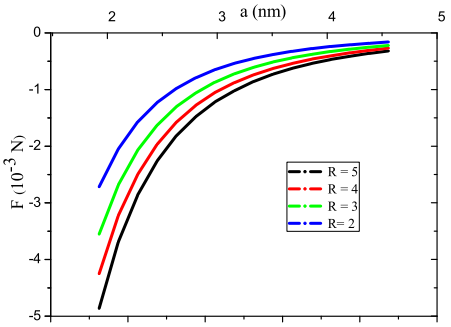

Fig. 1. The Casimir interaction force per unit length between the nanotube and a Au semispace.

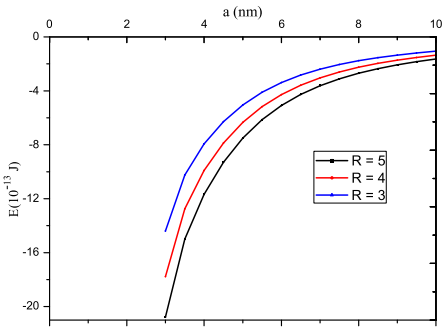

Fig. 2. The Casimir interaction free energy per unit length between the nanotube and a Au semispace.

It is noted that the results presenting in Ref.[1] were calculated in low temperature (nearly $0K$) and the fit functions were used in the distance from 2 nm to 10 nm. In this range, the PFA method becomes more accurate than lager distances because it has relation to the ratio of a to R. The smaller a/R is, the more accurate the computation is. The precision of PFA in such configuration applied in measurements was given in the Ref.[9].

IV. CONCLUSION AND DISCUSSION

In the foregoing, we have obtained the Lifshitz-types formulas describing the free energy and force of the Van der Waals and Casimir interaction between a material plate and a graphene plate, a single-wall carbon nanotube and material. The distinguishing feature of these formulas is that they describe graphene by using the reflection coefficents obtained from the specific boundary conditions for the electromagnetic oscillations on the infinitely thin plasma sheet. This approach permits to circumvent the use of the concept of dielectric permittivity commonly used in the Lifshitz theory of the van der Waals and Casimir force between macrobodies, but being not directly applicable to single-wall carbon nanostructures.

The obtained Lifshitz-type formulas for the van der Waals and Casimir energy and force were applied to the case of graphene interacting with the Au wall. The wall material

was described by the dielectric permittivity along the imagimary frequency axis computed using the tabulated optical data for the complex index of refraction for Au. In the case of Au, the interaction energy and force with graphene was also obtained using the plasma model dielectric function. The van der Waals and Casimir interaction of a material wall with a single-wall carbon nanotube in different radiuses in close proximity and fit functions, respectively. At separations less than 2 nm, there may be the attractive forces of chemical nature and short-range repulsive forces of exchange nature come into play. These forces depend on atomic structure of a surface and cannot be described macroscopically by means of the boundary conditions.

The results in this paper of Au-graphene interaction entirely match with [1]. The measure in this paper suggest some advantages in comparison to the approximate way used to estimate Casimir interaction in previous articles. As was recently noted in [1, 4], they applied PFA transformations in original Lifshitz expressions and computed by designing programs. Therefore, with each other configuration, they have to write a different program. While, offering fit functions for Casimir free energy and force between Au plate and graphene help us see form of Casimir energy and force and calculate other configurations by only these fit functions.

REFERENCES

[1] M. Bordag, B. Geyer, G. L. Klimchitskaya, and V. M. Mostepanenko, *arxiv*, 0611015v2 [cond-mat.other], (2006).
[2] A. Lambrecht, and S. Reynaud, *arxiv*, 0302073v1 [quant-ph], (2003).
[3] G. L. Klimchitskaya, U. Mohidder, and V. M. Mostepanenko, *arxiv*, 0902.4022v1 [cond-mat.other], (2009).
[4] E. V. Blagov, G. L. Klimchitskaya, and V. M. Mostepanenko, *arxiv*, 0704.1752v1 [cond-mat.mtrl-sci], (2007).
[5] M. Bordag, *arxiv*, 0511269v2 [hep-th], (2005).
[6] P. J. van Zwol, G. Palasantzas, and J. Th. M. De Hosson, *arxiv*, 0801.1384v1 [cond-mat.other], (2008).
[7] B. Geyer, G. L. Klimchitskaya, V. M. Mostepanenko, *arxiv*, 1002.2484v1 [cond-mat.other], (2010).
[8] V. M. Mostepanenko, *arxiv*, 0903.0815v1 [quant-ph], (2009).
[9] H. Gies, and K. Klingmuller, *arxiv*, 0601094v1 [quant-ph], (2006).
[10] E. V. Blagov, G. L. Klimchitskaya, and V. M. Mostepanenko, *Phys. Rev.* **B71** (2005) 235401.

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