Dispersive interactions in graphitic nanostructures

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Abstract

The Casimir interaction between graphitic nanostructures, such as carbon nanotubes and graphene sheets, is investigated at the quantum mechanical limit (T = 0 K) using a quantum electrodynamical approach for absorbing and dispersive media. It is found that the nanotube/nanotube interaction in a double wall carbon nanotube configuration is profoundly affected by the collective low frequency excitations of individual nanotubes. It is shown that pronounced, low frequency peaks in the nanotube electron energy loss spectra are a main factor contributing to the strength of the intertube attraction. The graphene/graphene force is also investigated. It is obtained that the graphene optical transparency is the main reason for the reduced attraction as compared to the one for perfect metals. This study presents a unified approach for electromagnetic interactions in graphitic nanostructures, which is able to account for their unique electronic and response properties and geometry configurations.

1. Introduction

Nanostructured graphitic derivatives have dominated many research fields with their potential for challenging fundamental discoveries and novel practical applications. Carbon nanotubes (CNTs) are quasi-one dimensional structures obtained by rolling atomically thin graphite sheets into a cylinder [1]. These can be single walled carbon nanotubes consisting of one graphitic sheet or multiwall carbon nanotubes consisting of two or more concentric sheets. The particular way of rolling is characterized by a chirality index (n,m), which determines the CNT characteristics. Also recently single layers of graphite – graphene – have been isolated using micromechanical cleavage [2]. At present, graphene is one of the most interesting materials, which may pave the way for future carbon based electronics [3].

A fundamental question in the understanding of the governing scientific laws of such nano-structured inert materials is how they interact with similar or different systems. This is important for the realization of new effects and devices, such as the proposed trapping of cold atoms [4] and their entanglement [5] near CNTs, exciton–plasmon coupling [6], surface profiling [7] and nanolithography applications [8]. The van der Waals/Casimir force is of particular interest here. It is a long ranged dispersive force, which couples neutral objects with or without permanent electric and/or magnetic moments via the vacuum fluctuations of the electromagnetic field. When the interacting objects are relatively close to each other, retardation effects coming from the finite speed of light are not important, and this is the regime of van der Waals interactions. The stability of graphitic materials and related devices has also been connected to dispersion interactions originating from Casimir/van der Waals forces [1–3].

Various approaches have been proposed to investigate how the electronic and dielectric properties of the interacting objects, together with their geometry, affect the Casimir force. For macroscopic objects with planar geometry, the discussions have been limited to applications of the Lifshitz theory [9]. For objects with curved surfaces and relatively close separations, the Proximity Force Approximation (PFA) has been adapted, which approximates the interaction through a series of parallel plates, resulting in a summation of energies using the Lifshitz formula [10]. This is essentially an additive approach applicable to objects at small distances with relatively large curvature.

Here we present a quantum electrodynamical (QED) approach suitable for dispersive and absorbing media [11]. This method allows taking into account the particular geometry of the interacting objects by solving the Fourier-domain operator Maxwell equations with appropriate boundary conditions together with the response properties of the interacting objects. In this paper, we show how this approach can be applied for calculating the Casimir interactions involving CNTs or graphene sheets. The generality of the method enables one to investigate the role of the geometry and response properties of the particular graphitic nanostructures.

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2. Model systems and formalism

2.1. Model systems

The double wall CNT is modeled by two infinitely long, infinitely thin, continuous concentric cylinders with radii \( R_{1,2} \) immersed in the vacuum (see Fig. 1(a)). The infinitely thin shells model has proven to be a suitable description for interactions between CNTs since the electromagnetic interaction wavelength is much greater than the transverse size of the system. This model was successfully employed to explain experimental data involving long range interactions between CNT and graphene layers [12–14]. Each cylinder is further characterized by the complex dynamic axial dielectric function \( \varepsilon_{\text{dyn}}(R_{1,2}, \omega) \) with the z-direction along the CNT axis. The transverse components of the dielectric function are strongly suppressed [15–19], as compared to the longitudinal component, due to the strong transverse depolarization effect in CNT. \textit{Ab initio} calculations [16] show that the transverse dielectric function is about 5 times smaller than the longitudinal dielectric function. When local field effects are also included, the suppression is even stronger (10–100 times) [17,18]. Experimental works also report that CNTs are almost completely transparent for the EM radiation polarized perpendicular to the nanotube axis [19]. Therefore, the transverse components of the dielectric function are neglected here.

The graphic layers are taken to be infinitely thin and parallel located in the x-y plane – Fig. 1(b). Each graphene is characterized by a two-dimensional conductivity tensor \( \sigma \) with components \( \sigma_{xx}, \sigma_{yy} \).

\[ \sigma_{xx} = \frac{1}{2} \left( \frac{1}{\varepsilon_{\text{die}}(0)} \right) \]

\[ \sigma_{yy} = \frac{1}{2} \left( \frac{1}{\varepsilon_{\text{die}}(0)} \right) \]

2.2. Quantization scheme

The QED approach used to calculate the interaction between dispersive and absorbing objects involves quantum mechanical quantization of the EM field. This procedure yields the second-quantized Hamiltonian [11]

\[ \hat{H} = \sum_{\ell=1,2} \int_{0}^{\infty} d\omega \left[ \hat{E}(R_{\ell}, \omega) \hat{E}^\dagger(R_{\ell}, \omega) - \frac{1}{2} \hat{E}^2(R_{\ell}, \omega) \right] \]

of the vacuum-type medium assisted EM field, with the bosonic operators \( \hat{E}^\dagger(x) \) creating surface EM excitations of frequency \( \omega \) at points \( R_{1,2} \), where the two objects are located. The operators satisfy the standard bosonic commutation relations

\[ \left[ \hat{E}(r, \omega), \hat{E}^\dagger(r', \omega') \right] = \delta_{\omega, \omega'} \delta_{r, r'} \]

\[ \left[ \hat{E}(r, \omega), \hat{E}(r', \omega') \right] = 0 = \left[ \hat{E}^\dagger(r, \omega), \hat{E}^\dagger(r', \omega') \right]. \]

The Fourier images of the electric and magnetic fields are considered as quantum mechanical observables of the corresponding electric and magnetic field operators. The latter ones satisfy the Fourier-domain operator form of Maxwell equations with the additional external source operators \( \hat{\rho} \) and \( \hat{J} \), which are associated with the presence of a pair of interacting objects(CNTs or graphene sheets in our case)

\[ \nabla \cdot \hat{B}(r, \omega) = 0 \]

\[ \nabla \cdot (\hat{\rho}(r, \omega) \hat{E}(r, \omega)) = \hat{\rho}(r, \omega) \]

\[ \nabla \times \hat{E}(r, \omega) = i \omega \hat{B}(r, \omega) \]

\[ \nabla \times \hat{B}(r, \omega) = -i \omega \mu_0 \hat{\rho}(r, \omega) \hat{E}(r, \omega) + \mu_0 \hat{J}(r, \omega) \]

The sources, called the charge and current noise densities, account for the medium-induced absorption. They are chosen in such a way as to ensure the correct QED equal-time commutation relations for the electric and magnetic field operators [11]. The noise current \( \hat{J} \) is related to the bosonic field \( f \) as [20,21]

\[ \hat{J}(R_{1}, \omega) = \frac{\omega}{\mu_0 c^2} \sqrt{\frac{\hbar}{2\pi\varepsilon_0}} \text{Im}[\hat{E}(R_{1}, \omega)]f(R_{1}, \omega) \]

where \( c, \mu_0 \) and \( \varepsilon \) are the vacuum dielectric constant, magnetic permeability and the speed of light, respectively, while \( i = 1, 2 \). For the CNT, the unit vector is along the tube’s axis, \( e = e_x \), reflects the cylindrical geometry of the system, and \( \varepsilon \rightarrow i\omega \). For graphene, the noise current is two-dimensional since the unit vector is \( e = x \) and \( R_{1} = (x_1, y_1, z_1) \) corresponds to its planar geometry. Also, \( \varepsilon \rightarrow \varepsilon_{2D} \), with \( \varepsilon_{2D} \) being the approximately isotropic two dimensional dielectric response of graphene.

2.3. Dyadic Green function technique

The QED approach further requires that we express the Fourier-domain electric field operator at an arbitrary point \( r \) of space as

\[ \hat{E}(r, \omega) = i\omega \mu_0 \sum_{i=1,2} \int dR_i \hat{G}(r, R_i, \omega) \cdot \hat{J}(R_i, \omega) \]

where \( \hat{G}(r, R_i, \omega) \) is the dyadic EM field Green’s function (GF), satisfying the wave equation

\[ \nabla \times \nabla \times \hat{G}(r, r', \omega) - \frac{\omega^2}{c^2} \hat{G}(r, r', \omega) = \delta(r-r') I \]

with \( I \) being the unit tensor. The boundary conditions for the EM field components at the CNT surfaces are further imposed required by standard electrodynamics.

\[ e_r \times \left[ \hat{E}(r, \omega)|_{R_1,2} - \hat{E}(r, \omega)|_{|_{R_1,2}} \right] = 0 \]

\[ e_r \times \left[ \hat{B}(r, \omega)|_{R_1,2} - \hat{B}(r, \omega)|_{R_1,2} \right] = \mu_0 \hat{J}(r, \omega)|_{R_1,2} \]

\[ e_r \times \left[ \hat{G}(r, r', \omega)|_{R_1,2} - \hat{G}(r, r', \omega)|_{R_1,2} \right] = 0 \]

\[ e_r \times \nabla \times \left[ \hat{G}(r, r', \omega)|_{R_1,2} - \hat{G}(r, r', \omega)|_{R_1,2} \right] = i\omega \mu_0 |_{|_{12}} \hat{G}(r, r', \omega)|_{R_1,2} \]

The boundary conditions for the two graphene sheets are found by considering the planar geometry of the sheets where upon the unit vector \( e_z \) is substituted by \( z \) in Eqs. (10)–(11). In both cases, the discontinuity in Eq. (13) fully accounts for the finite absorption and dispersion via the conductivity tensor \( \sigma^{(12)} \) of the two objects under consideration.

The method of scattering superposition is further used [22,23] and the dyadic GF is decomposed as \( \hat{G}^{(0)} = \hat{G}^{(0)} \hat{G}^{(12)} \hat{G}^{(12)} \), where \( \hat{G}^{(0)} \) and \( \hat{G}^{(12)} \) represent the contributions of the direct and scat-
tered waves, respectively, with a point-like field source located in region \((s)\) and the field registered in region \((f)\) (see Fig. 1).

For the concentric CNTs, the free and scattering dyadic GFs, \(G^{(0)}\) and \(G^{(p)}_{\text{rad}}\), are expanded into a series of even and odd vector cylindrical functions with unknown coefficients \([22,23]\). This splits the EM modes in the system into TE and TM polarizations, with Eqs. (12) and (13) yielding a set of 32 equations (16 for each polarization) with 32 unknown coefficients. Details for determining the dyadic CNT Green’s tensor are given in the Appendix. For parallel graphene sheets, due to the planar geometry, the dyadic GF can be expanded in terms of orthogonal functions \(\hat{M}(k) = \nabla \times [\mathbf{z}^k] \times [\mathbf{M}(k)]\). The exact expressions for the graphene/graohene Green’s function can be found in Ref. \([24]\), thus we do not provide further details here.

2.4. Maxwell stress tensor

The electromagnetic stress tensor is constructed next using the vacuum expectation values of the fields \([11,25]\):

\[
T_{i j}(r, \mathbf{r}^\prime) = T_i(r, \mathbf{r}^\prime) + T_j(r, \mathbf{r}^\prime) - \frac{1}{2} \nabla \nabla \cdot T_{i j}(r, \mathbf{r}^\prime) + T_{i j}(r, \mathbf{r}^\prime) \tag{14}
\]

where

\[
T_i(r, \mathbf{r}^\prime) = \varepsilon_0 \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \mathbf{E}(r, \omega) \otimes \mathbf{E}(r', \omega') \, d\omega d\omega' \tag{15}
\]

\[
T_{i j}(r, \mathbf{r}^\prime) = \frac{1}{\mu_0} \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \mathbf{B}(r, \omega) \otimes \mathbf{B}(r', \omega') \, d\omega d\omega' \tag{16}
\]

Using the expressions for the electric and magnetic fields and the useful property of the dyadic GF,

\[
\omega^2 \sum_k \int \frac{d\omega}{2\pi} \mathbf{E}(s, \omega) \mathbf{G}(r, \mathbf{r}, \omega) \mathbf{G}^*(\mathbf{r}', s, \omega) = \text{Im} \mathbf{G}(r, \mathbf{r}', \omega). \tag{17}
\]

The Maxwell stress tensor components are further expressed in terms of the dyadic GF as

\[
T_i(r, \mathbf{r}^\prime) = \frac{h}{\pi} \int_{\omega} \frac{d\omega}{2\pi} \text{Im} \mathbf{G}(r, \mathbf{r}, \omega) \tag{18}
\]

\[
T_{i j}(r, \mathbf{r}^\prime) = -\frac{1}{\pi} \int_{\omega} \frac{d\omega}{2\pi} \text{Im} \nabla \times \mathbf{G}(r, \mathbf{r}, \omega) \times \nabla' \tag{19}
\]

where \(\nabla\) introduces differentiation to the left.

For CNTs, we are interested in the radial component \(T_i\), which describes the radiation pressure of the virtual EM field on each nanotube surface. The net Casimir force per unit area exerted on one CNT is then calculated by subtracting the radiation pressures from both sides of the CNT surface \([25,26]\), in the limit \(r \to r^\prime\)

\[
p_i = \lim_{r^\prime \to r} \left[ \text{Im} \left( T^{(0)}_{i}(r, \mathbf{r}^\prime) - T^{(p)}_{i}(r, \mathbf{r}^\prime) \right) \right], \quad i = 1, 2 \tag{20}
\]

It is found that the pressure \(p_{12}\) from Eq. (20) are of equal magnitude and opposite direction indicating attraction between the cylindrical surfaces.

\[
|p_{12}| = \frac{h^2}{2\pi^2} \int_0^\infty d\omega \left[ \sum_{n} \left( 2 - \delta_{n0} \right) \left( \frac{n^2}{R_1^2} + \frac{n^2}{R_2^2} \right) \lambda_{n}(\mathbf{r}^\prime) \lambda_{n}(\mathbf{r}) \right] \tag{21}
\]

where \(I_n(x)\) and \(J_n(x)\) are the modified Bessel functions of the first and second kind, respectively, and their derivatives \(I_n'(x) = dh_n(x)/dx\) and \(J_n'(x) = dK_n(x)/dx\). Also, \(x^2 = k^2 + k^2, k = \omega/c, \) and \(k\) is the one dimensional wave vector along the nanotube axis. Note that the substitution \(\omega \to \hbar \omega\) has been executed in Eq. (21). The coefficients are given in the Appendix. We see that the Casimir force obtained by using the above approach accounts simultaneously for both the geometrical curvature effects (through the GF tensor) and the finite absorption and dissipation of each CNT (through their dielectric response).

For the graphene sheets, Eq. (21) is modified by substituting \(r, r^\prime\) with \(z, z^\prime\) directions. The electromagnetic pressure or Casimir force per unit area is also attractive,

\[
|p_{12}| = \frac{h^2}{2\pi^2} \int_{\infty}^0 d\omega \left| \frac{R_1^2}{\epsilon_{2h\omega}} - \frac{R_2^2}{\epsilon_{2h\omega}} \right|^2 \tag{22}
\]

where \(R_h = -\mu_0 \omega c / (2h + \mu_0 \omega c)\) and \(R_h = \mu_0 \sigma c^2 h_c / (2\mu_0 + \mu_0 \sigma + h_c)^2\) \([24]\) are the generalized reflection coefficients for the two suspended graphene sheets corresponding to the boundary conditions due to the transversal electric (E) and magnetic(B) modes. Here \(h_c^2(\omega) = k_c^2 + \omega^2 / c^2, \) with \(k_c\) being the two-dimensional wave vector and \(\sigma\) is the two-dimensional conductivity \([24]\). One notes that the finite temperature Casimir force may be found by making the following substitution \([27]\), \(\int d\omega \sim 2\pi \int d\beta / \beta^2 \) and \(\omega \to \omega_f = 2\pi \beta \hbar c / \beta^2\), where the prime means that the \(\beta = 0\) term is taken as one half the value, \(k_B\) is Boltzmann’s constant, \(T\) is the temperature and \(\hbar\) is Planck’s constant.

2.5. Response properties

The calculation of the pressure on the graphitic surfaces requires full knowledge of the frequency dependence of their dielectric response. For the CNTs, we use the nearest neighbor tight binding model for the carbon \(\pi\)-bands and the random phase approximation (RPA) to determine the chirality dependent dielectric response, with the electronic dissipation processes taken into account in the relaxation time approximation \([15]\). The energy dispersions of an \((n,m)\) CNT are obtained: \([1,15]\)

\[
E_n(l, k) = \pm \epsilon_0 \sqrt{1 + 4 \cos \left( \frac{2\pi N}{n} - \frac{n + 2m}{2n} \right) \cos \left( \frac{kL}{2} \right) } + 4 \cos^2 \left( \frac{kL}{2} \right) \tag{23}
\]

where \(\epsilon_0\) is the hopping energy, \(l = 0.213 \text{ nm}\) is 3/2 times the interatomic distance, \(N = 0, 1, \ldots, n-1\), and \(-\pi/l \leq k \leq \pi/l\). The minus and plus subscripts stand for the valence and conduction band respectively. The main contribution to the conductivity is given by the parallel dielectric function \([15]\), which is decomposed into a Drude part and a part originating from (transversely quantized) interband electronic transitions, \(\epsilon_{\text{opt}} = \epsilon_{\text{opt}} + \epsilon_{\text{opt}}^{\text{opt/Dr}}\).

Using the RPA, the interband transition term is found as

\[
\epsilon_{\text{opt}}(\omega) = 1 + \left( \frac{\omega_p^2}{\hbar^2} \right)^2 \frac{4\pi}{\omega_p^2} \sum_{n \neq m} \int_0^\infty \frac{d\omega}{2\pi} \frac{f(E_n(N, p)) - f(E_{N,m}(p))}{E_n(N, p) - E_{N,m}(p)} \tag{24}
\]

where \(\tau\) is a phenomenological relaxation time, \(f(E)\) is the Fermi distribution function, and \(\rho_s\) is the cubic density of carbon nanotubes. The quantity \(K_{\text{opt}}(N, p)\) corresponds to the matrix element of the momentum operator, and it is given in Ref. \([15]\) together with the hopping parameter \(\epsilon_0\) and the relaxation time \(\tau\). The Drude term is:
\[ I^P(\omega) = -\frac{(\hbar \omega_p)^2}{\hbar \omega_0 + i\hbar/\tau} \]  

where \( \omega_p \) is the plasma frequency.

\[ \sigma(\omega) = -\frac{i e^2}{\pi h^2 (\omega + i\Gamma)} \int_0^\infty dE \left( \frac{\partial f(E) - \partial f(-E)}{\partial E} \right) \]

\[ + \frac{i e^2 (\omega + i\Gamma)}{\pi h^2} \int_0^\infty dE \frac{f(E) - f(-E)}{(\omega + i\Gamma)^2 - 4E^2/h^2}, \]

where the first term corresponds to intra-band transitions, while the second one corresponds to inter-band transitions.

The result correctly reproduces the power law dependence of the pressure to the plates separation distance.

Next, the attractive force per unit area on the CNTs surfaces is numerically evaluated as a function of the inter-tube surface-to-surface distance for various pairs of CNTs. We have chosen to keep the inner CNT with the achiral (12,12) metallic nanotube, while changing the outer tube chirality. The results are shown in Fig. 2(a).

The total radiation pressure is \( |p| = \frac{\hbar c}{4\pi^2} \sum_{n=1}^\infty n^4 \int_0^\infty d\eta \frac{\eta}{\eta^2 - \frac{e^{-\eta d}}{e^{-\eta d}}} \approx \frac{\hbar c}{4\pi^2} (2d)^4 \), which is about 1/3 of the Casimir formula for parallel perfect metal plates \( |p| = \frac{\hbar c}{4\pi^2} \), which is monotonic for small separation distances.

The difference is attributed to utilizing the axial model (not the full dielectric function) for the nanotube dielectric response. The result correctly reproduces the power law dependence of the pressure on the plates separation distance \( d \).

Next, the attractive force per unit area on the CNTs surfaces is numerically evaluated as a function of the inter-tube surface-to-surface distance. For zigzag \((m,0)\) and armchair \((n,n)\) outer tubes this dependence is monotonic, while for chiral tubes the pressure decreases as a function of \( d \) in a rather irregular fashion. As the outer CNT is changed, one can imagine double wall CNTs consisting of metal/metal or metal/semiconductor combinations of different chiralities but of similar radial dimensions. One notes that the attraction is stronger if the outer CNT is an armchair \((n,n)\) one as compared to the attraction for the outer \((m,0)\) CNTs. At small separation distances the difference can be quite significant. For example, the attraction between \((27,4)@(12,12)\) and \((21,13)@(12,12)\) differ by \( \sim 20\% \) in favor of the second pair, even though the radial difference is only 0.2 Å. These differences become smaller as the inter-tube surface to surface separation becomes larger, and eventually become negligible as the Casimir force diminishes at large distances.

The pressure on the CNTs surfaces is also calculated, using the Drude contribution only, in each CNT dielectric response (insert...
in Fig. 2(a)). The attraction is stronger when the interband transitions are neglected, and the decrease of $p$ as a function of $d$ is monotonic. As the full dielectric response is considered, the pressure is affected differently due to the chirality dependent interband electronic transitions of each individual CNT. These differences become less significant at large surface to surface separations, and we find that for $d \sim 15$ Å, this difference is less than 10%.

To further investigate the role of the CNTs geometry and dielectric response on their mutual interaction, we consider different pairs of tubes with the same chiralities and different radial sizes, or tubes with similar radial dimensions and different chiralities. For CNTs with the same chiralities and different radial sizes, the increase in the surface to surface separation results in a monotonic decrease in their mutual interaction strength, as shown in Fig. 2(a). To study the case of CNT pairs with similar radial dimensions and different chiralities, we consider the additional semi-metallic (21,0) and semiconducting (20,0) inner tubes with various achiral outer tubes. They are of comparable radii, 8.22 Å and 7.83 Å, respectively, and similar to the (12,12) CNT radius which is 8.14 Å. The calculated pressure vs. the inter-tube separation distance is shown in Fig. 2(b). Depending on the outer CNTs type, it is found that the interaction is weaker when there are two zigzag concentric CNTs. The fact that some of these are semi-metallic and others are semiconducting does not seem to influence the magnitude and monotonic decrease of their mutual interaction with the separation distance. By comparing Fig. 2(a) and (b) one notices that the curves for $(m,0)@(12,12)$, $(n,n)@(21,0)$, and $(n,n)@(20,0)$ are practically overlapping, meaning that the specific location of the zigzag and armchair tubes (inner or outer) is of no significance to the interaction. The small deviations can be attributed to the small differences in the inner CNT radii. However, it is found that the strongest interaction occurs between two armchair CNTs. We have performed the same calculations for many different achiral tubes, and found that these features are not unique just for the considered CNTs. The strongest interaction always occurs between two armchair CNTs, provided that their radial dimensions are similar.

These results are indicative that the CNTs collective excitation properties have a strong effect on their mutual interaction, particularly for relatively small separation distances of interest here. The dominant contribution of plasmonic modes to the Casimir interactions has also been realized for planar [33,34] and linear [35] metallic systems. To further investigate the features originating from the CNTs collective excitation properties, we calculate the electron energy loss spectroscopy (EELS) spectra, given by $-\text{Im}[1/\varepsilon(i\omega)]$, using the formalism described in Section 2.5. The results for the representative CNT types are given in Fig. 3. Comparison of these spectra for various inner and outer CNTs combinations shows that the low frequency plasmon excitations, given by peaks in $-\text{Im}[1/\varepsilon(i\omega)]$, are key to the strength of their mutual interaction. It is found that, in general, armchair tubes always have strong, well pronounced interband plasmon excitations in the low frequency range (see Fig. 3(a) and (c)). Zigzag and most chiral CNTs have low frequency interband plasmons, too, but they are not as well pronounced as those in armchair tubes (Fig. 3(b) and (c)); their stronger plasmon modes are found at higher frequencies. For example, for the cases shown in Fig. 3, one finds well pronounced plasmon transitions in the (12,12) CNT at $\omega_1 = 2.18$ eV and $\omega_2 = 3.27$ eV, and at $\omega_1 = 1.63$ eV and $\omega_2 = 2.45$ eV in the (17,17) CNT. At the same time, no such well defined strong low frequency excitations in the (21,0) and (30,0) CNTs are found. Fig. 2(a) and (b) show that the attraction in (17,17)@(12,12) is much stronger than the attraction in (30,0)@(21,0), even though the radial sizes of the involved CNTs are approximately the same. One also notes that for the case of (17,17)@(21,0) there is only one such low frequency excitation coming from the armchair tube, and consequently the Casimir force has an intermediate value as compared to the above discussed two cases.

These results suggest that the strongest interaction occurs between CNTs with well pronounced overlapping low frequency plasmon excitations. This is also consistent with the conclusion of Ref. [35] for generic one-dimensional plasmonic structures. However, in our case we deal with the interband plasmons originating from the space quantization of the transverse electronic motion, and, therefore, having quite a different frequency-momentum dispersion law (constant) as compared to that normally assumed (linear) for plasmons [36]. Further, the interaction is weaker when only one of the CNTs supports strong low frequency interband plasmon modes. Finally, the weakest interaction happens when neither CNT has strong low frequency plasmons.

We also consider the graphene/graphene interaction. It turns out that the calculation of the Casimir force per unit area can be carried out analytically if one takes the universal conductivity value $\sigma_0$ [24]

$$|p| = \frac{3e^2}{32\pi nd^4}$$

(31)

Comparing this result to the force per unit area of two perfect conducting plates $p_0 = \pi^2 \hbar c/(240d^4)$ shows that the distance dependence is the same, but the magnitude is reduced by an order of the fine structure constant $\alpha = 1/137$. Recent studies have shown that at $T = 0$ K spatial dispersion may affect the graphene/graphene interaction to some extent [37]. Inclusion of spatial dispersion requires using the full conductivity Kubo expression $-\pi(k_z, \omega)$. Interestingly, the distance dependence is the same as in the case of without dispersion, $p \sim 1/d^4$, but the magnitude is reduced by about 20% [24,37].

4. Conclusions

We have presented a general QED approach to investigate Casimir interactions in graphitic nanostructures. The method is particularly attractive since it enables one to take into account the geometry of the system (via the dyadic Green’s function) and the finite response properties (via the conductivity or dielectric function) of each object.

It is found that unique energy dispersion and response properties of each graphitic nanostructure influence the Casimir force in a profound way. For CNTs, the attraction is dominated by the low energy (inter-band) plasmon excitations of both tubes. The key features are the existence of low frequency plasmons, their strong and well pronounced nature, and the overlap between the low frequency plasmon peaks belonging to the two CNTs. Thus, the
chiralities of concentric nanotubes, which are determined by their energy dispersion, play an important role in the nanotube/nanotube force responsible for the stability of CNT pairs in a double wall nanotube configuration. The graphene/graphene interaction is also significantly affected by the dielectric and electronic properties. Taking the universal conductivity values results in a reduced by an order of magnitude of the fine structure constant as compared to the Casimir attraction between two perfect metals with the same distance dependence. Inclusion of spatial dispersion further reduces the force.

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Appendix A. Dyadic Green function of the double-wall carbon nanotube

Using the method of scattering superposition [22,23], the dyadic Green function is decomposed as $G^{(2)} = G^{(0)} G^{(d)} + G^{(0)} G^{(s)\text{strat}}$, where $f_s = 1, 2, 3, 4$ (see Fig. 1). The unbounded part $G^{(0)}$ represents the contribution of the direct waves from sources in an unbounded medium, and the scattering part $G^{(d)}$ describes additional contribution of the multiple reflection and transmission waves from the CNT surfaces. The indices ($f$) and ($s$) stand for point-like field sources located in region ($f$) and fields located in region ($f$), according to Fig. 1.

In order to satisfy the homogeneous Helmholtz equation (Eq. (9)) and the radiation condition at infinity, the two contributions are taken to be in the following forms:

$$G^{(0)}(\mathbf{r}, \mathbf{r}', \omega) = \frac{e_0 \epsilon_0 (\mathbf{r} - \mathbf{r}')}{k^2} - \frac{i}{8\pi} \int_{\infty}^{\infty} dk \sum_{n=0}^{\infty} \frac{2 - \delta_n^0}{2} \left\{ M^{(1)}_{\text{un}}(k) M^{(1)}_{\text{un}}(-k) + N^{(1)}_{\text{un}}(k) N^{(1)}_{\text{un}}(-k) \right\}, r > r'$$

$$G^{(d)}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{2\pi} \int_{\infty}^{\infty} dk \sum_{n=0}^{\infty} \frac{2 - \delta_n^0}{2} \left\{ \varepsilon_0 J_n(k) \frac{\varepsilon_{\text{un}}}{\varepsilon_{\text{un}} + n^2} \right\}, r < r'$$

(A1)

$$\gamma_{1,2} = \frac{\alpha \mu_0 V_{22}^{(1,2)}}{\pi \varepsilon_{\text{un}} R_1}$$

(A6)

The rest of the coefficients can be obtained by applying the boundary conditions in Eqs. (12) and (13) to the GF expansion Eq. (A2).

References