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Impact of Mass-Gap on the Dispersion Interaction of Nanoparticles with Graphene Out of Thermal Equilibrium

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Abstract: We consider the nonequilibrium dispersion force acting on nanoparticles on the source side of a gapped graphene sheet. Nanoparticles are kept at the environmental temperature, whereas the graphene sheet may be either cooler or hotter than the environment. Calculation of the dispersion force as a function of separation at different values of the mass-gap parameter is performed using the generalization of the fundamental Lifshitz theory to out-of-thermal-equilibrium conditions. The response of the gapped graphene to quantum and thermal fluctuations in the electromagnetic field is described by the polarization tensor in $(2 + 1)$ -dimensional space–time in the framework of the Dirac model. The explicit expressions for the components of this tensor in the area of evanescent waves are presented. The nontrivial impact of the mass-gap parameter of graphene on the nonequilibrium dispersion force, as compared to the equilibrium one, is determined. It is shown that, unlike the case of pristine graphene, the nonequilibrium force preserves an attractive character. The possibilities of using the obtained results in the design of micro- and nanodevices, incorporating nanoparticles and graphene sheets for their functionality, is discussed.

Keywords: dispersion force; thermal nonequilibrium; nanoparticles; Lifshitz theory; graphene; polarization tensor; nanodevices



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1. Introduction

Investigations of interactions between nanoparticles and material surfaces of different nature are of profound importance for physics and its applications in nanotechnology, including bioelectronics (see, e.g., the following articles and reviews [1–17]). The microparticle–surface interaction includes several contributions, among which are mechanical contact forces, Born repulsion, and attractive dispersion forces [18,19]. At separations between a nanoparticle and a surface exceeding several nanometers, the dispersion forces, which are also called the van der Waals or Casimir–Polder forces, become dominant. These are determined by the quantum and thermal fluctuations in the electromagnetic field.

An entirely new material that finds increasing use in nanotechnology, is graphene, i.e., the plane sheet of carbon atoms arranged in a hexagonal lattice [20–22]. The dispersion (Casimir–Polder) interaction of graphene with different atomic systems [23–36] and nanoparticles [37–42] has been the subject of much investigation. The obtained results are finding ever-widening applications in bioelectronics [43–46].

The implementation of interactions between nanoparticles and graphene to new generation of nanodevices calls for the development of theoretical methods, which will make it possible to calculate the dispersion force as a function of all relevant parameters. These methods were developed in the framework of the Lifshitz theory [47–49] by expressing the dispersion force between an atom or a nanoparticle and a graphene sheet via the atomic (nanoparticle) electric polarizability and the polarization tensor of graphene [23–36]. In so

doing, the polarization tensor of graphene was found [50–53] on the basis of the first principles of thermal quantum field theory in the framework of the Dirac model [20–22].

The Lifshitz theory of dispersion forces is formulated for the case when the interacting bodies are in the state of thermal equilibrium with the environment. This condition, however, is violated when both of the interacting bodies (or at least one of them) are kept at temperatures different from that of the environment. The formalism generalizing the Lifshitz theory for systems out of thermal equilibrium was developed in [54–59]. In recent years, different aspects of the nonequilibrium dispersion forces acting between two material plates, a small sphere or an atom and a material plate, and between two spheres were investigated using this formalism [60–66]. Specifically, the temperature-dependent response functions of the interacting bodies was considered in [63,64].

The nonequilibrium dispersion force acting on spherical nanoparticles on the source side of an ideal (pristine) freestanding-in-vacuum graphene sheet was investigated quite recently [67]. The pristine character of graphene assumed in [67] means that its crystal lattice does not include any foreign atoms and the quasiparticles are massless, as was supposed in the original Dirac model [20–22]. Reference [67] suggested that the temperature of nanoparticles is the same as that of the environment, whereas the graphene sheet can be either cooler or hotter than the environment. It was shown that the impact of the nonequilibrium effects of the dispersion force decreases with increasing graphene–nanoparticle separation distance. Furthermore, according to the obtained results, at relatively short separations the effects of nonequilibrium may change the sign of the dispersion force by making it repulsive [67].

In this article, we applied the theory of nonequilibrium dispersion interaction to investigate the force acting on nanoparticles kept at the environmental temperature on the source side of the gapped graphene described by the Dirac model with light but massive quasiparticles. The temperature of a graphene sheet is assumed to be either lower or higher than that of the environment. To perform dispersion force computations, we present the explicit expressions for the polarization tensor of gapped graphene along the real frequency axis in the region of evanescent waves, which have not been considered in the literature with sufficient detail to date. We demonstrate that the value of the mass-gap parameter has a nontrivial impact on the nonequilibrium force, as compared to the equilibrium force, depending on the values of separation and graphene temperature. Unlike the case of pristine graphene, for a nonzero mass of quasiparticles, the nonequilibrium dispersion force preserves its attractive character.

The structure of the article is as follows. In Section 2, we present the expression of a nonequilibrium dispersion force acting on nanoparticles on the source side of the gapped graphene sheet in terms of the polarization tensor. In Section 3, the components of this tensor in the area of the evanescent waves are specified. Section 4 contains the computational results for the dispersion force acting on nanoparticles, which is shown as the function of separation for different values of the mass-gap parameter and at different temperatures. In Sections 5 and 6, the reader will find the discussion of the obtained results and our conclusions.

2. Nonequilibrium Dispersion Force on a Nanoparticle on the Source Side of Gapped Graphene

We consider the dispersion (Casimir–Polder) force acting on a spherical nanoparticle of radius R spaced above a graphene sheet at a separation $a \gg R$. The consideration of nanoparticles of other types (for instance, having a nonspherical shape) would need a more complicated theory using the scattering-matrix approach [58]. The area of graphene sheet is taken to be much larger than the separation to a nanoparticle squared. It is assumed that, at all temperatures T under consideration, it holds that $R \ll \hbar c / (k_B T)$, where k_B is the Boltzmann constant (for instance, at the environmental temperature $T_E = 300$ K, one has $\hbar c / (k_B T) \approx 7.6 \mu\text{m}$). Under this condition, within the range of separations a considered

below, the nanoparticle can be described by the static polarizability $\alpha(0)$, which takes the form [61]

$$\alpha(0) = R^3 \frac{\varepsilon(0) - 1}{\varepsilon(0) + 2}, \quad \alpha(0) = R^3 \tag{1}$$

for dielectric and metallic nanoparticles, respectively, where $\varepsilon(0)$ is the static dielectric permittivity of a nanoparticle material.

Below, we assume that nanoparticles have the same temperature T_E as the environment, whereas the graphene sheet has the temperature T_g , which is either lower or higher than T_E . As distinct from [67], where the case of a pristine graphene was considered, here the graphene sheet is characterized by a nonzero mass-gap parameter $\Delta = 2mv_F^2$, where m is the mass of quasiparticles and $v_F \approx c/300$ is the Fermi velocity [21,68,69].

The nonequilibrium dispersion force acting on a nanoparticle is represented in the form [56,58]

$$F_{\text{neq}}(a, \Delta, T_E, T_g) = F_M(a, \Delta, T_E, T_g) + F_r(a, \Delta, T_E, T_g), \tag{2}$$

where $F_M(a, \Delta, T_E, T_g)$ can be expressed as a sum over the discrete Matsubara frequencies, much as the equilibrium Casimir–Polder force [70,71], whereas $F_r(a, \Delta, T_E, T_g)$ is the contribution, which is given by an integral over the real frequency axis.

In fact, the effects of nonequilibrium contribute to both terms on the right-hand side of (2). Because of this, it is not reasonable to call the first of them “equilibrium” and the second—“nonequilibrium”, as occurs in the literature. Moreover, the division of F_{neq} into F_M and F_r is not unique and can be made in a number of ways. Below, we use the same division as in [67].

In this case, the first term in (2) is given by [67]

$$F_M(a, \Delta, T_E, T_g) = -\frac{2k_B T_E \alpha(0)}{c^2} \sum_{l=0}^{\infty} \int_0^{\infty} k dk e^{-2aq_l(k)} \left\{ \left[2q_l^2(k)c^2 - \zeta_{E,l}^2 \right] R_{\text{TM}}(i\zeta_{E,l}, k; \Delta, T_g) - \zeta_{E,l}^2 R_{\text{TE}}(i\zeta_{E,l}, k; \Delta, T_g) \right\}. \tag{3}$$

Here, k is the magnitude of the wave vector component along the graphene sheet, $q_l^2(k) = k^2 + \zeta_{E,l}^2/c^2$, $\zeta_{E,l} = 2\pi k_B T_E l/\hbar$ with $l = 0, 1, 2, \dots$ are the Matsubara frequencies at the environmental temperature T_E , and the prime on the summation sign multiplies the term with $l = 0$ by the factor $1/2$.

The quantities R_{TM} and R_{TE} are the reflection coefficients of the electromagnetic fluctuations on a graphene sheet for the transverse magnetic (TM) and transverse electric (TE) polarizations calculated at the pure imaginary Matsubara frequencies $\omega = i\zeta_{E,l}$, but at the temperature of graphene T_g . They are expressed via the components of the polarization tensor of graphene $\Pi_{ij}(\omega, k; \Delta, T_g)$ [51,52,72]

$$\begin{aligned} R_{\text{TM}}(\omega, k; \Delta, T_g) &= \frac{q(\omega, k)\Pi_{00}(\omega, k; \Delta, T_g)}{2\hbar k^2 + q(\omega, k)\Pi_{00}(\omega, k; \Delta, T_g)}, \\ R_{\text{TE}}(\omega, k; \Delta, T_g) &= -\frac{\Pi(\omega, k; \Delta, T_g)}{2\hbar k^2 q(\omega, k) + \Pi(\omega, k; \Delta, T_g)}, \end{aligned} \tag{4}$$

where $q^2(\omega, k) = k^2 - \omega^2/c^2$, and the quantity Π is defined as

$$\Pi(\omega, k; \Delta, T_g) = k^2 \Pi_i^i(\omega, k; \Delta, T_g) - q^2(\omega, k)\Pi_{00}(\omega, k; \Delta, T_g) \tag{5}$$

with the summation over the repeated index $i = 0, 1, 2$. The explicit expressions for the polarization tensor in the required frequency regions are given in Section 3.

Note that the polarization tensor Π_{ij} , describing the response of graphene to quantum and thermal fluctuations of the electromagnetic field, strongly depends on temperature T_g as a parameter. When applied to the nonequilibrium dispersion forces, a similar situation was previously considered for the phase-change [63] and metallic [64] materials.

The second term on the right-hand side of (2), according to the division accepted in [67], takes the form [58]

$$F_r(a, \Delta, T_E, T_g) = \frac{2\hbar\alpha(0)}{\pi c^2} \int_0^\infty d\omega \Theta(\omega, T_E, T_g) \int_{\omega/c}^\infty k dk e^{-2nq(\omega, k)} \text{Im} \left\{ \left[2q^2(\omega, k)c^2 + \omega^2 \right] R_{\text{TM}}(\omega, k; \Delta, T_g) + \omega^2 R_{\text{TE}}(\omega, k; \Delta, T_g) \right\}. \quad (6)$$

Here, the quantity $\Theta(\omega, T_E, T_g)$ is defined as

$$\Theta(\omega, T_E, T_g) = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_E}\right) - 1} - \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_g}\right) - 1}. \quad (7)$$

The important property of the division (2) accepted in [67] is that the quantity F_r , expressed in terms of real frequencies, is determined by the contribution of only the evanescent waves for which $k > \omega/c$. As a result, the exponent in (6) has the real power. This is advantageous as compared to the standard Lifshitz formula for equilibrium Casimir and Casimir–Polder forces written in terms of real frequencies, containing the contributions of both the evanescent and propagating ($k < \omega/c$) waves [71]. For the latter contribution, the quantity $q(\omega, k)$ is purely imaginary, resulting in the integral of the quickly oscillating function, which makes integration difficult.

3. Polarization Tensor in the Area of Evanescent Waves

The nonequilibrium dispersion force (2) acting on nanoparticles on the source of a gapped graphene sheet can be computed by Equations (3)–(7). For this purpose, one should know the component of the polarization tensor Π_{00} and the combination of its components Π defined in (5) for a graphene sheet with the nonzero mass-gap parameter Δ . As mentioned in Section 1, the polarization tensor of graphene was found in [50–53] in the framework of the Dirac model. In doing so, Ref. [50] was devoted to the case of zero-temperature, $T = 0$. In [51], the polarization tensor of graphene was obtained at nonzero temperatures at all discrete Matsubara frequencies. These results, however, did not admit a continuation to the entire plane of complex frequencies and, specifically, were inapplicable along the real frequency axis. Thus, they can be used for the calculation of the equilibrium Casimir and Casimir–Polder forces and the contribution F_M to the nonequilibrium force, but not the contribution F_r .

The polarization tensor of graphene with nonzero Δ valid over the entire plane of complex frequencies was derived in [52], where the most attention was paid to the region of propagating waves $k < \omega/c$ in connection with the topical applications to the reflectivity [73–76] and conductivity [77–80] properties of graphene. Below, we present a more detailed exposition of the results of [52], which are relevant to the area of evanescent waves ($k > \omega/c$) that determines the contribution (6) to the nonequilibrium dispersion force.

Before dealing with the polarization tensor, a few remarks concerning the area of application of this quantity for the calculation of dispersion forces are in order. In [50–53], the polarization tensor of graphene was derived in the framework of the Dirac model. This model provides a physically adequate description of graphene at energies below approximately 3 eV [81]. Thus, the energies $\hbar\omega$ providing the major contribution to the dispersion force should be below this limit. The characteristic frequency determining the dispersion force is $\omega_c = c/(2a)$ [70,71]. It can easily be seen that the respective characteristic energy $\hbar\omega_c$ is below 1 eV at all separations $a > 100$ nm. Therefore, at separations, say, $a > 200$ nm, one can safely use the Dirac model and its consequences in calculations of dispersion forces. This was confirmed by the fact that measurements of the dispersion interaction with graphene were found to be in very good agreement with theoretical predictions computed using the polarization tensor [82,83].

Now, we present explicit expressions for the quantities Π_{00} and Π in the frequency region of evanescent waves $\omega/c < k$. Similar to [30], we present these quantities as the sums of two contributions

$$\begin{aligned} \Pi_{00}(\omega, k; \Delta, T_g) &= \Pi_{00}^{(0)}(\omega, k; \Delta) + \Pi_{00}^{(1)}(\omega, k; \Delta, T_g), \\ \Pi(\omega, k; \Delta, T_g) &= \Pi^{(0)}(\omega, k; \Delta) + \Pi^{(1)}(\omega, k; \Delta, T_g). \end{aligned} \tag{8}$$

Here, the contributions with an upper index (0) are defined at zero-temperature, $T = 0$, whereas the quantities with an upper index (1) have the meaning of the thermal corrections. In doing so, both contributions depend on the mass-gap parameter of graphene Δ . With vanishing temperature, both $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ go to zero.

The analytic continuation of the polarization tensor of graphene to the frequency region of evanescent waves takes different forms in the interval

$$\frac{\omega}{c} < k \leq \frac{\omega}{v_F} \approx 300 \frac{\omega}{c} \tag{9}$$

and in the interval

$$300 \frac{\omega}{c} \approx \frac{\omega}{v_F} < k < \infty. \tag{10}$$

First, we consider the interval (9), which is often called the plasmonic region [84]. In this region, the first contributions to (8) take the form [52]

$$\begin{aligned} \Pi_{00}^{(0)}(\omega, k; \Delta) &= -\frac{2\alpha k^2}{cp^2(\omega, k)} \Phi(\omega, k, \Delta), \\ \Pi^{(0)}(\omega, k; \Delta) &= \frac{2\alpha k^2}{c} \Phi(\omega, k, \Delta), \end{aligned} \tag{11}$$

where

$$p^2(\omega, k) = \frac{\omega^2}{c^2} - \frac{v_F^2}{c^2} k^2 \geq 0 \tag{12}$$

and $\alpha = e^2/(\hbar c)$ is the fine structure constant. The function Φ is defined as

$$\Phi(\omega, k, \Delta) = \Delta - \hbar cp(\omega, k) \left[1 + \frac{\Delta^2}{\hbar^2 c^2 p^2(\omega, k)} \right] \left[\operatorname{arctanh} \frac{\Delta}{\hbar cp(\omega, k)} + i \frac{\pi}{2} \right] \tag{13}$$

for $\hbar cp(\omega, k) \geq \Delta$ and as

$$\Phi(\omega, k, \Delta) = \Delta - \hbar cp(\omega, k) \left[1 + \frac{\Delta^2}{\hbar^2 c^2 p^2(\omega, k)} \right] \operatorname{arctanh} \frac{\hbar cp(\omega, k)}{\Delta} \tag{14}$$

for $\hbar cp(\omega, k) < \Delta$.

The second contributions to (8) in the plasmonic region are more complicated. It is convenient to define their real and imaginary parts separately. We start from defining the real parts of $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ which, in turn, have different forms under the conditions $\hbar cp(\omega, k) \geq \Delta$ and $\hbar cp(\omega, k) < \Delta$.

Thus, if the condition $\hbar cp(\omega, k) \geq \Delta$ is satisfied, one obtains from [52] after identical transformations,

$$\operatorname{Re} \Pi_{00}^{(1)}(\omega, k; \Delta, T_g) = \frac{8\alpha \hbar c^2}{v_F^2} (I_1 + I_2 + I_3), \tag{15}$$

where the following notations are introduced:

$$\begin{aligned}
 I_1 &= \int_{\frac{\Delta}{2\hbar c}}^{u^{(-)}(\omega,k)} \frac{du}{e^{\beta(T_g)u} + 1} \left[2 - \frac{B_1(2cu + \omega) + B_1(2cu - \omega)}{cp(\omega, k)} \right], \\
 I_2 &= \int_{u^{(-)}(\omega,k)}^{u^{(+)}(\omega,k)} \frac{du}{e^{\beta(T_g)u} + 1} \left[2 - \frac{B_1(2cu + \omega)}{cp(\omega, k)} \right], \\
 I_3 &= \int_{u^{(+)}(\omega,k)}^{\infty} \frac{du}{e^{\beta(T_g)u} + 1} \left[2 - \frac{B_1(2cu + \omega) - B_1(2cu - \omega)}{cp(\omega, k)} \right].
 \end{aligned}
 \tag{16}$$

Here,

$$\begin{aligned}
 u^{(\pm)}(\omega, k) &= \frac{1}{2c} [\omega \pm v_F k \sqrt{A(\omega, k; \Delta)}], \quad A(\omega, k; \Delta) = 1 - \frac{\Delta^2}{\hbar^2 c^2 p^2(\omega, k)}, \\
 B_1(x) &= \frac{x^2 - v_F^2 k^2}{\sqrt{x^2 - v_F^2 k^2 A(\omega, k; \Delta)}}, \quad \beta(T_g) = \frac{\hbar c}{k_B T_g}.
 \end{aligned}
 \tag{17}$$

It can be seen that all the integrals I_j are the functions of ω, k, Δ , and T_g .

Under the same condition $\hbar c p(\omega, k) \geq \Delta$, we obtain from [52]

$$\text{Re } \Pi^{(1)}(\omega, k; \Delta, T_g) = \frac{8\alpha \hbar \omega^2}{v_F^2} (J_1 + J_2 + J_3),
 \tag{18}$$

where the quantities J_j are given by

$$\begin{aligned}
 J_1 &= \int_{\frac{\Delta}{2\hbar c}}^{u^{(-)}(\omega,k)} \frac{du}{e^{\beta(T_g)u} + 1} \left\{ 2 - \frac{cp(\omega, k)[B_2(2cu + \omega) + B_2(2cu - \omega)]}{\omega^2} \right\}, \\
 J_2 &= \int_{u^{(-)}(\omega,k)}^{u^{(+)}(\omega,k)} \frac{du}{e^{\beta(T_g)u} + 1} \left[2 - \frac{cp(\omega, k)B_2(2cu + \omega)}{\omega^2} \right], \\
 J_3 &= \int_{u^{(+)}(\omega,k)}^{\infty} \frac{du}{e^{\beta(T_g)u} + 1} \left\{ 2 - \frac{cp(\omega, k)[B_2(2cu + \omega) - B_2(2cu - \omega)]}{\omega^2} \right\}.
 \end{aligned}
 \tag{19}$$

Here, the function $B_2(x)$ is defined as

$$B_2(x) = \frac{x^2 - v_F^2 k^2 [1 - A(\omega, k; \Delta)]}{\sqrt{x^2 - v_F^2 k^2 A(\omega, k; \Delta)}}.
 \tag{20}$$

If the opposite condition, $\hbar c p(\omega, k) < \Delta$, is satisfied, the real parts of $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ take the following form [52]

$$\begin{aligned} \operatorname{Re} \Pi_{00}^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar c^2}{v_F^2} \int_{\frac{\Delta}{2\hbar c}}^{\infty} \frac{du}{e^{\beta(T_g)u} + 1} \left[2 - \frac{B_1(2cu + \omega) - B_1(2cu - \omega)}{cp(\omega, k)} \right], \\ \operatorname{Re} \Pi^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar\omega^2}{v_F^2} \int_{\frac{\Delta}{2\hbar c}}^{\infty} \frac{du}{e^{\beta(T_g)u} + 1} \left\{ 2 - \frac{cp(\omega, k)[B_2(2cu + \omega) - B_2(2cu - \omega)]}{\omega^2} \right\}. \end{aligned} \tag{21}$$

This concludes the consideration of the real parts of $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ in the plasmonic region (9). The imaginary parts of $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ are given by the unified expressions

$$\begin{aligned} \operatorname{Im} \Pi_{00}^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar c}{v_F^2 p(\omega, k)} \theta[\hbar cp(\omega, k) - \Delta] \int_{u^{(-)}(\omega, k)}^{u^{(+)}(\omega, k)} \frac{du}{e^{\beta(T_g)u} + 1} \frac{(2cu - \omega)^2 - v_F^2 k^2}{\sqrt{v_F^2 k^2 A(\omega, k; \Delta) - (2cu - \omega)^2}}, \\ \operatorname{Im} \Pi^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar cp(\omega, k)}{v_F^2} \theta[\hbar cp(\omega, k) - \Delta] \int_{u^{(-)}(\omega, k)}^{u^{(+)}(\omega, k)} \frac{du}{e^{\beta(T_g)u} + 1} \frac{(2cu - \omega)^2 + v_F^2 k^2 [1 - A(\omega, k; \Delta)]}{\sqrt{v_F^2 k^2 A(\omega, k; \Delta) - (2cu - \omega)^2}}, \end{aligned} \tag{22}$$

which are valid over the entire region (9). Here, $\theta(x)$ is the step function equal to 1 for $x \geq 0$ and to 0 for $x < 0$.

Next, we consider the polarization tensor in the interval (10). In this case, the first contributions to (8) are given by [52]

$$\begin{aligned} \Pi_{00}^{(0)}(\omega, k; \Delta) &= \frac{\alpha\hbar k^2}{\tilde{p}(\omega, k)} \Psi(\omega, k, \Delta), \\ \Pi^{(0)}(\omega, k; \Delta) &= \alpha\hbar k^2 \tilde{p}(\omega, k) \Psi(\omega, k, \Delta), \end{aligned} \tag{23}$$

where

$$\tilde{p}^2(\omega, k) = \frac{v_F^2}{c^2} k^2 - \frac{\omega^2}{c^2} \geq 0 \tag{24}$$

and Ψ is defined as

$$\Psi(\omega, k, \Delta) = 2 \left\{ \frac{\Delta}{\hbar c \tilde{p}(\omega, k)} + \left[1 - \frac{\Delta^2}{\hbar^2 c^2 \tilde{p}^2(\omega, k)} \right] \arctan \frac{\hbar c \tilde{p}(\omega, k)}{\Delta} \right\}. \tag{25}$$

Similar to the plasmonic interval (9), in the interval (10) the quantities $\Pi_{00}^{(1)}$ and $\Pi^{(1)}$ are the complex-valued functions. Here, we present their explicit expressions without separating the real and imaginary parts [52]

$$\begin{aligned} \Pi_{00}^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar c^2 \tilde{p}(\omega, k)}{v_F^2} \int_{\frac{\Delta}{\hbar c \tilde{p}(\omega, k)}}^{\infty} \frac{dv}{e^{D(\omega, k, T_g)v} + 1} \left[1 - \frac{1}{2} \sum_{\lambda=\pm 1} \frac{1 - v^2 - 2\lambda \frac{\omega}{c \tilde{p}(\omega, k)} v}{\sqrt{1 - v^2 - 2\lambda \frac{\omega}{c \tilde{p}(\omega, k)} v + \frac{v_F^2 k^2 \Delta^2}{c^4 \hbar^2 \tilde{p}^4(\omega, k)}}} \right], \\ \Pi^{(1)}(\omega, k; \Delta, T_g) &= \frac{8\alpha\hbar c^2 \tilde{p}(\omega, k)}{v_F^2} \int_{\frac{\Delta}{\hbar c \tilde{p}(\omega, k)}}^{\infty} \frac{dv}{e^{D(\omega, k, T_g)v} + 1} \left\{ \frac{\omega^2}{c^2} - \frac{1}{2} \sum_{\lambda=\pm 1} \frac{[\tilde{p}(\omega, k)v + \lambda \frac{\omega}{c}]^2 + \frac{v_F^2 k^2 \Delta^2}{c^4 \hbar^2 \tilde{p}^2(\omega, k)}}{\sqrt{1 - v^2 - 2\lambda \frac{\omega}{c \tilde{p}(\omega, k)} v + \frac{v_F^2 k^2 \Delta^2}{c^4 \hbar^2 \tilde{p}^4(\omega, k)}}} \right\}, \end{aligned} \tag{26}$$

where

$$D(\omega, k, T_g) = \frac{\hbar c \tilde{p}(\omega, k)}{2k_B T_g}. \tag{27}$$

For a calculation of the contribution F_M to the nonequilibrium dispersion force (2), which is given by (3), one also needs to obtain the values of the polarization tensor at the pure imaginary Matsubara frequencies. These are easily obtained from (8) and the respective expressions (23)–(27) found in the interval (10) where we put $\omega = i\tilde{\zeta}_{E,l}$. In this case, the definitions (24) and (27) take the form

$$\tilde{p}^2(i\tilde{\zeta}_{E,l}, k) \equiv \tilde{p}_l^2(k) = \frac{v_F^2}{c^2} k^2 + \frac{\tilde{\zeta}_{E,l}^2}{c^2}, \quad D(i\tilde{\zeta}_{E,l}, k, T_g) = \frac{\hbar c \tilde{p}_l(k)}{2k_B T_g}. \tag{28}$$

Thus, all expressions for the polarization tensor appearing in both contributions F_M and F_r to the nonequilibrium dispersion force through the reflection coefficients (4) are presented.

4. Computational Results for the Dispersion Force on Nanoparticles from Graphene

Here, we present the computational results for the nonequilibrium dispersion force F_{neq} acting on nanoparticles of radius R on the source side of a graphene sheet characterized by the mass-gap parameter Δ , which takes the typical values of 0.1 and 0.2 eV [82,83]. The temperature of nanoparticles is assumed to be the same as that of the environment, i.e., $T_E = 300$ K, whereas the temperature of a graphene sheet can be either cooler, $T_g = 77$ K, or hotter, $T_g = 500$ K, than the environmental temperature. These temperatures are chosen as a representative example. The first is the temperature of liquid nitrogen, whereas the second is close to that employed in the experiment measuring the nonequilibrium Casimir–Polder force [85]. The developed formalism allows for computation of the nonequilibrium dispersion interaction for any experimental temperatures. In line with the assumptions made in Sections 2 and 3, computations were performed in the separation range from 200 nm to 2 μ m and it is assumed that R is sufficiently small. The polarizabilities of dielectric and metallic nanoparticles are presented in (1).

Numerical computations were performed by Equations (2)–(4), (6) and (7) using the expressions for the polarization tensor presented in Section 3. For this purpose, we worked out a program written in the C++ programming language. The program utilizes the Gauss–Kronrod and double-exponential quadrature methods from the GNU Scientific Library [86] and Boost C++ Libraries [87] for numerical integration. High-precision computation is achieved with the help of the Boost Multiprecision Library [88]. The program also employs the OpenMP Library [89] for parallelization. The results presented below were obtained using computational resources of the Supercomputer Center of the Peter the Great Saint Petersburg Polytechnic University.

The computational results for F_{neq} are normalized to the classical limit of the equilibrium dispersion force acting on a nanoparticle on the source side of an ideal metal plane [71]

$$F_c(a, T_E) = -\frac{3k_B T}{4a^4} \alpha(0). \tag{29}$$

The normalized values do not depend on the static polarizability of a nanoparticle $\alpha(0)$. The absolute values of F_{neq} for the nanoparticles made of some specific material can be obtained using Equations (1) and (29) by fixing the values of R and $\epsilon(0)$. In doing so, the value of R is restricted by the conditions $R \ll a$ and $R \ll \hbar c / (k_B T)$, considered in the beginning of Section 2.

In Figure 1, the F_{neq}/F_c ratio is shown as a function of the nanoparticle–graphene separation by the two bottom (blue) lines, which are plotted for graphene sheets with the mass-gap parameter Δ equal to 0.2 and 0.1 eV, kept at temperature $T_g = 77$ K.

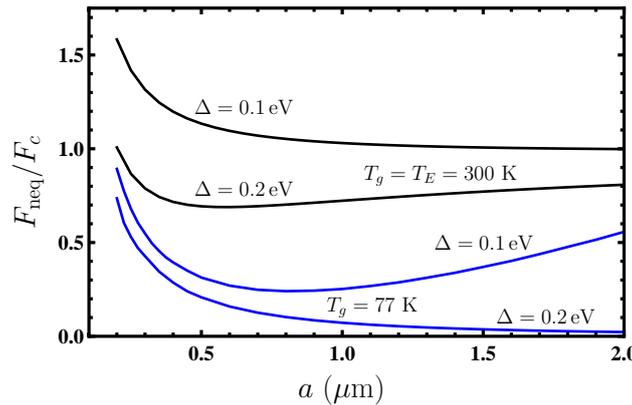


Figure 1. The ratio of nonequilibrium force acting on a nanoparticle on the source side of cooled to $T_g = 77$ K gapped graphene sheets with $\Delta = 0.2$ and 0.1 eV to the classical limit of an equilibrium at $T_E = 300$ K force acting between the same nanoparticle and an ideal metal plane is shown by the two blue bottom lines as the function of separation. The two black top lines show the ratio of the equilibrium force between a nanoparticle and the gapped graphene sheets kept at $T_E = 300$ K to the same classical limit.

For comparison, the two top (black) lines in Figure 1 show the ratio F_{eq}/F_c for the same nanoparticles and graphene sheets computed at a state of thermal equilibrium, i.e., when the temperatures of graphene and nanoparticles are equal to the environmental temperature, $T_g = T_E = 300$ K. In this case, the quantity F_{eq} is computed as

$$F_{eq}(a, \Delta, T_E) = -\frac{2k_B T_E \alpha(0)}{c} \sum_{l=0}^{\infty} \int_0^{\infty} k dk e^{-2a q_l(k)} \left\{ \left[2q_l^2(k) c^2 - \zeta_{E,l}^2 \right] R_{TM}(i\zeta_{E,l}, k; \Delta, T_E) - \zeta_{E,l}^2 R_{TE}(i\zeta_{E,l}, k; \Delta, T_E) \right\}. \quad (30)$$

Equation (30) is obtained from (3) by putting $T_g = T_E$.

As shown in Figure 1, for a cooled graphene sheet the change in the value of Δ has a lesser impact on F_{neq} than on F_{eq} at short separations but has a greater impact on F_{neq} than on F_{eq} at large separations. As opposed to the case of cooled sheet of a pristine graphene [67], for a gapped graphene with sufficiently large Δ the nonequilibrium dispersion force remains attractive.

Now let us admit that the graphene sheet is heated up to $T_g = 500$ K, whereas nanoparticles preserve the environmental temperature $T_E = 300$ K. In this case, the computational results for the ratio F_{neq}/F_c are shown in Figure 2 as the functions of separation by the two red lines plotted for graphene sheets with the mass-gap parameter Δ equal to 0.2 and 0.1 eV. The two black lines, which show the ratio F_{eq}/F_c , are reproduced from Figure 1. As explained above, they are plotted for graphene sheets with $\Delta = 0.2$ and 0.1 eV in thermal equilibrium with the environment at $T_g = T_E = 300$ K.

From Figure 2, it can be seen that, for a heated graphene sheet, the change in the value of Δ has a lesser impact on F_{neq} than on F_{eq} over the entire separation region being considered. By comparing Figures 1 and 2, one can conclude that the magnitude of a nonequilibrium dispersion force acting on a nanoparticle on the source side of gapped graphene increases with increasing temperature.

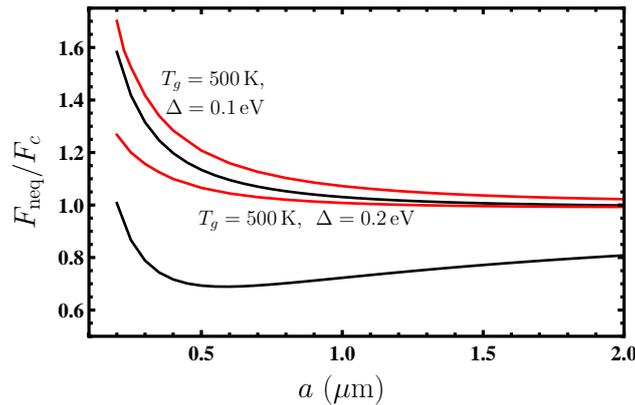


Figure 2. The ratio of nonequilibrium force acting on a nanoparticle on the source side of heated to $T_g = 500$ K gapped graphene sheets with $\Delta = 0.2$ and 0.1 eV to the classical limit of an equilibrium at $T_E = 300$ K force acting between the same nanoparticle and an ideal metal plane is shown by the two red lines as the functions of separation. The two black lines reproduced from Figure 1 show the ratio of the equilibrium force between a nanoparticle and the gapped graphene sheets kept at $T_E = 300$ K to the same classical limit.

Now, we investigate the relative role of the first and second contributions F_M and F_r in (2), which represents the total value of F_{neq} . We begin with F_M , computed by Equations (3) and (4), and the respective expressions (8), (23)–(27) for the polarization tensor calculated at the pure imaginary Matsubara frequencies $i\zeta_{E,J}$. Similar to the case of an equilibrium force, F_M is always negative, i.e., contributes to the attraction. The computational results for the ratio F_M/F_c are shown as the functions of separation in Figure 3 by the two pairs of blue and red lines computed at the graphene temperature $T_g = 77$ K and 500 K, respectively. In each pair, the lower line represents a graphene sheet with $\Delta = 0.2$ eV and the upper line represents a graphene sheet with $\Delta = 0.1$ eV.

As is seen in Figure 3, at both temperatures, the contribution F_M decreases in magnitude with increasing separation. In the considered separation region, this decrease occurs to the relatively small values at $T_g = 77$ K and to the classical limit (29) at $T_g = 500$ K. In doing so, the sign of F_M remains negative, which corresponds to the attractive force.

The role of the contribution F_r is somewhat different. The sign of F_r in (6) is determined by the sign of the quantity Θ in (7) and of the imaginary parts of R_{TM} and R_{TE} defined in (4). Thus, F_r can be both negative and positive. The quantity Θ is negative for $T_g > T_E$ and positive for $T_g < T_E$. As to the sign of $\text{Im} R_{\text{TM}}$ and $\text{Im} R_{\text{TE}}$, it depends on the relative contributions of the frequency regions (9) and (10). In the region (9), $\text{Im} R_{\text{TM,TE}}$ is positive and in the region (10), it is negative. The computational results for F_r are obtained by Equations (6), (4) and respective expressions for the polarization tensor at the real frequencies presented in Section 3.

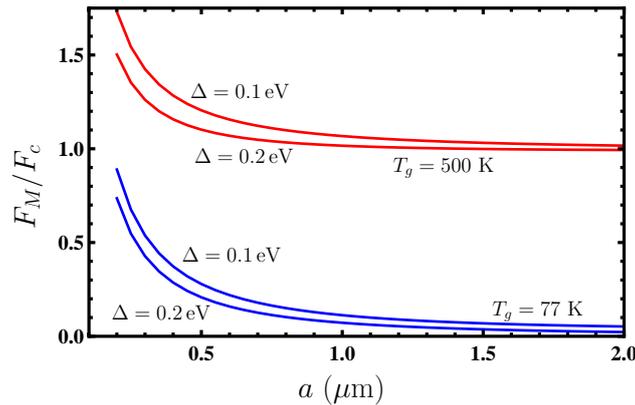


Figure 3. The ratio of the first contribution to the nonequilibrium force acting on a nanoparticle on the source side of cooled to $T_g = 77$ K and heated to $T_g = 500$ K gapped graphene sheets to the classical limit of an equilibrium at a $T_E = 300$ K force acting between the same nanoparticle and an ideal metal plane is shown by the pairs of blue and red lines, respectively, as the function of separation. In each pair, the lower line represents a graphene sheet with the mass-gap parameter $\Delta = 0.2$ eV and the upper line represents a graphene sheet with $\Delta = 0.1$ eV.

In Figure 4a, we plot the ratio F_r/F_c as the function of separation at the graphene temperature $T_g = 77$ K and in Figure 4b—for $T_g = 500$ K (the blue and red pairs of lines, respectively). In both cases, the lower and upper lines are for the graphene sheets with $\Delta = 0.2$ and 0.1 eV, respectively.

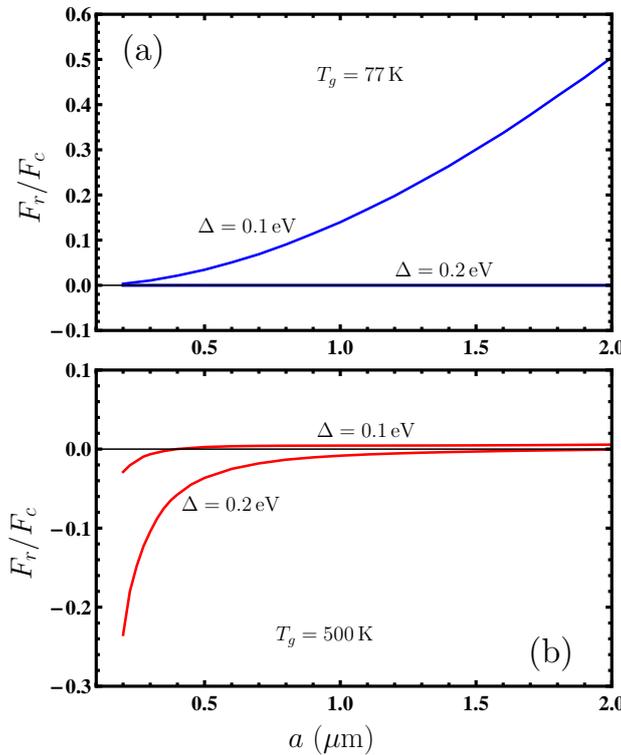


Figure 4. The ratio of the second contribution to the nonequilibrium force acting on a nanoparticle on the source side of (a) cooled to $T_g = 77$ K and (b) heated to $T_g = 500$ K gapped graphene sheets to the classical limit of an equilibrium at $T_E = 300$ K force acting between the same nanoparticle and an ideal metal plane is shown by the pairs of blue and red lines, respectively, as the function of separation. In each pair, the lower line represents a graphene sheet with the mass-gap parameter $\Delta = 0.2$ eV and the upper line represents a graphene sheet with $\Delta = 0.1$ eV.

From Figure 4a, one can see that, for a graphene sheet with $\Delta = 0.2$ eV at $T_g = 77$ K, the contribution F_r remains negligibly small at all considered separations, whereas it increases monotonously with increasing separation for a graphene sheet with $\Delta = 0.1$ eV. The sign of F_r remains negative. Here, the main contribution to F_r given by the frequency region (10) is negative, leading to $F_r < 0$.

In Figure 4b, the sign of F_r is positive for a graphene sheet with $\Delta = 0.2$ eV and changes from positive to negative for graphene with $\Delta = 0.1$ eV. This means that, at the considered separations, the main contribution to F_r for a graphene sheet with $\Delta = 0.2$ eV given by the frequency region (10) is positive, leading to $F_r > 0$. If $\Delta = 0.1$ eV, the relative role of the frequency regions (9) and (10) is different depending on separation. At short distances, the dominant region is (10) and $F_r > 0$, whereas at separations exceeding approximately $0.5 \mu\text{m}$, the dominant contribution is given by the region (9) and $F_r < 0$.

By comparing Figure 1 with Figures 3 and 4a, it is seen that at short separations the major contribution to F_{neq} for a graphene sheet at $T_g = 77$ K is given by F_M for both values of the mass-gap parameter. At large separations, the major contribution to F_{neq} is given by F_r for graphene with $\Delta = 0.1$ eV, whereas the relatively small values of F_{neq} for graphene with $\Delta = 0.2$ eV are determined by F_M .

In a similar way, by comparing Figure 2 with Figures 3 and 4b, we conclude that at short separations the major contributions to F_{neq} for graphene sheets at $T_g = 500$ K with both values of Δ are also given by F_M . These contributions, however, are slightly decreased by the impact of F_r , which is of the opposite sign. At large separations, the major contribution to F_{neq} is again given by F_M for both values of Δ , but for $\Delta = 0.1$ eV its magnitude is slightly increased at the expense of F_r .

At the intermediate separation distances, the value of the nonequilibrium dispersion force acting on a nanoparticle on the source side of gapped graphene sheet is determined by the joint action of both contributions F_M and F_r .

5. Discussion

In this article, we investigated the dispersion (Casimir–Polder) force acting on a nanoparticle on the source side of a gapped graphene sheet in the nonequilibrium situations when the graphene temperature is not equal to the nanoparticle temperature coinciding with the temperature of the environment. Cases when the graphene temperature is lower and higher than that of the environment were both considered.

It was shown that the nonzero value of the mass-gap parameter results in new properties of the nonequilibrium dispersion force as compared to the case of thermal equilibrium. Specifically, for a cooled graphene sheet, the variation in the mass-gap parameter has a lesser and greater impact on the nonequilibrium force than on the equilibrium one at short and large separations, respectively. For a heated graphene sheet, the variation in the mass-gap parameter results in a lesser impact on the nonequilibrium force than on the equilibrium one at all separations considered from 200 nm to $2 \mu\text{m}$. As opposed to the case of pristine graphene, for a gapped graphene sheet the nonequilibrium dispersion force preserves an attractive character at all considered separations.

We emphasize that the above results were obtained using the dielectric response of graphene expressed via the polarization tensor. The latter quantity was found in the framework of the Dirac model on the solid foundation of quantum field theory with no recourse to any phenomenological methods. Thus, in the application region of the Dirac model discussed in Section 3, these results possess the highest degree of reliability. In fact, graphene and other 2D materials, such as silicene, stanene, and germanene [90–95], are unique in that some of their properties can be investigated based on the most fundamental physical principles. The nonequilibrium dispersion force acting on nanoparticles on the source side of gapped graphene considered above presents one more example of this kind.

6. Conclusions

To conclude, the above results provide the possibility of controlling the nonequilibrium dispersion interaction between nanoparticles and a graphene sheet by varying the mass-gap parameter of this sheet and its temperature. The need for such control is apparent when noting that both nanoparticles of different kinds and graphene are already widely used in various micro- and nanodevices, including the field-effect transistors, integrated nanoparticle–biomolecule systems, electrochemical sensors and biosensors etc. [6,7,18,19,39–46]. The theoretical methods used in the design of these micro- and nanodevices are often based on phenomenology and computer simulation, rather than on fundamental physical principles. It is hoped that the employment of the methods of fundamental physics will further accelerate the progress in this rapidly developing field of applied science.

In the future, it would be interesting to extend the obtained results to graphene sheets deposited on substrates made of metallic and dielectric materials and to consider the case of doped graphene characterized by some nonzero chemical potential. This will provide further possibilities to control the nonequilibrium dispersion interaction in micro- and nanodevices incorporating nanoparticles and graphene sheets for their functionality.

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