

Effects of Spatial Dispersion on the Casimir Force between Graphene Sheets

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Abstract – The asymptotic dispersion force F between two graphene sheets at a separation d is unusual: at $T = 0$ K, $F \sim Cd^{-p}$, where $p=4$, unlike the 2D insulating ($p=5$) or metallic ($p = 7/2$) cases. Here it is shown that these anomalous low-temperature properties of p are retained when spatial dispersion is included in the conductivity. Furthermore, it is shown that the prefactor C is only weakly decreased (by 20%) upon spatial dispersion inclusion. For larger temperatures and nonzero chemical potential, such dispersion has even a lesser effect on the graphene/graphene force. The opening of a bandgap in the graphene electronic structure, however, can cause larger sensitivity to spatial dispersion at elevated temperatures.

Introduction . – Long-ranged dispersive interactions, such as the Casimir [1] force or the van der Waals [2] force, originate from electromagnetic field fluctuations. They are present between all types of objects at any distance, regardless of whether there are permanent electric and/or magnetic moments. Despite their universal nature, the dimensionality, dielectric and magnetic response properties, and geometry of the interacting systems can influence the dispersive force in profound ways, thus offering possibilities to tailor the sign, magnitude, and distance dependences of the interaction [3, 4].

Single layers of graphite have been recently isolated [5, 6], and their dispersive forces present not only challenging theoretical problems, but they are also important for graphene based devices [7], [8]. The electromagnetic fluctuation forces in graphene have been considered both at low and high temperature regimes as well as with the inclusion of a chemical potential or a band gap [9–17]. A distance power law has been obtained for the graphene/graphene Casimir force at the quantum limit, where the force per unit area (F) goes as the inverse distance (d) to the fourth power, $F \sim d^{-4}$, a behavior distinct from 2D metals or 2D insulators [17]. At the same time, due to the graphene gapless electronic structure, the fluctuation forces are thermal in nature even at room temperature [16]. This is in stark contrast to the Casimir

forces in most matter whereupon quantum fluctuation effects are dominant even at relatively high temperatures.

Concerning Casimir interactions in general, the inclusion of spatial dispersion in the response properties of the materials has received significant attention recently, since it was shown that the dispersion may play an important role [18, 19]. In this work we investigate how the spatial dispersion, in combination with modifications in the graphene electronic structure through a nonzero chemical potential or an induced energy gap, influence the graphene-graphene Casimir interaction. In practice, a finite chemical potential is induced by doping [20, 21] or by the application of external fields [5]. Energy band gaps on the other hand can be brought about by the growth of graphene on certain substrates [22], via adsorption [23] or hydrogenation [24]. The response properties of graphene for the calculations here are taken into account via the conductivity obtained from the linear response to the electromagnetic field [25], from which both the small and large spatial dispersion forces are investigated. **Spatial dispersion is found to be mostly important at low temperatures. At higher temperatures, such effects maybe apparent if a bandgap is induced in graphene.**

Graphene Conductivity. – An important factor in the Casimir force is the dielectric response properties of

the materials involved. For the graphene/graphene system, these properties are described via the optical conductivity calculated within the Kubo [26] formalism. Consider the case when there is a band gap Δ induced at the graphene Fermi level. Near the K-point of the Brillouin zone, assuming small wave vector excitations, the Hamiltonian can be written as

$$H = \begin{pmatrix} \Delta & v_0(p_x - ip_y) \\ v_0(p_x + ip_y) & -\Delta \end{pmatrix}, \quad (1)$$

where \mathbf{p} is the two-dimensional momentum operator and $v_0 = 3\gamma_0 a/2 \approx 10^6 m/s$ ($a = 0.142 nm$ is the CC distance and $\gamma_0 = 2.4 eV$ is the nearest neighbor tight binding overlap integral [27]). The Hamiltonian, Eq.(1), corresponds to a two-band model with eigenvalues and eigenvectors given respectively as:

$$E_s = s\sqrt{\Delta^2 + (v_0\hbar k)^2} = sE, \quad (2)$$

$$|\mathbf{k}, s\rangle = \frac{E - s\Delta}{\sqrt{E_0^2 + (E - s\Delta)^2}} \begin{pmatrix} \frac{E_0 e^{-i\theta}}{E - s\Delta} \\ s \end{pmatrix}, \quad (3)$$

where the wave function is $\psi(\mathbf{r}, s) = |\mathbf{k}, s\rangle e^{i\mathbf{k}\cdot\mathbf{r}}$, the two-dimensional wave vector is $\mathbf{k} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}}$ (\hat{x} , \hat{y} are unit vectors), $e^{i\theta} = (k_x + ik_y)/k$, $E_0 = v_0\hbar k$, and $s = \pm$. If $\Delta = 0$, one recovers the gapless Dirac-like model suitable for perfect graphene. Using this two-band model and applying linear response theory, the dyadic two dimensional conductivity is found [25] to be

see eq. (4)

where $f_0(E_s) = 1/(e^{(E_s - \mu)/k_B T} + 1)$ is the equilibrium Fermi distribution function, k_B is the Boltzmann constant and T is the temperature. The velocity matrix elements are $\mathbf{v}_{ss'} = \langle s, \mathbf{k} | \hat{\mathbf{v}} | s', \mathbf{k} \rangle$, where $\hat{\mathbf{v}} = \frac{\partial H}{\partial \mathbf{p}}$. The first term in Eq.(4) accounts for intraband transitions, while the second one accounts for interband transitions. From hence forth, imaginary frequency will be used, which is the relevant quantity for calculating Casimir forces.

In the limit when $\hbar v_0 q \rightarrow 0$, the optical conductivity of graphene, $\sigma_0(i\omega)$, is isotropic and it is found as:

$$\begin{aligned} \sigma_{0,intra}(i\omega) = & \frac{e^2 \ln(2)}{\hbar^2 \pi \omega \beta} + \frac{e^2}{\hbar^2 \pi \omega \beta} \ln(\cosh(\Delta\beta) + \cosh(\mu\beta)) - \\ & \frac{e^2 \Delta^2}{\hbar^2 \pi \omega} \int_{\Delta}^{\infty} \frac{dE}{E^2} \frac{\sinh(E\beta)}{\cosh(\mu\beta) + \cosh(E\beta)}, \end{aligned} \quad (5)$$

$$\begin{aligned} \sigma_{0,inter}(i\omega) = & \frac{e^2 \omega}{\pi} \int_{\Delta}^{\infty} dE \frac{\sinh(E\beta)}{\cosh(\mu\beta) + \cosh(E\beta)} \frac{1}{(\hbar\omega)^2 + 4E^2} + \\ & \frac{e^2 \omega \Delta^2}{\pi} \int_{\Delta}^{\infty} \frac{dE}{E^2} \frac{\sinh(E\beta)}{\cosh(\mu\beta) + \cosh(E\beta)} \frac{1}{(\hbar\omega)^2 + 4E^2} \end{aligned} \quad (6)$$

where $\beta = 1/k_B T$. One notes that when $\mu = 0$ and $\Delta = 0$, for $k_B T \ll \hbar\omega$, $\sigma_0(i\omega)$ acquires a universal value $\sigma_0(i\omega) \approx$

$\sigma_0 \equiv e^2/(4\hbar)$. In Fig(1(a)), results are shown for $\sigma_0(i\omega)$ as a function of frequency. The largest differences appear at small ω , where the conductivity is most significantly reduced when $\Delta \neq 0$ ($\mu = 0$) and augmented when $\mu \neq 0$ ($\Delta = 0$). For larger ω , the conductivity approaches σ_0 . **If the conductivity does not include spatial dispersion, the dielectric function will still depend on the wavenumber. Therefore, to avoid confusion, in this work, it is made clear that spatial dispersion on the Casimir force refers to the inclusion of spatial dispersion in the conductivity, instead of on the dielectric function.**

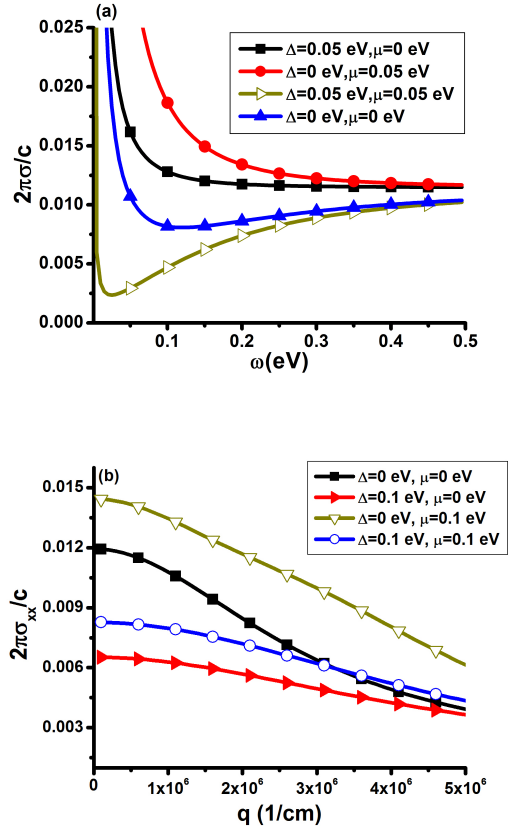


Fig. 1: (a) The isotropic conductivity $\sigma_0(i\omega)$ as a function of frequency (in eV) for different values of Δ and μ at $T = 300 K$. (b) $\sigma_{xx}(i\omega)$, as a function of q for finite Δ and μ with $\hbar\omega = 0.162 eV$ corresponding to $T = 300 K$.

If spatial dispersion is taken into account, $\overleftrightarrow{\sigma}$ is not isotropic. For graphene, however, we find that σ_{xx} and σ_{yy} have very similar magnitude and behavior over large wave vector and frequency regions, therefore only σ_{xx} is shown in Fig(1(b)). The conductivity, σ_{xx} , starts changing in a more pronounced way for $q > 10^6 cm^{-1}$. It is noted that σ_{xx} is the conductivity in the direction of the \mathbf{E} field parallel to the **wave propagation**, while σ_{yy} corresponds to the direction of the \mathbf{E} field perpendicular to the **wave propagation**.

$$\begin{aligned} \overleftrightarrow{\sigma}(\omega, \mathbf{q}) &= \frac{i\hbar e^2}{\pi^2} \times \sum_{s=\pm} \int d^2k \frac{\mathbf{v}_{ss}\mathbf{v}_{ss} (f_0[E_s(\mathbf{k}-\mathbf{q}/2)] - f_0[E_s(\mathbf{k}+\mathbf{q}/2)])}{[E_s(\mathbf{k}+\mathbf{q}/2) - E_s(\mathbf{k}-\mathbf{q}/2)][\hbar\omega - E_s(\mathbf{k}+\mathbf{q}/2) + E_s(\mathbf{k}-\mathbf{q}/2)]} + \\ &\frac{2i\hbar^2 e^2 \omega}{\pi^2} \int d^2k \frac{\mathbf{v}_{+,-}\mathbf{v}_{-,+} (f_0[E_+(\mathbf{k}-\mathbf{q}/2)] - f_0[E_-(\mathbf{k}+\mathbf{q}/2)])}{[E_-(\mathbf{k}+\mathbf{q}/2) - E_+(\mathbf{k}-\mathbf{q}/2)][\hbar^2\omega^2 - [E_-(\mathbf{k}+\mathbf{q}/2) - E_+(\mathbf{k}-\mathbf{q}/2)]^2]}, \end{aligned} \quad (4)$$

$$F = -\frac{ik_B T}{2\pi} \sum_{n=-\infty}^{\infty} \int_0^{\infty} h(i|\omega_n|) q dq \left\{ \left[\frac{e^{-2ih(i|\omega_n|)d}}{\rho_E(i|\omega_n|)^2} - 1 \right]^{-1} + \left[\frac{e^{-2ih(i|\omega_n|)d}}{\rho_B(i|\omega_n|)^2} - 1 \right]^{-1} \right\}, \quad (7)$$

Graphene Casimir Force and Dispersion. – The Casimir force per unit area [3] between two graphene sheets separated by a distance d is

see eq. (7)

where $h(i|\omega_n|) = i\sqrt{\epsilon(i|\omega_n|)\mu(i|\omega_n|)(\omega_n/c)^2 + q^2}$ with $\omega_n = 2\pi n k_B T / \hbar$ and \mathbf{q} is the two-dimensional wave vector in the xy -plane. $\rho_{E,B}$ are the generalized reflection coefficients for two suspended graphenes corresponding to the boundary conditions due to the transverse electric (**E**) and magnetic (**B**) field modes,

$$\begin{aligned} \rho_E(i\omega) &= -\frac{2\pi\sigma_{yy}(i\omega, \mathbf{q})\omega/[h(i\omega)c^2]}{1 + 2\pi\sigma_{yy}(i\omega, \mathbf{q})\omega/[h(i\omega)c^2]}, \\ \rho_B(i\omega) &= \frac{2\pi\sigma_{xx}(i\omega, \mathbf{q})h(i\omega)/\omega}{1 + 2\pi\sigma_{xx}(i\omega, \mathbf{q})h(i\omega)/\omega}. \end{aligned} \quad (8)$$

More details concerning the derivation procedure of these expressions can be found in Refs. ([15], [28]).

Thermal Limit. The thermal fluctuation forces are first considered, which correspond to the zero Matsubara term ($n = 0$) of Eq.(7) in the strong dispersion limit, where $\hbar\omega \ll k_B T$, $\hbar v_0 q$. In most materials purely thermal fluctuation effects are important at distances larger than their characteristic thermal wavelength, $\lambda_T = \hbar c / (k_B T) \sim 7 \mu m$. Instead, due to the Dirac-like Hamiltonian of graphene and its two dimensional nature, the characteristic thermal wavelength is significantly reduced - $\sim \lambda_T / 200$. As a result, thermal fluctuation forces become important at relatively small scales [16], $d \approx 30 nm$. Therefore the quasi-static response is a reasonable approximation for a large distance range.

In the quasi-static response limit of $\hbar\omega \ll \hbar v_0 q \ll k_B T$, the σ_{xx} is

$$\sigma_{xx}(i\omega, \mathbf{q}) = \frac{\omega q_s}{2\pi q^2}. \quad (9)$$

This corresponds to the longitudinal plasmon excitations in the graphene static dielectric function $\epsilon(q) = 1 + q_s/q$ obtained via the Random Phase Approximation(RPA) method [29]. Note that in the limit of $k_B T, \hbar v_0 q \ll \hbar\omega$ $\sigma = \sigma_0$, but the dielectric function will still depend on the

wave number. For gapped graphene [12],

$$\begin{aligned} q_s(\Delta) &= \frac{4\alpha c}{\hbar v_0^2} \left\{ 2k_B T \ln \left(2 \cosh \left(\frac{\Delta}{2k_B T} \right) \right) \right\} - \\ &\frac{4\alpha c}{\hbar v_0^2} \left\{ \Delta \tanh \left(\frac{\Delta}{2k_B T} \right) \right\}, \end{aligned} \quad (10)$$

where $\alpha \approx 1/137$ is the fine structure constant. Using Eq.(7) and Eq.(9) the thermal fluctuation stress between two graphene sheets is obtained to be

$$F(d) = \frac{k_B T}{16\pi d^3} \int_0^{\infty} \frac{x^2 dx}{e^x (x + 2dq_s)^2 / (2dq_s)^2 - 1}. \quad (11)$$

The main contribution to the integral in Eq.(11) occurs when $x \equiv 2dq_s \sim 1$. Given the restrictions for the conductivity of Eq.(9), $q \ll 4 \times 10^5 \text{ cm}^{-1}$ at room temperature, which corresponds to a distance of $d \gg 10 \text{ nm}$. Eq.(11) becomes a reasonable approximation by around $d > 50 \text{ nm}$. One finds that as $q_s d \gg 1$, the stress approaches the thermal stress between two perfect metals, i.e., $F_T = k_B T \zeta(3) / (8\pi d^3)$.

A similar calculation can be executed for the problem of finding the thermal fluctuation force $f(d)$ between a graphene sheet and a polarizable atom with polarizability $\chi(\omega)$. The Casimir interaction between graphene and an atom has received some attention recently [30], partially due to the potential applications of two dimensional nanostructures being used for hydrogen storage. The force is given [31] by

see eq. (12)

Using Eq.(9), the thermal fluctuation force, $n = 0$ term, in this case is

$$f(d) = \frac{k_B T \chi(0)}{8d^4} \int_0^{\infty} x^3 dx e^{-x} \left[\frac{2dq_s}{x + 2dq_s} \right],$$

$$\begin{aligned} f(d) &= \frac{k_B T \chi(0)}{8d^4} [(2dq_s)^3 - (2dq_s)^2 + 2(2dq_s)] - \\ &\frac{k_B T \chi(0)}{8d^4} [(2dq_s)^4 e^{2dq_s} E_1(2dq_s)]. \end{aligned} \quad (13)$$

where $E_1(x)$ is the exponential integral. Again as $q_s d \gg 1$, the force between atom and graphene becomes $f_T =$

$$f(d) = -k_B T \sum_{n=-\infty}^{\infty} \chi(i|\omega_n|) \int_0^{\infty} k dk h^2(i|\omega_n|) \left[2\rho_B(i|\omega_n|) - \left(\frac{\omega_n}{\hbar(i|\omega_n|)c} \right)^2 [\rho_E(i|\omega_n|) - \rho_B(i|\omega_n|)] \right] e^{2idh(i|\omega_n|)}. \quad (12)$$

$3k_B T \chi(0)/(4d^4)$, which is the thermal interaction between an atom and a perfectly conducting plate.

The normalized forces, F/F_T and f/f_T , as a function of $2dq_s$ are shown in Fig.(2). One finds that for large distances spatial dispersion is less important, and the force goes to the one expected for ideal metallic surfaces. For short distances the electron screening shields the force such that it goes to zero at very small distances. From Fig.(2(a)) it is seen that dispersion is significant when $q_s d \approx 10$ or less. For the case of gapless graphene, this corresponds to a distance of $d \approx 20 \text{ nm}$ at room temperature, in which case higher Matsubara frequencies need to be considered. Hence, for the case of graphene, dispersion does not play a significant role in the region where the fluctuation force is thermal. Spatial dispersion becomes important for graphene if q_s decreases.

It has been noted that while for good conductors and dielectrics thermal Van-der-Waal/Casimir forces are not heavily influenced by dispersion effects, the latter may have a strong influence on the force for poor conductors [32,33]. A similar result occurs for graphene, where upon the conduction properties of the material are decreased by introducing a band gap.

By inducing an energy band gap, the effect of spatial dispersion in graphene is increased by effectively decreasing q_s , as shown in Fig.(2(b)). It is clear that the influence of dispersion increases as q_s gets small with the effect that the thermal fluctuation forces between graphene sheets are substantially decreased. For example for $\Delta = 0.05 \text{ eV}$, a typical value for the gap, one obtains a distance for dispersion to have strong effects of $d \approx 40 \text{ nm}$, within the range where thermal fluctuation forces are dominant. **The final result may not be quantitatively accurate since Eq.(11) is not precise for such scales. Still the qualitative conclusion of increasing dispersion effects by inducing a band gap holds true.** This effect is analogous to 3-D materials, whereupon the influence of dispersion in the fluctuation forces of a conductor become strong were it to become a poorer conductor.

T = 0 K. When the temperature is zero, the summation in F (Eq.(7)) is substituted by an integral, $\sum_n = [\hbar/(2\pi k_B T)] \int_0^{\infty} d\omega$. The $T = 0 \text{ K}$ case corresponds to purely quantum mechanical contributions to the Casimir stress. If the graphene conductivity is given by the universal value $\sigma_0 = e^2/(4\hbar)$, the graphene/graphene Casimir force per unit area is found as [15–17]

$$F_g = \frac{3e^2}{32\pi d^4} = F_0 \kappa(\alpha) \quad (14)$$

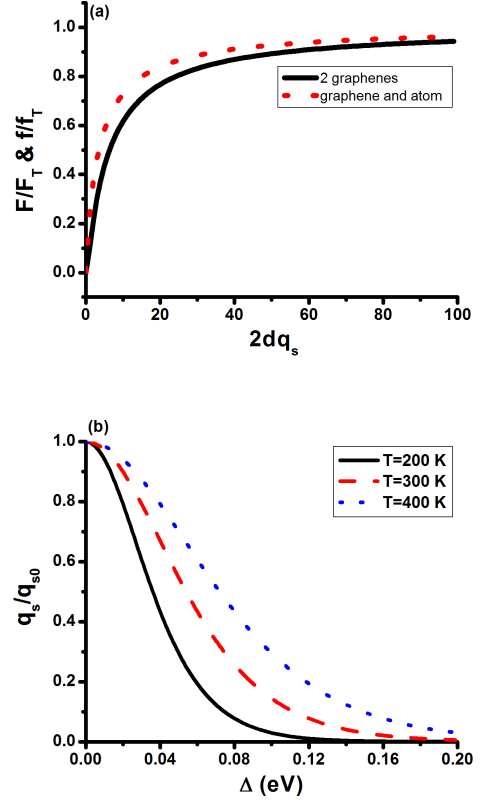


Fig. 2: (a) Thermal stress between two graphenes normalized to the thermal stress between two metals and thermal force between graphene and atom normalized to the thermal force between metal and an atom. (b) q_s normalized to the value at zero band gap q_{s0} as a function of the energy band gap Δ for different temperatures, $T = 200 \text{ K}$, $T = 300 \text{ K}$, $T = 400 \text{ K}$.

where $F_0 = \pi^2 \hbar c / (240d^4)$ is the force per unit area between two perfectly conducting metallic sheets and $\kappa(\alpha) = 720\alpha / (32\pi^3)$ with $\alpha = 1/137$ being the fine structure constant. It is interesting that the force in this limit does not depend on any quantum mechanical characteristics nor the speed of light. Comparing F_g to F_0 shows that the distance dependence of the graphene/graphene force is the same as for metallic plates in the retarded regime, however, the magnitude is reduced by an order of the fine structure constant. Incidentally, this differs from the non-retarded “2D” metal and doped graphene result– $F \sim d^{-7/2}$ [14, 17]

The presence of μ or Δ alters the graphene conductivity, which can change the Casimir interaction significantly. Using the isotropic $\sigma_0(i\omega)$ from Eqs.(5, 6), it is found that

F/F_0 increases almost linearly as a function of d when $\mu \neq 0$, while for $\Delta \neq 0$ and $\mu \neq 0$ the normalized Casimir stress has nonlinear dependences - Fig.(3(a)). This happens because at shorter distances the effect of the band gap is more pronounced, while at larger distances the finite chemical potential has a stronger effect. It is found that F/F_0 can be diminished by increasing the band gap of the graphene sheets (Fig.(3(b))) or it can be enhanced by increasing the chemical potential (Fig.(3(c))). These changes can be quite substantial, providing that the system supports large μ or Δ .

It is interesting to consider to what extent spatial dispersion affects the graphene/graphene Casimir interaction. In the absence of a band gap or chemical potential, dimensional analysis dictates that the force may be written as

$$F = F_0 g(\alpha, v_0/c), \quad (15)$$

where the scaling factor $g(\alpha, v_0/c)$ now depends on the fine structure constant, and the ratio of v_0/c . If one uses Eq.(4), the scaling factor is evaluated as $f(\alpha, v_0/c) \approx 0.0043$. Note that the distance dependence is still $F \sim d^{-4}$. Comparing the scaling factors κ and g shows that the inclusion of spatial dispersion reduces the graphene/graphene Casimir attraction by $\approx 20\%$. If one were to approximate the conductivity of graphene via RPA, then inclusion of dispersion would reduce the graphene/graphene interaction by $\approx 9\%$. Figs.(3(b),3(c)) further show that dispersion effects are rather insignificant as μ and Δ increase.

T \neq 0K. Finally, the full finite temperature Casimir interaction is considered. Eq.(7) indicates that the largest contribution to the force occurs when $qd \sim 1$. On the other hand it was shown that for finite frequencies, the conductivity varies sharply as a function of wavenumber when $q_s > 10^6 \text{ cm}^{-1}$ - Fig(1(b)). Therefore, dispersion effects start becoming important for Matsubara terms in Eq.(7) greater than zero at a distance of $d_s \sim 1/q_s = 0.01 \mu\text{m}$. Fig.(4(a)) shows the Casimir interaction force per unit area between two graphene sheets where spatial dispersion is only included in the force for the $n = 0$ thermal term and also where spatial dispersion is included for all Matsubara frequency terms. If the distance is reduced much further the force reduces back to the zero temperature result.

Much more influential parameters to the Casimir interaction are the induced chemical potential or energy band gap. The effects are displayed in Fig.(4(b)), which shows the stress between graphenes for different band gaps, and chemical potentials. In addition, the role of the chemical potential is to increase the magnitude of the force while the energy band gap decreases it (not shown graphically). The characteristic behavior is similar as for the quantum $T = 0 \text{ K}$ limit.

Conclusion. – The Casimir interaction between two graphene sheets has been investigated at room and zero

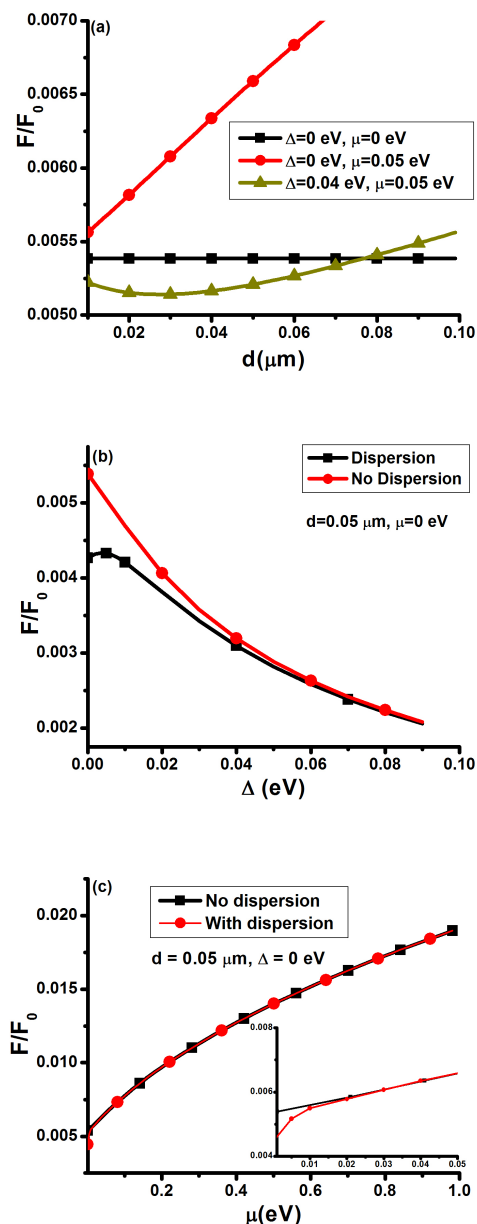


Fig. 3: (a) Casimir stress normalized to F_0 at $T=0$ and calculated using the isotropic conductivity $\sigma_0(i\omega)$ for different Δ and μ . The flat line indicates the normalized stress obtained via the universal conductivity σ_0 ; (b) Casimir stress normalized to F_0 at $T=0$ as a function of Δ calculated using $\sigma_0(i\omega)$ and $\sigma(i\omega, \mathbf{q})$ ($\mu = 0$); (c) Casimir stress normalized to F_0 as a function of μ calculated using $\sigma_0(i\omega)$ and $\sigma(i\omega, \mathbf{q})$ ($\Delta = 0$)

temperatures by using linear response theory with a conductivity response function in order to determine how spatial dispersion affects the interaction. **In the quantum mechanical regime, spatial dispersion reduces the Casimir force and it preserves its d^{-4} distance dependence. In the thermal regime, the Casimir interaction may be well approximated by using a frequency only dependent con-**

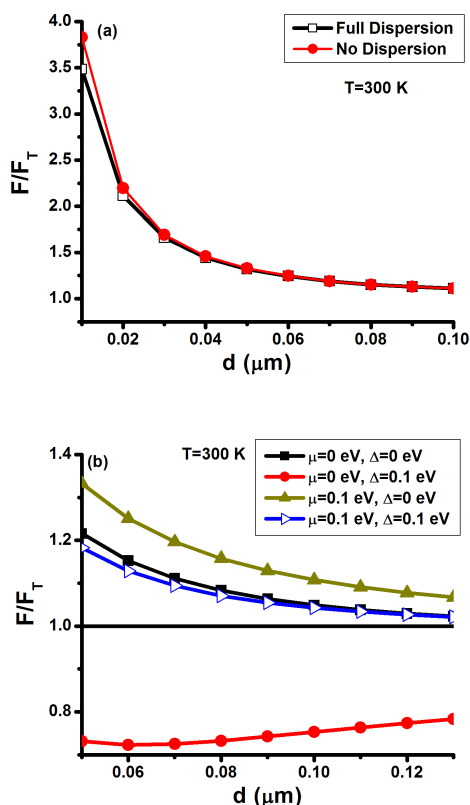


Fig. 4: (a) Casimir stress normalized to the idealized stress F_0 at $T = 300\text{ K}$ with and without the inclusion of dispersion for Matsubara terms greater than zero. (b) Casimir stress normalized to the idealized stress F_0 at $T = 300\text{ K}$.

ductivity. Spatial dispersion corrections start appearing at distances of $d \sim 0.01\ \mu\text{m}$ at room temperature. A finite chemical potential can enhance the Casimir interaction substantially and further inhibit spatial dispersion. If a band gap is induced at finite temperature, however, graphene exhibits similar characteristics to a poor metal and dispersion effects start becoming more important, that is the thermal fluctuation forces are reduced by the presence of electronic charge screening.

In the present work, dispersion has been investigated using the 2-band model. Yet at shorter distances, in the order of 10 nm or less, higher band transitions become important for the Van-der Waals/Casimir interaction. The inclusion of such effects without spatial dispersion have already been investigated in a previous work [10].

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