SURFACE PLASMON RETARDATION IN GRAPHENE BILAYER

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The aim of this work was to

- derive and investigate dispersion equation for plasmons in single- and multilayer graphene systems;
- calculate plasmon phase velocity.

Presentation structure:

- 1) Motivation. Why did we need it?
- 2) Method. How did we get it?
- 3) Results. How could we use it?

Motivation

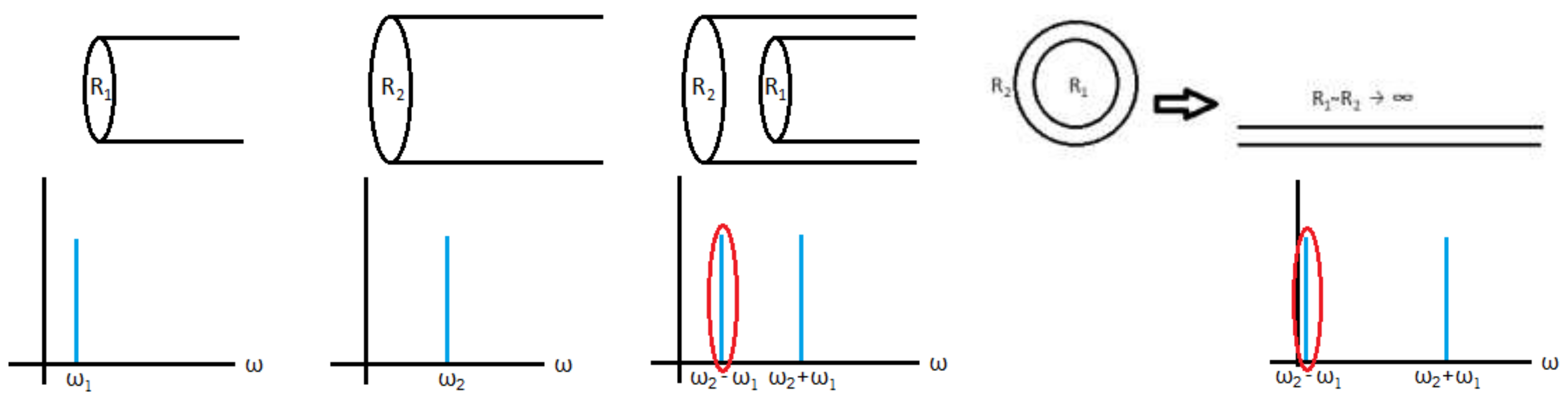
Slepyan G.Ya., Maksimenko S.A., Lakhtakia A., Yevtushenko O., Gusakov A.V. Electrodynamics of carbon nanotubes: Dynamic conductivity, impedance boundary conditions and surface wave propagation // Phys. Rev. B. -1999. **-60**, N 24. –P. 17136-17149.

Batrakov K.G., Maksimenko S.A., Kuzhir P.P., Thomsem C. Carbon nanotube as a Cherenkov-type light emitter and free electron laser// Phys. Rev. B. -2009. **-70**, N 12. -P. 125408-125420.

Batrakov K. G., Kuzhir P. P., Maksimenko S. A. Stimulated emission of electron beam in nanotube bundles// Physica E – 2008. –V.40. –No.7. –P.2370-2374.

Batrakov K.G., Kibis O.V., Kuzhir P.P., Maksimenko S.A., M. Rosenau da Costa and Portnoi M.E. Mechanisms of terahertz emission from carbon nanotubes// Physica B: condensed Matter — 2010. – V. 405, No 14. – P. 3043–3056.

Batrakov K. G., Kuzhir P. P., Maksimenko S. A. Toward the nano-FEL: undulator and Cherenkov mechanisms of light emission in carbon nanotubes// Physica E – 2008. –V.40. –No.5, –P.1065-1068.



CHERENKOV RADIATION IN NANOSCALE (?)

Requirements:

1) Ballistic transport (~10^{-6} m)

Micrometer-Scale Ballistic Transport in Encapsulated Graphene at Room Temperature / *Alexander S. M., R.V. Gorbachev, S.V. Morozov, L. Britnell, R. Jalil, L.A. Ponomarenko, P. Blake, K.S. Novoselov, K. Watanabe, T. Taniguchi, A.K. Geim//* Nano Lett. – 2011. -V. 11, No. 6. -P. 2396-2399.

2) High density of breakdown current(~10^7-10^9A/cm)

Breakdown current density of graphene nanoribbons / *R. Murali, Y. Yang, K. Brenner, T. Beck, J.D. Meindl//* App. Phys. Lett. – 2009. –V. 94, No. 24. –P. 243114- 243117.

3) Electromagnetic wave retardation(?)

SELF-CONSISTENT PROBLEM

- Electromagnetic waves dynamics in the medium can be described by system of equations consisting of Maxwell's equations (microscopic) and quantum mechanical equations (in Heisenberg picture) for wave functions in secondary quantization representation.

$$\left(\frac{\partial^2}{c^2\partial t^2}-\Delta\right)\Phi(\vec{r},t)=4\pi\rho(\vec{r},t); \qquad \rho(\vec{r},t)=e\left\langle 0\left|\widehat{\Psi}^{+}\widehat{\Psi}\right|0\right\rangle;$$

$$\widehat{\Psi}\equiv\widehat{\Psi}(\vec{r},t)=\sum_{\vec{k}}\Psi_s(\vec{r},\vec{k})\widehat{b}_{\vec{k}s}(t); \quad \widehat{H}=\sum_{\vec{k}}E_{\vec{k}s}\widehat{b}^{+}_{\vec{k}s}\widehat{b}_{\vec{k}s}+\int\Psi^{+}(\vec{r},t)\widehat{H}_{\text{int.}}\Psi(\vec{r},t)d\vec{r};$$

$$\frac{d\widehat{b}^{+}_{\vec{k}s}}{dt}=\frac{i}{\hbar}\left[\widehat{H},\widehat{b}^{+}_{\vec{k}s}\right]; \qquad \widehat{H}_{\text{int.}}=e\Phi.$$

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$$\hat\Psi\equiv\hat\Psi(\vec r,t)=\sum_{\vec k}\Psi_s(\vec r,\vec k)b_{\vec k s}(t);\quad \hat H=\sum_{\vec k}E_{\vec k s}\hat b^+_{\vec k s}\hat b_{\vec k s}+\int\Psi^+(\vec r,t)\hat H_{\text{int.}}\Psi(\vec r,t)d\vec r;$$

$$\frac{d\hat b^+_{\vec k s}}{dt}=\frac{i}{\hbar}\left[\hat H,\hat b^+_{\vec k s}\right];\qquad \hat H_{\text{int.}}=e\Phi.$$

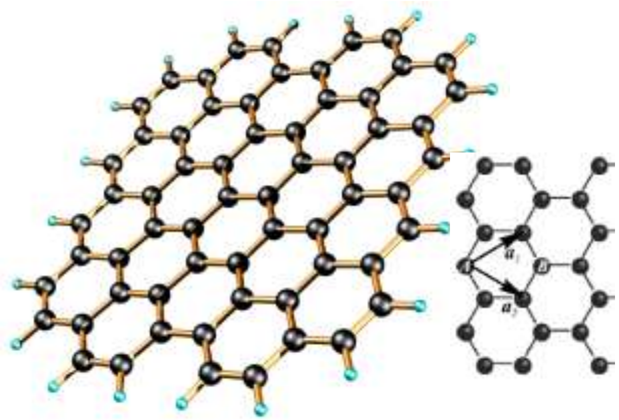
TIGHT-BINDING CALCULATION

- According to this method electrons are treated as strong interacted with atoms core. Therefore electron wavefunctions are presented as linear combination of the Bloch functions with unknown coefficients. Bloch functions in its turn are presented as a sum of atomic wave functions.

$$\Psi_s(\vec{r},\vec{k}) = \sum_{l=1}^{n} c_{\vec{k}s}^{l}(\vec{k})\psi_l(\vec{r},\vec{k}), \quad \psi_l(\vec{r},\vec{k}) = \frac{1}{\sqrt{N}}\sum_{m=1}^{N}\phi(\vec{r}-\vec{r}_{lm})\exp(i\vec{k}\cdot\vec{r}_{lm}) - \text{Bloch functions}$$

$$\phi(\vec{r}) = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_B}\right)^{\frac{5}{2}}\exp\left(-\frac{Z}{2a_B}r\right) - \text{atomic wavefunction.}$$

$$\begin{pmatrix} E_{\vec{k}s} & \gamma_0 f(k_x,k_y) \\ \gamma_0 f^*(k_x,k_y) & E_{\vec{k}s} \end{pmatrix}\begin{pmatrix} c_{\vec{k}s}^{A} \\ c_{\vec{k}s}^{B} \end{pmatrix} = 0; \quad \begin{pmatrix} E_0+\Delta-E_{\vec{k}s} & \gamma_0 f(k_x,k_y) & \gamma_1 & \gamma_4 f^*(k_x,k_y) \\ \gamma_0 f^*(k_x,k_y) & E_0-E_{\vec{k}s} & \gamma_4 f^*(k_x,k_y) & \gamma_4 f^*(k_x,k_y) \\ \gamma_1 & \gamma_4 f(k_x,k_y) & E_0+\Delta-E_{\vec{k}s} & \gamma_4 f^*(k_x,k_y) \\ \gamma_4 f(k_x,k_y) & \gamma_3 f^*(k_x,k_y) & \gamma_0 f(k_x,k_y) & E_0-E_{\vec{k}s} \end{pmatrix}\begin{pmatrix} c_{\vec{k}s}^{A_1} \\ c_{\vec{k}s}^{B_1} \\ c_{\vec{k}s}^{A_2} \\ c_{\vec{k}s}^{B_2} \end{pmatrix} = 0;$$

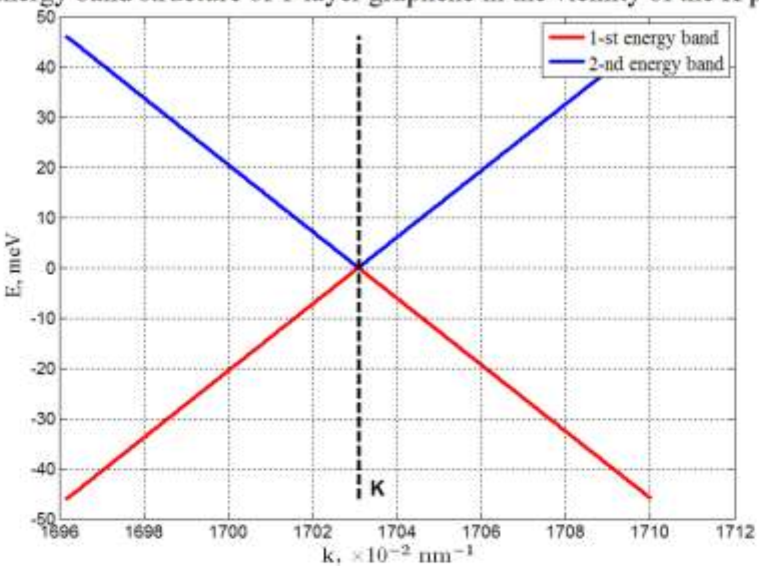


$$f(k_x,k_y) = \exp\left(\frac{ik_x a}{\sqrt{3}}\right) + 2\exp\left(\frac{ik_x a}{2\sqrt{3}}\right)\cos\left(\frac{ik_y a}{2}\right);$$

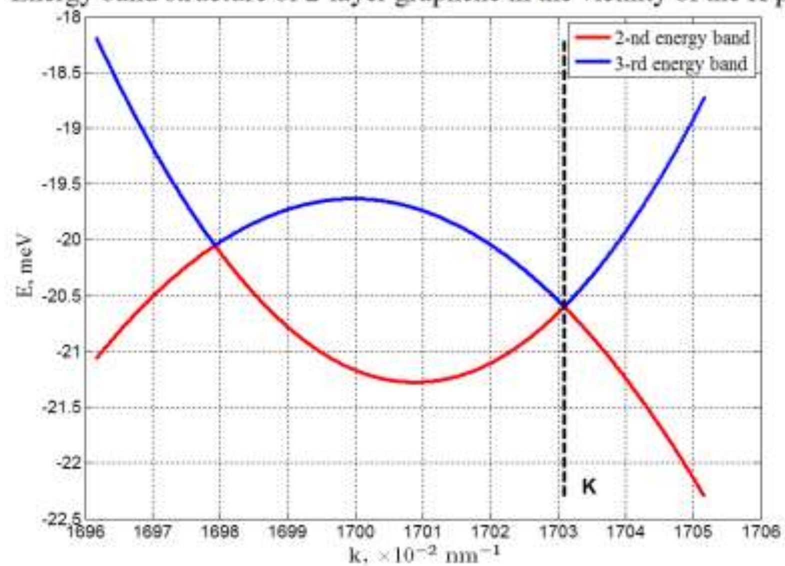
TIGHT-BINDING CALCULATION

- According to this method electrons are treated as strong interacted with atoms core. Therefore electron wavefunctions are presented as linear combination of the Bloch functions with unknown coefficients. Bloch functions in its turn are presented as a sum of atomic wave functions.

Energy band structure of 1-layer graphene in the vicinity of the K point



Energy band structure of 2-layer graphene in the vicinity of the K point



WAVE EQUATION SOLUTION

$$\left(\frac{\partial^2}{c^2\partial t^2}-\Delta\right)\Phi(\vec{r},t)=4\pi\rho(\vec{r},t);$$

- Let's use:

1) Fourier transformation time-dependent and 2d-space-dependent (r,t) – (k, z, ω)
2) Tight-binding approximation: smallness of the overlap integrals
3) Boundary conditions $\Phi(\vec{k},\omega,z)_{z\to\pm\infty}\to 0$

$$\left(\frac{d^2}{dz^2}-k^2\right)\Phi(\vec{k},z,\omega)=\sum_{i=1}^{\sigma}f_i(\vec{k},z,\omega)A_i;\qquad \Phi(\vec{k},\omega,z)=\sum_{i=1}^{\sigma}W_i(\vec{k},\omega,z)A_i(\vec{k},\omega);$$

$$W_i(\vec{k},\omega,z)=\exp(kz)\int_{\infty}^{z}\frac{\exp(-ky)f_i(\vec{k},\omega,y)}{2k}dy-\exp(-kz)\int_{-\infty}^{z}\frac{\exp(ky)f_i(\vec{k},\omega,y)}{2k}dy$$

$$f_i(\vec{k},z,\omega)=-\frac{4\pi e^2}{S}\sum_{\vec{k}_2,s_1,s_2}\sum_{m=1}^{\sigma}c^*_{\vec{k}_2s_2,m}c_{(\vec{k}_2+\vec{k})s_1,m}F_m(\vec{k},z)\frac{c^*_{(\vec{k}_2+\vec{k})s_1,i}\,c_{\vec{k}_2s_2,i}}{\hbar\omega+E_{\vec{k}_2s_2}-E_{\vec{k}_1s_1}}\left(n_{\vec{k}_2s_2}-n_{(\vec{k}_2+\vec{k})s_1}\right);$$

$$F_m(\vec{k},z)=\int\left|\phi(\vec{r}_{xy},z-z_m)\right|^2e^{-i\vec{k}\cdot\vec{r}_{xy}}d\vec{r}_{xy};$$

DISPERSION EQUATION

$$\Phi(\vec{k},\omega,z)=\sum_{i=1}^{\sigma}W_i(\vec{k},\omega,z)A_i(\vec{k},\omega);$$

Wave equation "solution" must be supplemented with a homogeneous system of algebraic equations with respect to variables A_i ingressed in wave equation solution and determined by it.

$$A_i(\vec{k},\omega)=\int\rho_i(\vec{k},z)\Phi(\vec{k},z,\omega)dz;$$

$$\rho_i(\vec{k},z)=\int\left|\phi(\vec{r}_{xy},z-z_i)\right|^2 e^{i\vec{k}\cdot\vec{r}_{xy}}d\vec{r}_{xy};$$

Dependence of plasmon frequency vs. its wave vector arises as natural requirement of the system solution existence: equality of the system matrix determinant to zero.

$$\begin{vmatrix} C_{11}-1 & C_{12} & \cdots & C_{1\sigma} \\ C_{21} & C_{22}-1 & \cdots & C_{2\sigma} \\ \vdots & \vdots & \ddots & \vdots \\ C_{\sigma 1} & C_{\sigma 2} & \cdots & C_{\sigma\sigma}-1 \end{vmatrix}=0,\quad C_{mn}=\int\rho_m(\vec{k},z)W_n(\vec{k},z,\omega)dz;$$

$$where\ \sigma-number\ of\ atoms\ in\ the\ unit\ cell;$$

1-LAYER GRAPHENE DISPERSION EQUATION

- Considering the system in long wave approximation and at low temperatures the following equation can be obtained:

$$1-\frac{2\pi e^2}{kS}P(\vec{k},\omega)Q(k)=0; \qquad k\cdot r\rightarrow 0$$

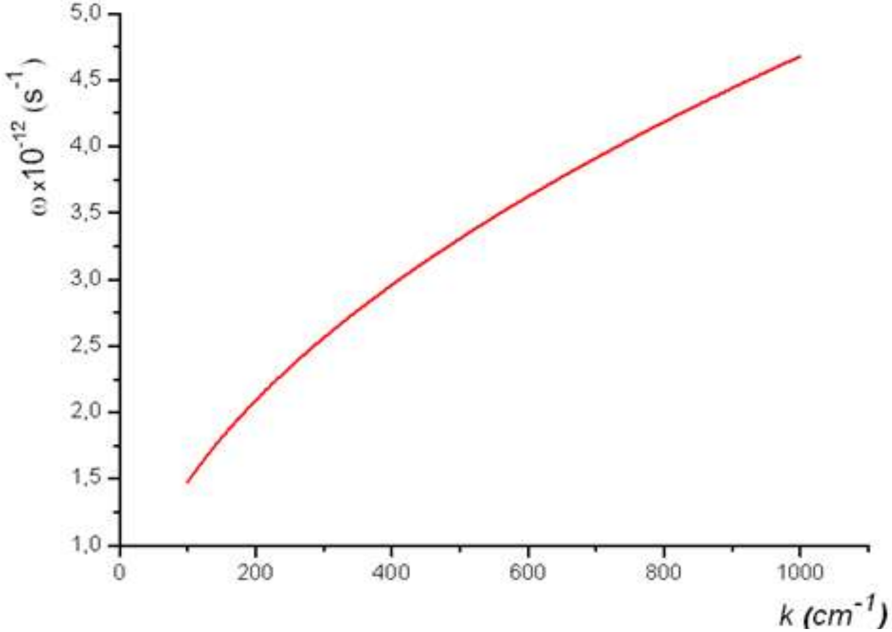
$$P(\vec{k},\omega)=\sum_{\vec{k}_2}\left\{\frac{n_{\vec{k}_2,1}-n_{\vec{k}_2+\vec{k},1}}{\hbar\omega+E_{\vec{k}_2,1}-E_{\vec{k}_2+\vec{k},1}}+\frac{n_{\vec{k}_2,2}-n_{\vec{k}_2+\vec{k},2}}{\hbar\omega+E_{\vec{k}_2,2}-E_{\vec{k}_2+\vec{k},2}}\right\};$$

$$Q(k)=\int\rho(z)\left\{e^{kz}\int_z^{\infty}e^{-kz'}\rho(z')dz'+e^{-kz}\int_{-\infty}^{z}e^{kz'}\rho(z')dz'\right\}dz;$$

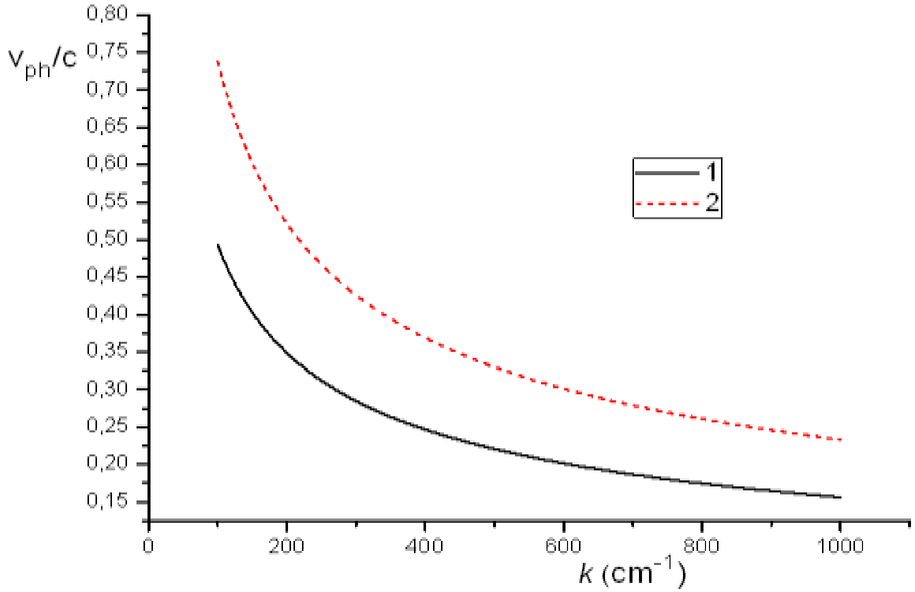
$$\rho(z)=\int\left|\phi(\vec{r}_{xy},z)\right|^2 d\vec{r}_{xy};$$

Results

1-LAYER GRAPHENE



Density of doped electrons 10^{12} cm^{-2}



Densities of doped electrons (1) 10^{12} cm^{-2} (2) $5\cdot10^{12}$ cm^{-2}

2-LAYER GRAPHENE DISPERSION EQUATION

- Considering system in long wave approximation the following equation can be obtained:

$$k \cdot r \to 0$$

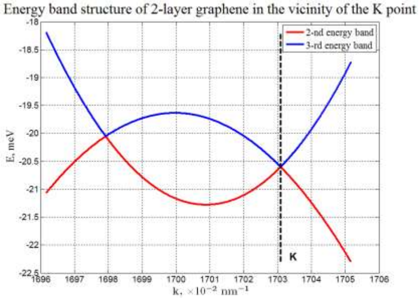
$$\left(1-\frac{2\pi e^2}{k}\Pi_1\right)\left(1-\frac{2\pi e^2}{k}\Pi_2\right)-\frac{4\pi^2 e^4}{k^2}\Pi_1\Pi_2\exp(-2kd)=0;$$

$$\Pi_i=\sum_{\vec{k}_2<k_F}\frac{1}{S}\left(\frac{1}{\hbar\omega+E_{(\vec{k}_2+\vec{k}),i}-E_{\vec{k}_2,i}}-\frac{1}{\hbar\omega+E_{\vec{k}_2,i}-E_{(\vec{k}_2+\vec{k}),i}}\right);$$

$$\Pi_i=\frac{\Gamma_i}{\omega^2};$$

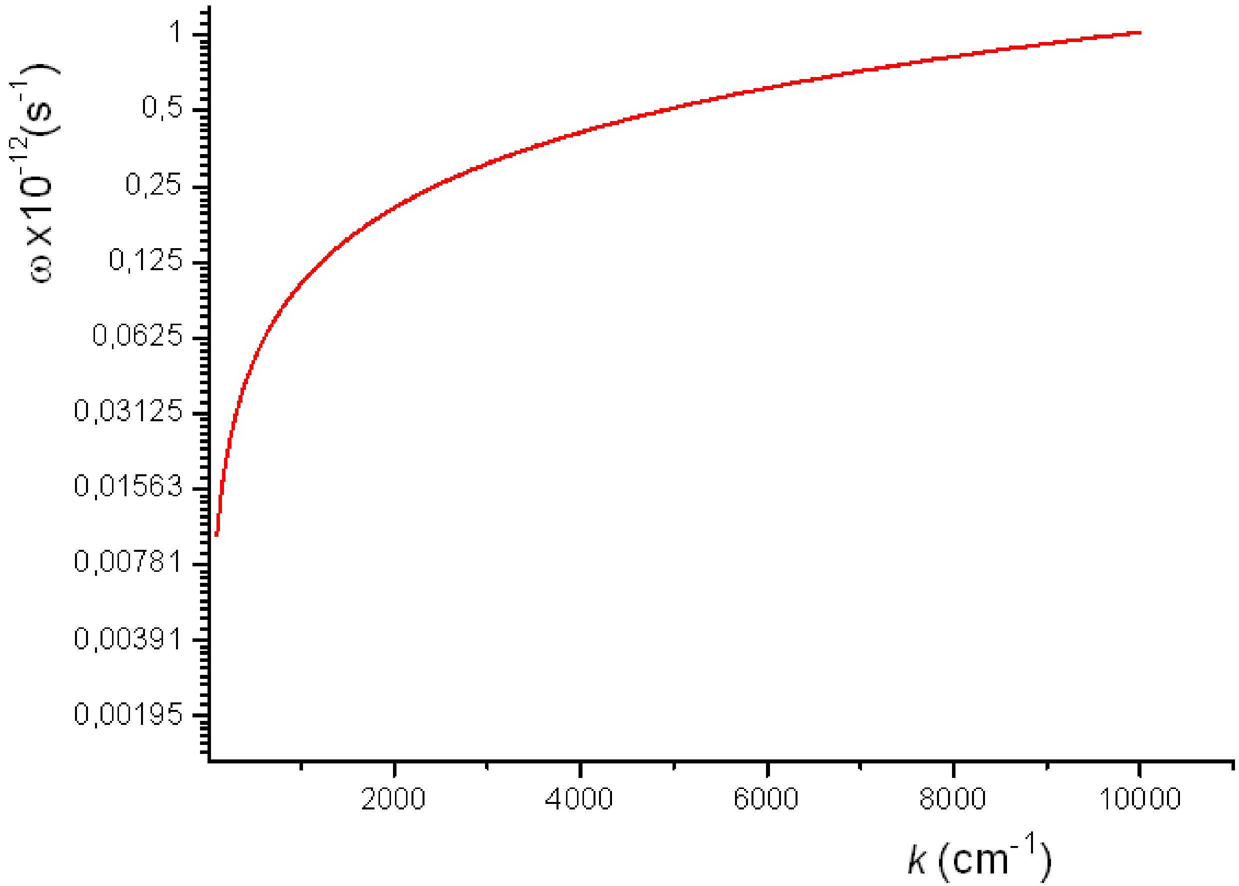
$$\omega_{1,2}^2=\frac{\Gamma_1+\Gamma_2}{2}\pm\sqrt{\left(\frac{\Gamma_1+\Gamma_2}{2}\right)^2-\Gamma_1\Gamma_2\left(1-\exp(-2kd)\right)};$$

Energy band structure of 2-layer graphene in the vicinity of the K point



Results

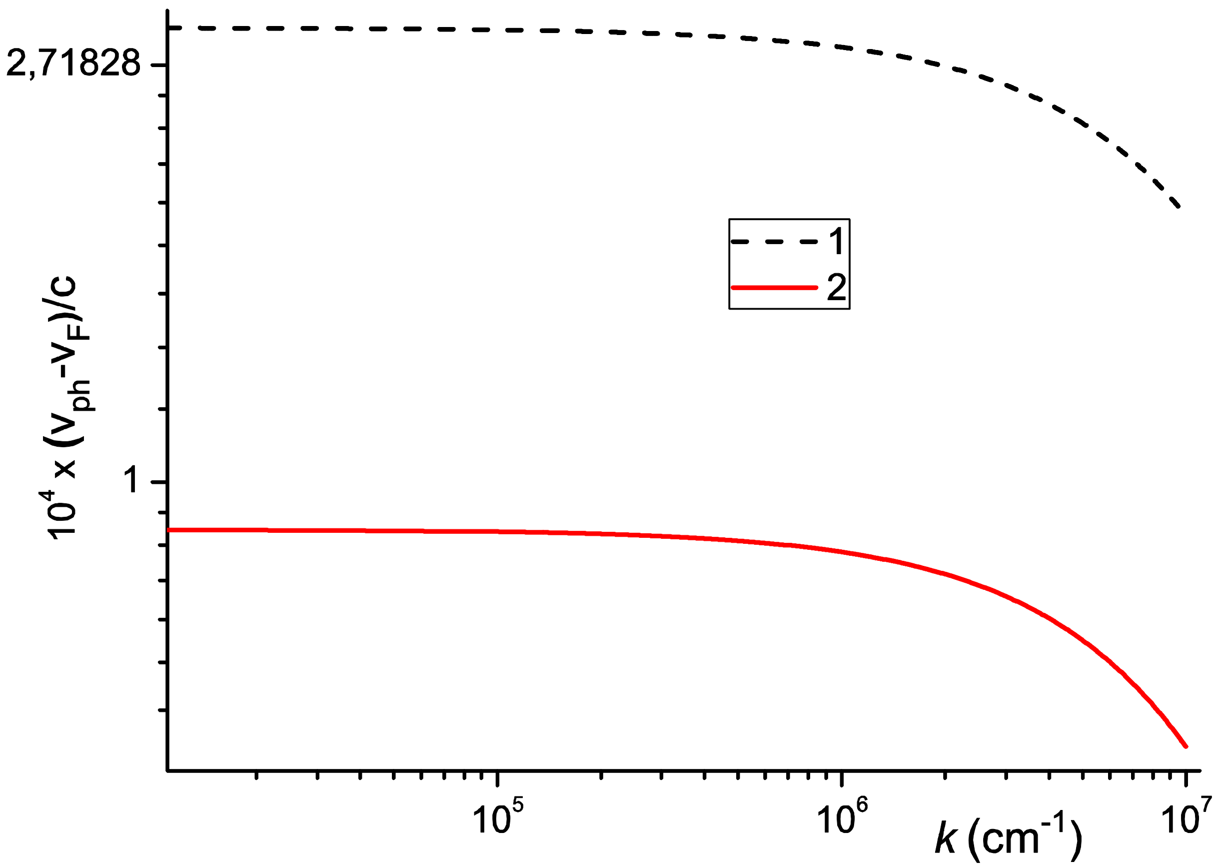
2-LAYER GRAPHENE



The plasmon frequency ω (1/s) vs. its wave vector k (1/cm) for 2-layer graphene.

Results

2-LAYER GRAPHENE



The deviation of plasmon phase velocity v_{ph} from the Fermi velocity v_F for 2-layer graphene: densities of electrons (1) 10^{12} cm^{-2} (2) $5 \cdot 10^{12}$ cm^{-2}

Conclusions

- In the double layer graphene nanoplates proximity of the electromagnetic wave phase velocity to the Fermi velocity in graphene v_F can be achieved.

- Double layer graphene nanoplates are promising candidates for the nano-sized Cherenkov-type terahertz emitters.

Thank you for attention