Efficient curvilinear coordinate method for grating diffraction simulation

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Plan

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Motivation

- Active research on control of light beams with metasurfaces
- Using 2D-materials in fabricating of metasurfaces (the most common material is graphene)
- EM wave-plasmon coupling

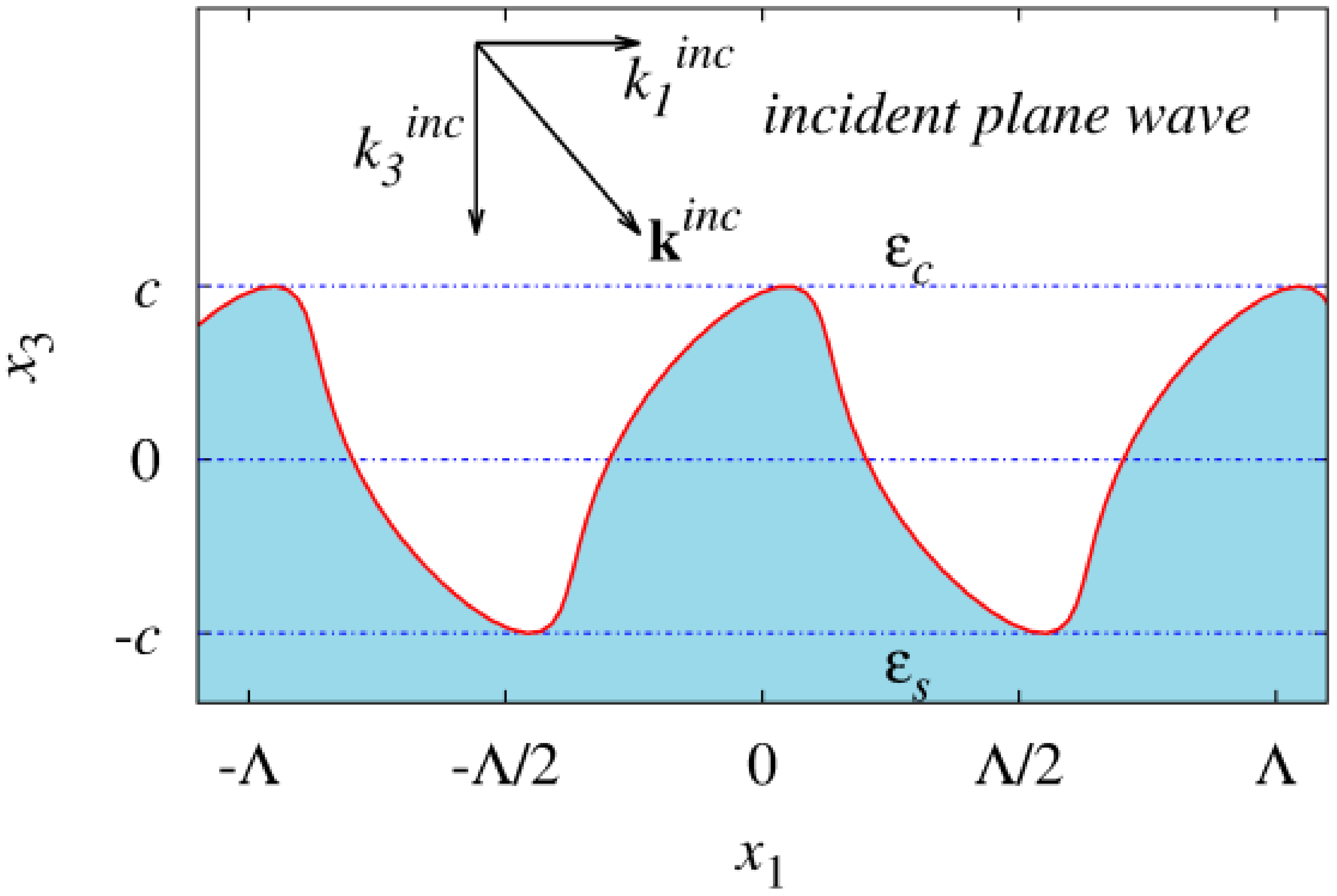
Formulation of the diffraction problem

A monochromatic plane wave with time factor $e^{-i\omega t}$ is incident on a periodically corrugated interface between two semi-infinite homogeneous media.

Diffraction is described by Maxwell's equations:

$$\xi^{\alpha\beta\gamma}\frac{\partial E_\gamma}{\partial x^\beta} = i\omega\mu g^{\alpha\beta} H_\beta$$

$$\xi^{\alpha\beta\gamma}\frac{\partial H_\gamma}{\partial x^\beta} = -i\omega\varepsilon g^{\alpha\beta} E_\beta$$



GSMCC

GSMCC [1] is a combination of two methods: GSM and C-method.

We introduce a curvilinear space in a grating region. At the same time one of curvilinear coordinate planes should coincide with corrugation interface. Therefore Maxwell's in new coordinates equations become:

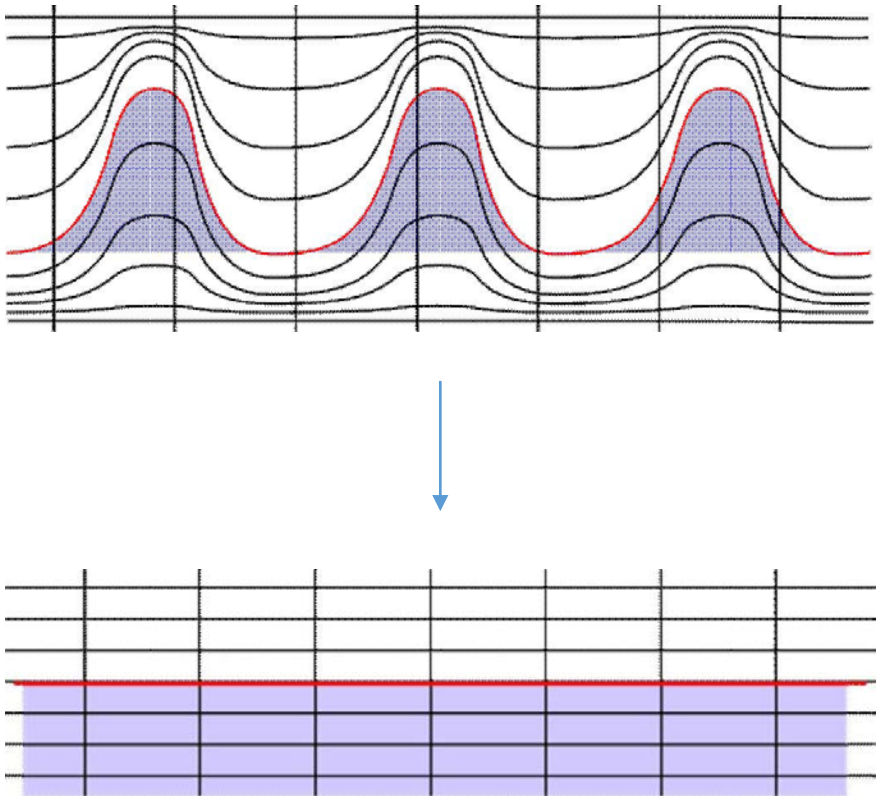
$$\xi^{\tau\vartheta\theta}\tilde{\nabla}_{\vartheta}\tilde{E}_{\theta} = -M^{\alpha} + i\omega\mu_b g^{\alpha\beta}\tilde{H}_{\beta}$$

$$\xi^{\tau\vartheta\theta}\tilde{\nabla}_{\vartheta}\tilde{H}_{\theta} = J^{\alpha} - i\omega\varepsilon_b g^{\alpha\beta}\tilde{E}_{\beta}$$

Where generalized metric sources are described as:

$$J^{\alpha} = -i\omega\varepsilon_b\left(\frac{\varepsilon}{\varepsilon_b}\sqrt{\tilde{g}}\tilde{g}^{\alpha\beta} - g^{\alpha\beta}\right)\tilde{E}_{\beta}$$

$$M^{\alpha} = -i\omega\mu_b\left(\sqrt{\tilde{g}}\tilde{g}^{\alpha\beta} - g^{\alpha\beta}\right)\tilde{H}_{\beta}$$



1. The whole development of GSMCC was made in [1].

GSMCC

Further we consider Fourier-space reciprocal to $\tilde{x}^1$ and $\tilde{x}^2$. After solving wave-equation we get integral representation for E and H. Considering expression in Fourier-space reciprocal to $\tilde{x}^3$, we get modal representation $\begin{pmatrix} \tilde{E}_m \\ \tilde{H}_m \end{pmatrix}$. Then we reduce size of system $\begin{pmatrix} \tilde{E}_m \\ \tilde{H}_m \end{pmatrix} = Q_m \begin{pmatrix} \tilde{a}_m^e \\ \tilde{a}_m^h \end{pmatrix}$.

Numerical solution may be obtained by limiting number of modes from $-\frac{N_O}{2}$ to $\frac{N_O}{2}$ and replacing integral by a finite sum. Finally we get a discretized equation for amplitudes: $a^{out} = a^{inc} + TPVQ(I - RPVQ)^{-1} a^{inc}$. An accurate definition of R, P, V, Q and T matrixes may be found in [1]. Thus, the complexity of the method is defined by complexity of matrix inversion in discretized equation.

Solution with graphene layer

A graphene monolayer adds current into Maxwell's equations:

$$\xi^{\alpha\beta\gamma}\frac{\partial H_\gamma}{\partial x^\beta} = -i\omega\varepsilon g^{\alpha\beta}E_\beta + g^{\alpha\beta}j_\beta$$

Transformed Maxwell's equations:

$$\xi^{\tau\vartheta\theta}\tilde{\nabla}_\vartheta\widetilde{H}_\theta = \sqrt{\tilde{g}}\tilde{g}^{\tau\beta}\left(\tilde{j}_\beta - i\omega\varepsilon\tilde{E}_\beta\right)$$

Let us find relations between $\tilde{j}_\beta$ and $\tilde{E}_\beta$:

$$\begin{cases} j_2 = -j_\beta = \sigma(\omega)\delta(\tilde{x}_3)E_2^a \\ j_\tau = \sigma(\omega)\delta(\tilde{x}_3)E_\tau \end{cases}$$ - 2

$$E_\tau = \frac{1}{\sqrt{1+(f')^2}}\tilde{E}_1^a$$

$$\begin{cases} j_1 = \dfrac{j_\tau}{\sqrt{1+(f')^2}} \\ j_3 = \dfrac{j_\tau}{\sqrt{1+(f')^2}}f' \end{cases}$$

$$\begin{cases} \tilde{j}_1 = \sigma(\omega)\delta(\tilde{x}_3)\tilde{E}_1^a \\ \tilde{j}_2 = \sigma(\omega)\delta(\tilde{x}_3)\tilde{E}_2^a \\ \tilde{j}_3 = \sigma(\omega)\delta(\tilde{x}_3)\dfrac{f'}{1+(f')^2}\tilde{E}_1^a \end{cases}$$

2. The expression for current and conductance in a graphene monolayer is derived in [3].

Solution with graphene layer

Thus, we get:

$$\tilde{j}_\alpha = \sigma(\omega)\delta(\tilde{x}_3){K_\alpha}^\beta \tilde{E}^a_\beta, \text{ where } {K_\alpha}^\beta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{f'}{1+(f')^2} & 0 & 0 \end{pmatrix}$$

Substitution current into the second Maxwell's equation provides us with:

$$\xi^{\alpha\beta\gamma}\tilde{\nabla}_\beta \tilde{H}_\gamma = \tilde{\varepsilon}^{\alpha\gamma}\tilde{E}_\gamma, \text{ where } \tilde{\varepsilon}^{\alpha\gamma} = \sqrt{\tilde{g}}\,\tilde{g}^{\alpha\beta}\left(\sigma(\omega)\delta(\tilde{x}_3){K_\beta}^\gamma - i\omega\varepsilon\delta^\gamma_\beta\right)$$

Explicit form of $\tilde{\varepsilon}^{\alpha\gamma}$:

$$\tilde{\varepsilon}^{\alpha\gamma} = \sqrt{1+2(f')^2}\begin{pmatrix} \frac{\sigma(\omega)\delta(\tilde{x}_3)}{1+(f')^2} - i\omega\varepsilon & 0 & 0 \\ 0 & \sigma(\omega)\delta(\tilde{x}_3) - i\omega\varepsilon & 0 \\ 0 & 0 & -i\omega\varepsilon \end{pmatrix}$$

Solution with graphene layer

Let's consider modes of EM wave with TM polarization under the surface (derivation is the same above the surface):

$$\widetilde{H}_{2q} = b_q^{\pm} \exp\left(i\psi_q^b(\tilde{x}_1) \pm i\beta_q^b \tilde{x}_3\right)$$

$\widetilde{H}_{2q}(\tilde{x}_1 + \Lambda) = \widetilde{H}_{2q}(\tilde{x}_1) e^{ik_1^{inc}\Lambda}$ - quasi-periodicity condition.

Substitution of magnetic field into the Maxwell's equation provides us with expression for E and differential equation on phase distribution $\psi_q^b(\tilde{x}_1)$, which can be solved [3].

Dispersion equations follow from quasi-periodicity condition:

$$\beta_q^b = \sqrt{\omega^2 \varepsilon_b \mu_b - k_{1q}^2}, k_{1q} = k_1^{inc} + \frac{2\pi q}{\Lambda}$$

3. Detailed solution of this equation can be found in [2].

Solution with graphene layer

Finally, we get these expressions for E and H:

$$\widetilde{H}_{2q}^{c} = c_q^{+} exp\left[ik_{1q} + i\beta_q^c[\tilde{x}_3 + f(\tilde{x}_1)]\right] + c_q^{-} exp\left[ik_{1q} - i\beta_q^c[\tilde{x}_3 + f(\tilde{x}_1)]\right]$$

$$\tilde{E}_{1q}^{c} = \frac{k_{1q}f'(\tilde{x}_1) - \beta_q^c}{\omega\varepsilon_c} c_q^{+} exp\left[ik_{1q} + i\beta_q^c[\tilde{x}_3 + f(\tilde{x}_1)]\right]$$

$$+ \frac{k_{1q}f'^{(\tilde{x}_1)} + \beta_q^c}{\omega\varepsilon_c} c_q^{-} exp\left[ik_{1q} - i\beta_q^c[\tilde{x}_3 + f(\tilde{x}_1)]\right]$$

Let’s assume this denotations:

$$A_q^{\pm} = exp\left[ik_{1q}\tilde{x}_1 \pm i\beta_q^a[\tilde{x}_3 + f(\tilde{x}_1)]\right], B_q^{\pm} = exp\left[ik_{1q}\tilde{x}_1 \pm i\beta_q^b[\tilde{x}_3 + f(\tilde{x}_1)]\right]$$

$$\frac{\beta_q^a \pm k_{1q}f'(\tilde{x}_1)}{\omega\varepsilon_a} = f_q^{\pm}, \frac{\beta_q^b \pm k_{1q}f'(\tilde{x}_1)}{\omega\varepsilon_b} = g_q^{\pm}$$

Solution with graphene layer

Boundary conditions:

$\tilde{E}_1^a\big|_{\tilde{x}_3=0} = \tilde{E}_1^b\big|_{\tilde{x}_3=0}$ – continuity of $\tilde{\mathrm{E}}_1$ (tangent) component.

$\tilde{H}_2^a\big|_{\tilde{x}_3=0} - \tilde{H}_2^b\Big|_{\tilde{x}_3=0} = \frac{4\pi}{c}\int_{-0}^{+0} \tilde{j}^1\, d\tilde{x}_3$ – jump of $\tilde{\mathrm{H}}_2$ (tangent) component.

After substitution of modal representation for the EM-wave they transform to:

$$\sum_{q=-\infty}^{\infty}\left(\frac{1}{\varepsilon_a}\left[-f_q^- a_q^+ A_q^+ + f_q^+ a_q^- A_q^-\right] - \frac{1}{\varepsilon_b}\left[-g_q^- b_q^+ B_q^+ + g_q^+ b_q^- B_q^-\right]\right)\Bigg|_{\tilde{x}_3=0} = 0$$

$$\sum_{q=-\infty}^{\infty}\left(a_q^+ A_q^+ + a_q^- A_q^- - b_q^+ B_q^+ - b_q^- B_q^-\right)\Bigg|_{\tilde{x}_3=0} = \frac{4\pi\sigma(\omega)}{c}\left(\frac{E_\tau}{\sqrt{1+(f')^2}}\right)\Bigg|_{\tilde{x}_3=0}$$

Solution with graphene layer

Multiplying:

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda} \left\{ \frac{\varepsilon_b}{\varepsilon_a} \left[-f_q^- a_q^+ A_q^+ B_p^+ + f_q^+ a_q^- A_q^- B_p^+ \right] - \left[-g_q^- b_q^+ B_q^+ B_p^+ + g_q^+ b_q^- B_q^- B_p^+ \right] \right\} \Bigg|_{\tilde{x}_3=0} = 0$$

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda} \left\{ \left[g_p^- a_q^+ A_q^+ B_p^+ + g_p^- a_q^- A_q^- B_p^+ \right] - \left[g_p^- b_q^+ B_q^+ B_p^+ + g_p^- b_q^- B_q^- B_p^+ \right] \right\} \Bigg|_{\tilde{x}_3=0} = \frac{4\pi\sigma(\omega)}{c} \frac{g_p^- B_p^+}{2\beta_p^b \Lambda} \left(\frac{E_\tau}{\sqrt{1+(f')^2}} \right) \Bigg|_{\tilde{x}_3=0}$$

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda} \left\{ \frac{\varepsilon_b}{\varepsilon_a} \left[-f_q^- a_q^+ A_q^+ B_p^- + f_q^+ a_q^- A_q^- B_p^- \right] - \left[-g_q^- b_q^+ B_q^+ B_p^- + g_q^+ b_q^- B_q^- B_p^- \right] \right\} \Bigg|_{\tilde{x}_3=0} = 0$$

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda} \left\{ \left[g_p^+ a_q^+ A_q^+ B_p^- + g_p^+ a_q^- A_q^- B_p^- \right] - \left[g_p^+ b_q^+ B_q^+ B_p^- + g_p^+ b_q^- B_q^- B_p^- \right] \right\} \Bigg|_{\tilde{x}_3=0} = \frac{4\pi\sigma(\omega)}{c} \frac{g_p^+ B_p^-}{2\beta_p^b \Lambda} \left(\frac{E_\tau}{\sqrt{1+(f')^2}} \right) \Bigg|_{\tilde{x}_3=0}$$

Solution with graphene layer

Combining:

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda}\left(\left\{\frac{\varepsilon_b}{\varepsilon_a}\left[-f_q^- a_q^+ \frac{A_q^+}{B_p^+} + f_q^+ a_q^- \frac{A_q^-}{B_p^+}\right] - \left[\left(g_p^- - g_q^-\right) b_q^+ \frac{B_q^+}{B_p^+} + \left(g_p^- + g_q^+\right) b_q^- \frac{B_q^-}{B_p^+}\right]\right\} + \left[g_p^- a_q^+ \frac{A_q^+}{B_p^+} + g_p^- a_q^- \frac{A_q^-}{B_p^+}\right]\right)\Bigg|_{\tilde{x}_3=0} = \frac{4\pi\sigma(\omega)}{c}\frac{g_p^-}{2\beta_p^b \Lambda B_p^+}\left(\frac{E_\tau}{\sqrt{1+(f')^2}}\right)\Bigg|_{\tilde{x}_3=0}$$

– sum of 1 and 2.

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda}\left\{\frac{\varepsilon_b}{\varepsilon_a}\left[-f_q^- a_q^+ \frac{A_q^+}{B_p^+} + f_q^+ a_q^- \frac{A_q^-}{B_p^+}\right] + \left[\left(g_p^- + g_q^-\right) b_q^+ \frac{B_q^+}{B_p^+} + \left(g_p^- - g_q^+\right) b_q^- \frac{B_q^-}{B_p^+}\right] - \left[g_p^- a_q^+ \frac{A_q^+}{B_p^+} + g_p^- a_q^- \frac{A_q^-}{B_p^+}\right]\right\}\Bigg|_{\tilde{x}_3=0} = -\frac{4\pi\sigma(\omega)}{c}\frac{g_p^-}{2\beta_p^b \Lambda B_p^+}\left(\frac{E_\tau}{\sqrt{1+(f')^2}}\right)\Bigg|_{\tilde{x}_3=0}$$

– difference between 1 and 2.

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda}\left(\left\{\frac{\varepsilon_b}{\varepsilon_a}\left[-f_q^- a_q^+ \frac{A_q^+}{B_p^-} + f_q^+ a_q^- \frac{A_q^-}{B_p^-}\right] - \left[\left(g_p^+ - g_q^-\right) b_q^+ \frac{B_q^+}{B_p^-} + \left(g_p^+ + g_q^+\right) b_q^- \frac{B_q^-}{B_p^-}\right]\right\} + \left[g_p^+ a_q^+ \frac{A_q^+}{B_p^-} + g_p^+ a_q^- \frac{A_q^-}{B_p^-}\right]\right)\Bigg|_{\tilde{x}_3=0} = \frac{4\pi\sigma(\omega)}{c}\frac{g_p^+}{2\beta_p^b \Lambda B_p^-}\left(\frac{E_\tau}{\sqrt{1+(f')^2}}\right)\Bigg|_{\tilde{x}_3=0}$$

– sum of 3 and 4.

$$\sum_{q=-\infty}^{\infty} \frac{1}{2\beta_p^b \Lambda}\left\{\frac{\varepsilon_b}{\varepsilon_a}\left[-f_q^- a_q^+ \frac{A_q^+}{B_p^-} + f_q^+ a_q^- \frac{A_q^-}{B_p^-}\right] + \left[\left(g_p^+ + g_q^-\right) b_q^+ \frac{B_q^+}{B_p^-} + \left(g_p^+ - g_q^+\right) b_q^- \frac{B_q^-}{B_p^-}\right] - \left[g_p^+ a_q^+ \frac{A_q^+}{B_p^-} + g_p^+ a_q^- \frac{A_q^-}{B_p^-}\right]\right\}\Bigg|_{\tilde{x}_3=0} = -\frac{4\pi\sigma(\omega)}{c}\frac{g_p^+}{2\beta_p^b \Lambda B_p^-}\left(\frac{E_\tau}{\sqrt{1+(f')^2}}\right)\Bigg|_{\tilde{x}_3=0}$$

– difference between 3 and 4.

Solution with graphene layer

Normalizing (the same relations are right for b-modes) [4]:

$$\frac{1}{\Lambda}\int_{0}^{\Lambda}\left(f_q^{\mp}+f_p^{\mp}\right)\frac{A_q^{\pm}}{A_p^{\pm}}\bigg|_{\tilde{x}_3=0} d\tilde{x}_1 = 2\beta_p^a\delta_{pq}$$

$$\frac{1}{\Lambda}\int_{0}^{\Lambda}\left(f_p^{\pm}-f_q^{\mp}\right)\frac{A_q^{\pm}}{A_p^{\mp}}\bigg|_{\tilde{x}_3=0} d\tilde{x}_1 = 0$$

Integrating over the period of the structure:

$$b_p^{+} = \frac{1}{2\beta_p^b\Lambda}\int_0^{\Lambda}\left(\sum_{q=-\infty}^{\infty}\left\{\left(g_p^{-}+\frac{\varepsilon_b}{\varepsilon_a}f_q^{-}+\frac{4\pi\sigma(\omega)}{c(1+(f')^2)}g_p^{-}f_q^{-}\right)a_q^{+}\frac{A_q^{+}}{B_p^{+}}+\left(g_p^{-}-\frac{\varepsilon_b}{\varepsilon_a}f_q^{+}-\frac{4\pi\sigma(\omega)}{c(1+(f')^2)}g_p^{-}f_q^{+}\right)a_q^{-}\frac{A_q^{-}}{B_p^{+}}\right\}\Bigg|_{\tilde{x}_3=0}\right)d\tilde{x}_1$$

$$b_q^{-} = \frac{1}{2\beta_p^b\Lambda}\int_0^{\Lambda}\left(\sum_{q=-\infty}^{\infty}\left\{\left(g_p^{+}-\frac{\varepsilon_b}{\varepsilon_a}f_q^{-}+\frac{4\pi\sigma(\omega)}{c(1+(f')^2)}g_p^{+}f_q^{-}\right)a_q^{+}\frac{A_q^{+}}{B_p^{-}}+\left(g_p^{+}+\frac{\varepsilon_b}{\varepsilon_a}f_q^{+}-\frac{4\pi\sigma(\omega)}{c(1+(f')^2)}g_p^{+}f_q^{+}\right)a_q^{-}\frac{A_q^{-}}{B_p^{-}}\right\}\Bigg|_{\tilde{x}_3=0}\right)d\tilde{x}_1$$

4. Normalizing is approved in appendix of [2].

Plans for the future

- Consider EM-wave-plasmon coupling and enhanced anomalous transmission effect
- Conduct an experiment with a graphene-metal structure and compare numerical and experimental results

References

1. «Efficient curvilinear coordinate method for grating diffraction simulation», Optics Express 21(21), 25236-47 (2013)
2. «General analytical solution for the electromagnetic grating diffraction problem», Optics Express 25(12), 13435-13447 (2017)
3. «Optical far-infrared properties of a graphene monolayer and multilayer», Physical review. B, Condensed matter 76(15), (2007)