BEHAVIOUR OF SPP WAVES FREQUENCY SPECTRUM FOR DIELECTRIC/METAL/DIELECTRIC STRUCTURES

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Introduction

Agenda

- Goals and current achievements
- Problem formulation and mathematical model
- Simulation results
- Conclusions

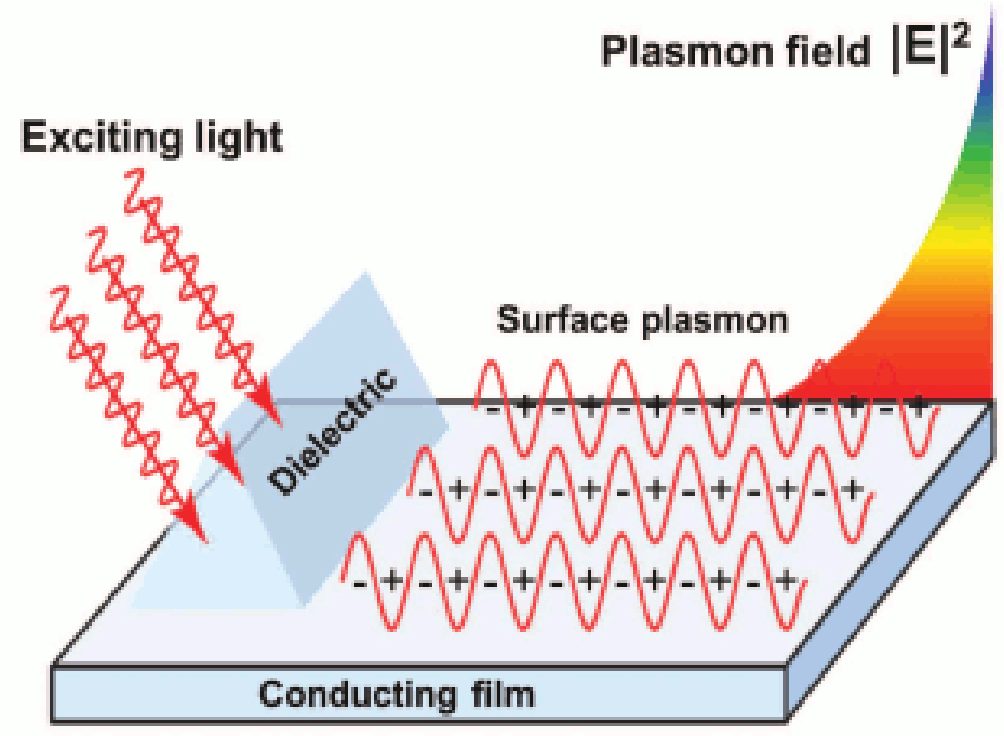

Fig 1. Plasmon wave propagation scheme [2].

[1] S. Maier., “Plasmonics: Fundamentals and Application.,” Springer - Verlag, 2007;
J. Jackson, “Classical Electrodynamics.”, John Wiley & Sons, 2007.
[2] D. V. Sotnikov, A. V. Zherdev, B. B. Dzantiev, 2015, published in Uspekhi Biologicheskoi Khimii, 2015, Vol. 55, pp. 391-420.

Problem formulation

System of Maxwell's equations [1]:

$$div\vec{D} = \vec{\rho},\ div\vec{B} = 0,$$

$$rot\vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J},\ rot\vec{E} = \frac{\partial \vec{B}}{\partial t}. \quad (1)$$

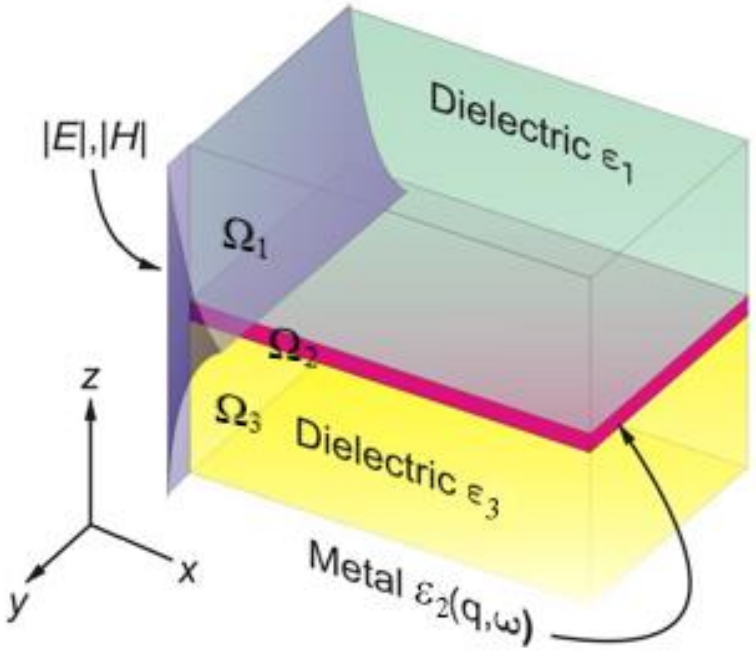

Fig 2. Dielectric/metal/dielectric structure [3].

Non-local dependence [1]:

$$\vec{D}(\vec{r},t) = \int_{\Omega} d\vec{r}' \int_{t} dt' \varepsilon(\vec{r},\vec{r}',t-t')\vec{E}(\vec{r}',t'). \quad (2)$$

[1] S. Maier., “Plasmonics: Fundamentals and Application.,” Springer - Verlag, 2007;
J. Jackson, “Classical Electrodynamics.”, John Wiley & Sons, 2007.
[3] P. Kostrobij, V. Polovyi et al, Math. Model. Comput. Vol. 5, No. 2, pp. 184-192 (2018).

Wave equations for TM-mode

$$\vec{H} = \left(0, H_y, 0\right),\ \vec{E} = \left(E_x, 0, E_z\right),$$
$$\vec{H} = H\left(z\right)\mathrm{e}^{ik_x x}\mathrm{e}^{-i\omega t}. \qquad (3)$$

TM polarization [1]

Wave equations in different domains

$$\frac{\partial^2 H_y}{\partial z^2} + \left(k_0^2 \varepsilon_1\left(\omega\right) - k_x\right) H_y = 0, \quad z < -L/2,$$
$$\frac{\partial^2 H_y}{\partial z^2} + \left(k_0^2 \varepsilon_2\left(\omega, z\right) - k_x\right) H_y = 0, \quad -L/2 < z < L/2, \qquad (4)$$
$$\frac{\partial^2 H_y}{\partial z^2} + \left(k_0^2 \varepsilon_3\left(\omega\right) - k_x\right) H_y = 0, \quad z > L/2.$$

[1] S. Maier., “Plasmonics: Fundamentals and Application.,” Springer - Verlag, 2007;
J. Jackson, “Classical Electrodynamics.”, John Wiley & Sons, 2007.

Dielectric function

Diagonal component of the dielectric tensor [4]:

$$\varepsilon\left(\omega,\vec{r},\vec{r}'\right)=\left(1-\frac{\omega_p^2}{n_e\omega^2}\sum_{n=1}^{n_{\max}} f_n\left|\varphi_n\left(\vec{r}'\right)\right|^2\right)\delta\left(\vec{r}-\vec{r}'\right), \quad (5.1)$$

$$\varphi\left(x,y,z\right)=\sqrt{\frac{2}{S}}e^{ik_x}e^{ik_y}\varphi_{II,n}\left(z\right). \quad (5.2)$$

$$f_n=1, \quad \vec{r}=\left(x,y,z\right).$$

Dielectric function of a metal film:

$$\varepsilon_2\left(\omega,L\right)=1-\frac{\omega_p^2}{2\pi n_e\omega^2}\sum_{i=1}^{n_{\max}}\left(k_F^2-k_i^2\right)\left|\overline{\varphi}_{II,i}\left(L\right)\right|^2. \quad (6)$$

l - the width of the potential well

[4] V. P. Kurbatsky, “Dielectric tensor of low-dimensional metal systems”, J. Exp. Theor. Phys, pp. 148–158, 2017.

Model: bound states and dispersion relation

Dispersion relation [1]:

$$e^{-4k_1 L/2} = \frac{k_1/\varepsilon_1 - k_2/\varepsilon_2}{k_1/\varepsilon_1 + k_2/\varepsilon_2} \cdot \frac{k_3/\varepsilon_3 - k_2/\varepsilon_2}{k_3/\varepsilon_3 + k_2/\varepsilon_2},$$

$$k_i = \sqrt{k_x^2 - k_0^2 \varepsilon_i}, \quad k_0 = \omega/c, \qquad (7)$$

Energy levels and quantum numbers:

$$\alpha_n = \frac{\pi n}{l}, \; n = 1, 2, \ldots, n_{\max}.$$

$$n_{\max} = \left[\frac{l k_F}{\pi} \right]. \qquad (8)$$

The width of the potential well for a system of interacting electrons:

$$l = l_{slab} + 2d,$$

$$d = \frac{3\pi}{8k_F} + \frac{\pi^2}{8k_F^2 l} \text{ [5]}. \qquad k_F = \frac{\sqrt{2m\mu}}{\hbar}, \qquad (9)$$

μ - chemical potential for the system of interacting electrons.

[1] S. Maier., “Plasmonics: Fundamentals and Application.,” Springer - Verlag, 2007; J. Jackson, “Classical Electrodynamics.”, John Wiley & Sons, 2007.
[5] Kostrobij P. P., Markovych B. M. Effect of Coulomb interaction on chemical potential of metal film. Philosophical Magazine. 98 (21), (2018).

Results: frequency spectrum for *SiO2/Ag/Si*

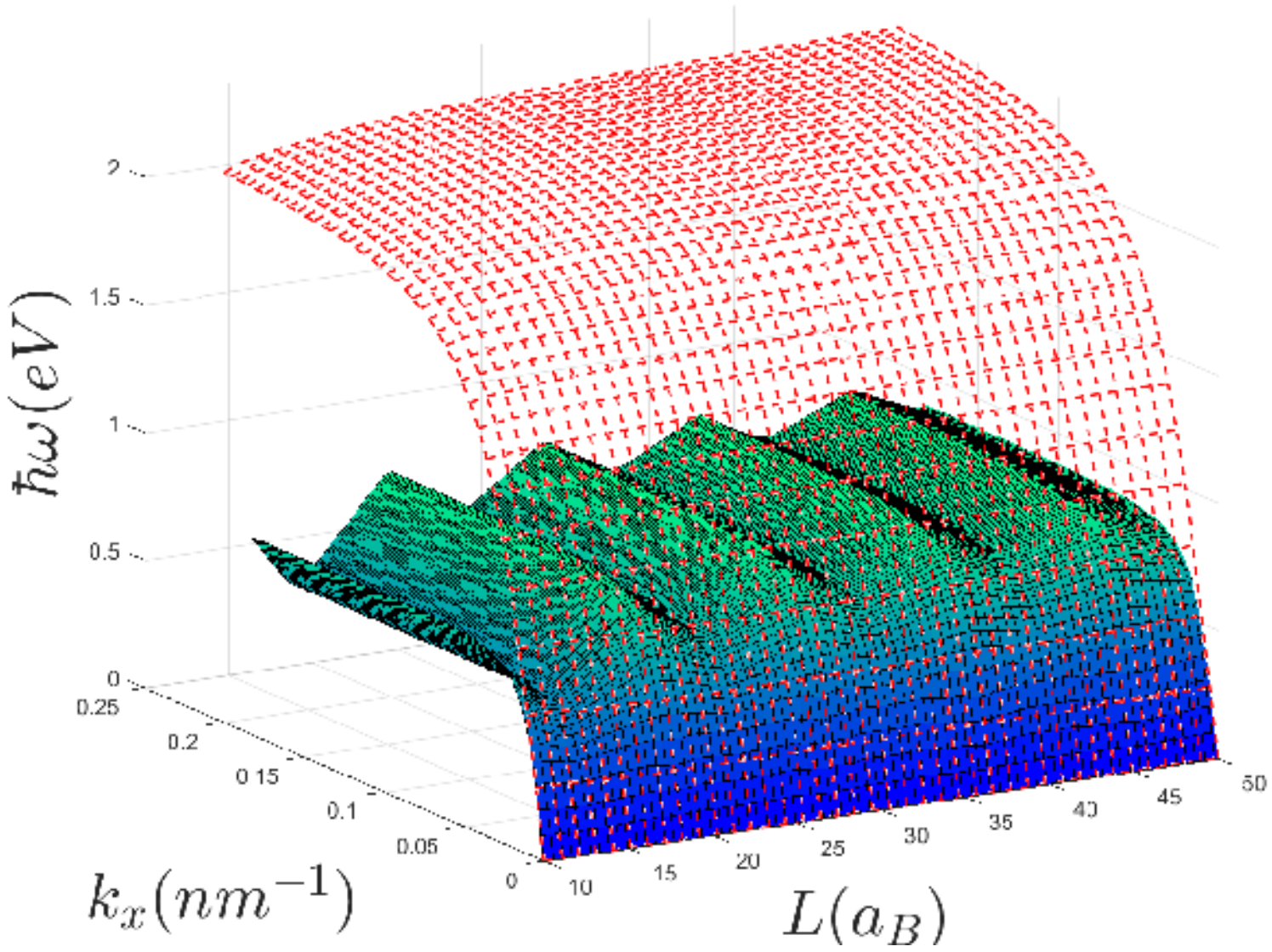

Fig 3. Blue lines - considering the Coulomb correlation, red - without.

Results: frequency spectrum for *SiO2/Ag/Si*

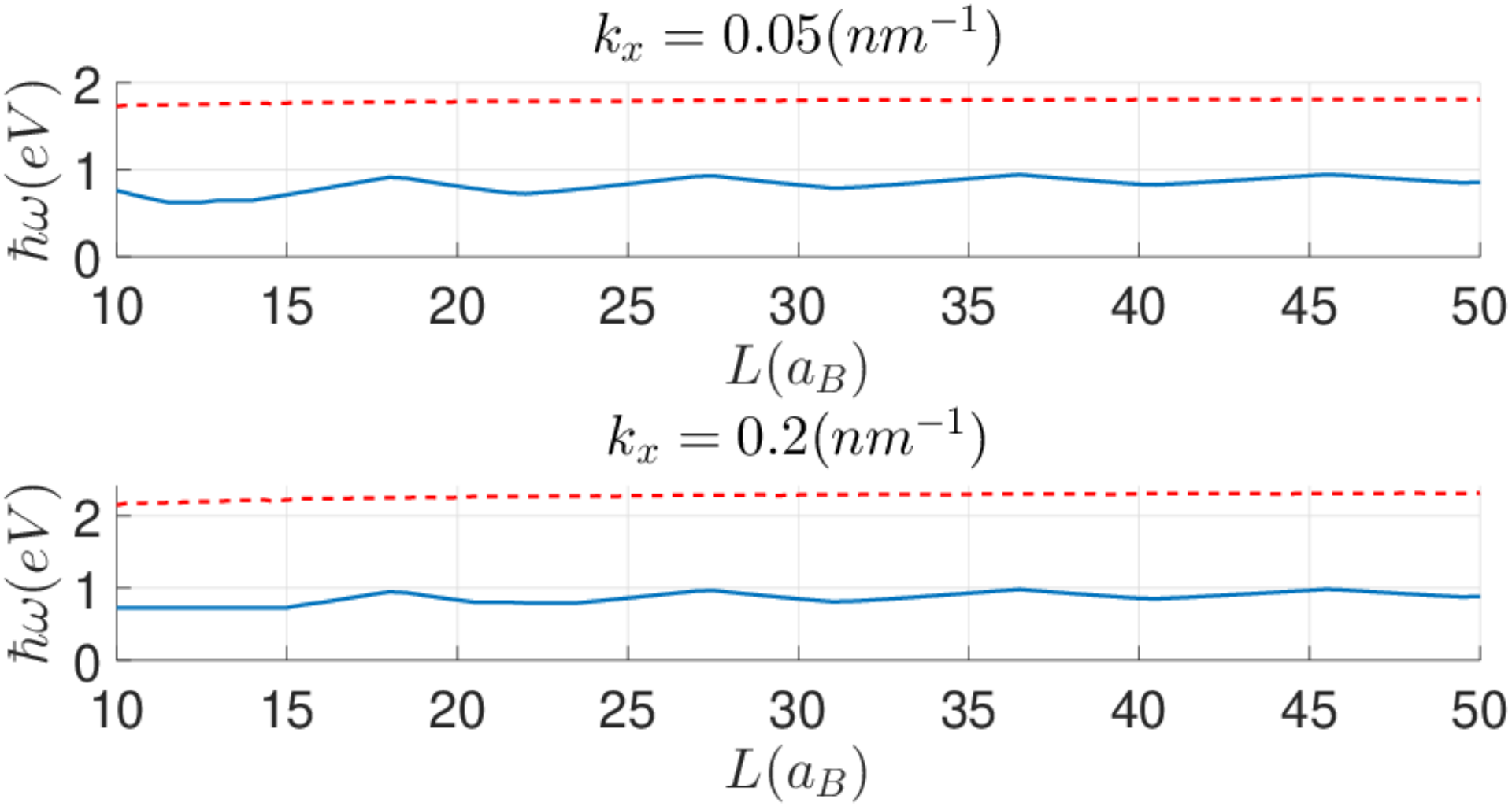

Fig 4. Blue lines - considering the Coulomb correlation, red - without.

Results: frequency spectrum for *SiO2/Ag/Si* comparison with the experiment

$k_x \approx 0.028nm^{-1}$				$k_x \approx 0.049nm^{-1}$			
k_x	**(a)**	**(b)**	**(e)**	k_x	**(a)**	**(b)**	**(e)**
0.0278	0.696	1.288	0.62	0.0487	0.889	1.784	0.8

Tab. 1. (a) – considering the Coulomb correlation, (b) – without, (c) – experiment.

Results: frequency spectrum for *SiO2/Ag/Si*

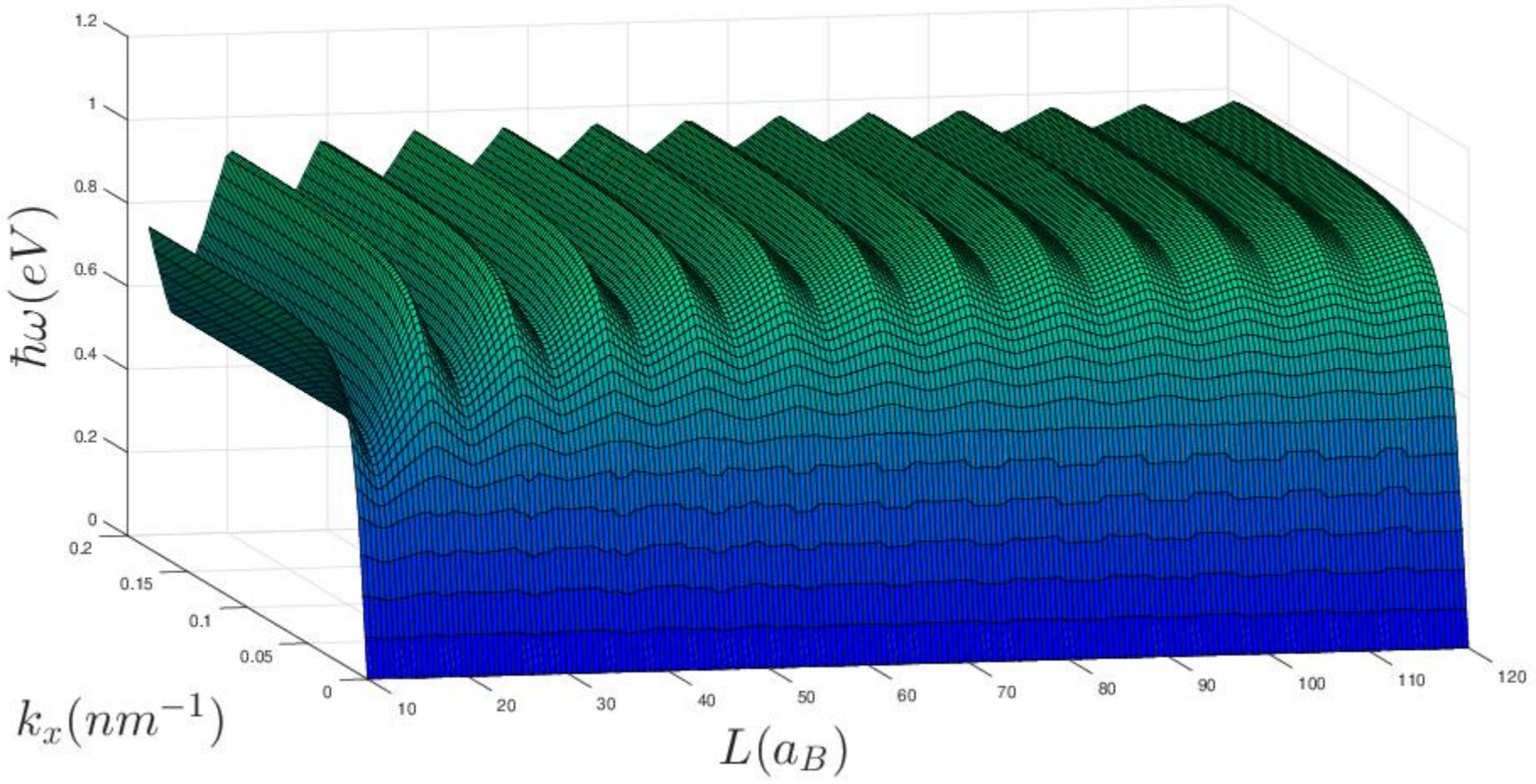

Fig 5. Blue lines - considering Coulomb correlations.

Results: what about asymmetric potential well of a finite depth?

Ansatz:

$K = \frac{k_F}{k_F^0}$ - model coefficient. (10)

k_F^0 - Fermi wave vector in the finite well w/o Coulomb correlations [5].

Energy levels:

$$\alpha L = \pi n - \left(\arcsin\frac{\alpha}{s_1} + \arcsin\frac{\alpha}{s_2} \right),\ n = 1, 2, \ldots, n_{\max}.$$

$$U_\alpha = \alpha^2\hbar^2 / 2m, \quad s_i = \frac{\sqrt{2mW_i}}{\hbar},\ i = 1, 2. \quad (11)$$

W_i - electron work function of dielectrics.

Number of bound states (energy levels):

$$n_{\max} = \left[\frac{1}{\pi} \left(L \min(s_1, s_2) + \arcsin\frac{\min(s_1, s_2)}{s_1} + \arcsin\frac{\min(s_1, s_2)}{s_2} \right) \right]. \quad (12)$$

Results: what about asymmetric potential well of a finite depth?

Wave vector	w/o Coulomb	with Coulomb	Diff
0,006826619	0,336062257	0,336732637	-0,00067038
0,009102159	0,417619227	0,418923173	-0,001303946
0,011377698	0,482458367	0,484491972	-0,002033605
0,013653238	0,533014478	0,535781158	-0,00276668
0,015928778	0,572160605	0,575605273	-0,003444668
0,018204317	0,602518939	0,606560715	-0,004041776
0,020479857	0,626221036	0,630774436	-0,0045534
0,022755397	0,644903193	0,64988884	-0,004985647
0,025030937	0,659787984	0,665136696	-0,005348712
0,027306476	0,671779534	0,677432962	-0,005653428
0,029582016	0,681545992	0,687455732	-0,00590974
0,031857556	0,689583451	0,695709643	-0,006126192
0,034133095	0,696263099	0,702572986	-0,006309887

Tab. 2a. – comparation for $l_{slab} = 10\ Bohr\ rad$.

Wave vector	w/o Coulomb	with Coulomb	Diff
0,006826619	0,342163	0,3412441	0,0009189
0,009102159	0,4296499	0,4278141	0,0018358
0,011377698	0,5014816	0,4985405	0,0029411
0,013653238	0,5592256	0,555124	0,0041016
0,015928778	0,6051573	0,5999293	0,005228
0,018204317	0,6415978	0,6352628	0,006335
0,020479857	0,670588	0,663457	0,007131
0,022755397	0,6937918	0,6858863	0,0079055
0,025030937	0,7125119	0,7039437	0,0085682
0,027306476	0,7277484	0,7186153	0,0091331
0,029582016	0,7402623	0,7306482	0,0096141
0,031857556	0,7506326	0,7406081	0,0100245
0,034133095	0,7593011	0,7489252	0,0103759

Tab. 2b. – comparation for $l_{slab} = 25\ Bohr\ rad$.

Conclusions

- Even a rather "rough" consideration of Coulomb correlations, namely, their influence on the chemical potential leads to significant changes in the frequency spectrum of SPPs in comparison with the classical approach and the correct consideration of electroneutrality in a non-interacting electronic system.
- The oscillatory spectrum pattern with increasing film thickness becomes less visible.
- Taking into account the Coulomb interaction leads to a significant improvement in the correlation of theoretical and experimental results.

References

- [1] S. Maier., “Plasmonics: Fundamentals and Application.,” Springer - Verlag, 2007; J. Jackson, “Classical Electrodynamics.”, John Wiley & Sons, 2007.
- [2] D. V. Sotnikov, A. V. Zherdev, B. B. Dzantiev, 2015, published in Uspekhi Biologicheskoi Khimii, 2015, Vol. 55, pp. 391-420.
- [3] P. Kostrobij, V. Polovyi et al, Math. Model. Comput. Vol. 5, No. 2, pp. 184-192 (2018).
- [4] V. P. Kurbatsky, “Dielectric tensor of low-dimensional metal systems”, J. Exp. Theor. Phys, pp. 148–158, 2017.
- [5] Kostrobij P. P., Markovych B. M. Effect of Coulomb interaction on chemical potential of metal film. Philosophical Magazine. 98 (21), 1991–2002 (2018).