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Dielectric Function of Two-Dimensional Nanostructure, Including Single Layer Quantum Well

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In this work, we calculate the dielectric function, depending on frequency, wave-vector and temperature in a two-dimensional nanostructure, including a single-layer quantum well. For this purpose, we used the theoretical expressions, also taking into account the exchange interactions of particles in a quantum well (a layer) placed in a boundless medium. These expressions include the response function, the Fourier transform of the Coulomb potential, and the local field correction factor. As it follows from our calculations, a considered nanostructure forms an active material, increasing and decreasing the electromagnetic field for some types of photons and also not allowing some types of photons to pass into the material. The temperature dependence of the dielectric function shows that increasing the temperature changes the interaction of the electromagnetic field with the structure.

topics: temperature depended dielectric function, nanostructures, multiparticle interactions

1. Introduction

Nanotechnologies and nanostructures are responsible for many outstanding properties that can be used in a wide range of practical applications. In this work, we consider a two-dimensional particle system with a quantum well, interacting with the two-dimensional gas of particles (holes) of the environment. The calculations were carried out using the theoretical expressions from [1] that include the response function, Fourier transform of the Coulomb potential and the local field correction factor. These expressions take the form

$$\varepsilon(q,\omega,T) = 1 - \frac{\nu(q)\,\chi^0(q,\omega,T)}{1+\nu(q)\,\chi^0(q,\omega,T)\,G(q)} \tag{1}$$

where $G(q)$ — a local field correlation factor containing exchange correlation effects, χ^0 — noninteracting electronic response function [2], and $\nu(q)$ — the Fourier transform of the Coulomb interaction such that

$$\nu(q) = \frac{2\pi e^2}{\varepsilon_s\, q}\, F(q\,l), \tag{2}$$

$$F(x) = \frac{3x+\frac{8\pi^2}{x}}{x^2+4\pi^2} - \frac{32\pi^4}{x^2}\,\frac{1-\mathrm{e}^{-x}}{x^2+4\pi^2} \tag{3}$$

where L — the quantum layer thickness, ε_s — a background dielectric constant, $F(x)$ — the form factor of an infinite rectangular quantum well [3]. In [4] we showed that the most important parameter in such studies is the size of the well, its form can be expressed by the structure factor, and the value of the potential barrier does not change the energies more than about 10%. Therefore, we consider the infinite rectangular quantum well. The expressions for the real and imaginary part of response function (χ^0) are given in [6, 7] for dimensionless temperature, wave vector, energy and chemical potential, depending on the temperature. These functions have the following forms

$$\mathrm{Im}\big(\chi^0\,(q,\omega)\big) = \frac{\sqrt{\pi}\,t\,N_0}{2Q}\left[F_{-\frac{1}{2}}\left(\frac{A_+}{2}\right) - F_{-\frac{1}{2}}\left(\frac{A^-}{2}\right)\right],$$

$$F_{-1/2}\,(x) = \frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}y\,\frac{y^{-1/2}}{\exp\,(y-x)+1},$$

$$A^\pm = \mu(t) - \frac{1}{4}\left(\frac{\Omega}{Q}\pm Q\right)^2,$$

$$\mu(t) = t\,\ln\left(\mathrm{e}^{1/t}-1\right),\quad N_0 = \frac{m^*}{\pi\hbar^2}, \tag{4}$$

$$\mathrm{Re}\big(\chi^0\,(q,\omega)\big) = N_0\left[\frac{-1}{\exp\,(-\mu/t)+1} + \frac{\mathrm{sign}(a_+)M_t(a_+^2)}{Q}\,\frac{\mathrm{sign}(a_-)\,M_t(a_-^2)}{Q}\right],$$

$$a_\pm = \frac{1}{2}\left(\frac{\Omega}{Q}\pm Q\right),$$

$$M_t(x) = \int_0^x \mathrm{d}z\,\frac{\sqrt{x-z}}{4t\,\cosh^2\left(\frac{z-\mu}{2t}\right)}. \tag{5}$$

We used (1)–(5) for the investigations of the real part of the dielectric function and to analyze its dependence on different parameters.

2. Results and discussions

2.1. The dependence of $\mathrm{Re}(\varepsilon)$ on the frequency

For our investigations, we used the following parameters

$$L = 20 \times 10^{-9}\ \mathrm{m}, \quad \varepsilon_0 = 8.85 \times 10^{-12}\ \mathrm{F/m},$$

$$\varepsilon_s = 3.5 \times 10^{-3}, \quad G(Q) = \begin{cases} 0.21, & \text{if } Q \leq 2, \\ 0.42, & \text{otherwise}, \end{cases} \tag{6}$$

and we calculated the real part of the dielectric function at room temperature, as a function of frequency for different wave vectors. The obtained family of curves is shown in Fig. 1.

As we can see for particles with a large momentum (curve 4 in Fig. 1), the dielectric function does not change significantly with frequency, but it undergoes a general trend, i.e., it is constant for low frequencies and weakly dependent on the frequency of the high frequency region. For some small momenta (curves 1 and 2 in Fig. 1), we observe the area with the special point $\min(\mathrm{Re}(\varepsilon))$ for the dielectric function, where the nonlinear effect of the quantum layer on the two-dimensional electron gas can be observed. On the other hand, for high frequencies, the curves go towards the limit value, which, as our calculations have shown, is constant and independent of frequency, wave vector and temperature. For all values shown in Fig. 1, we obtain positive values of the dielectric function. In Fig. 1, we also see nonmonotonic dependence of the real part of the dielectric function on the wave vector. This nonmonotony is vividly illustrated in Fig. 2, which shows the obtained dependence of the dielectric function on the frequency for small wave vectors: curve 1) for $q = 0.12$; curve 2) for $q = 0.15$; curve 3) for $q = 0.17$; curve 4) for $q = 0.2$.

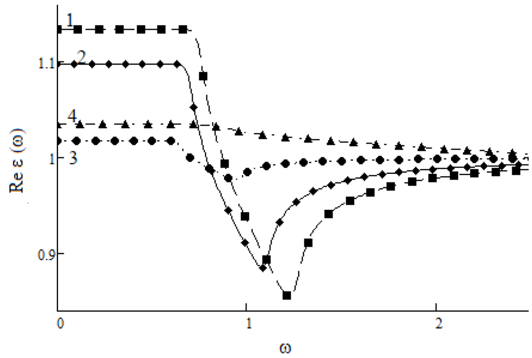

Fig. 1. The real part of the dielectric function of a two-dimensional electron gas in a medium with a quantum well for wave vectors $0.4 < q < 1.5$: 1 — $q = 0.4$, 2 — $q = 0.45$, 3 — $q = 0.5$, 4 — $q = 1.5$.

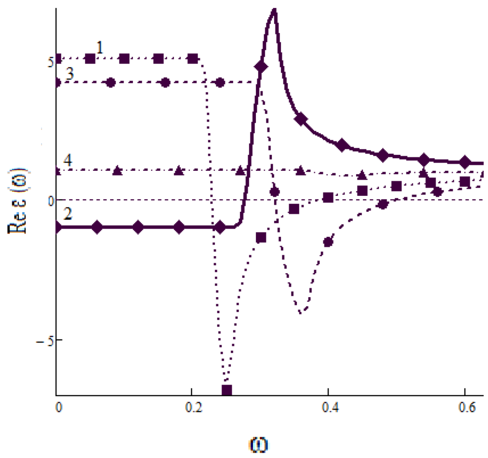

Fig. 2. The real part of the dielectric function of a two-dimensional electron gas in a medium with a quantum well for wave vectors $0.12 < q < 0.2$: 1 — $q = 0.12$, 2 — $q = 0.15$, 3 — $q = 0.17$, 4 — $q = 0.2$.

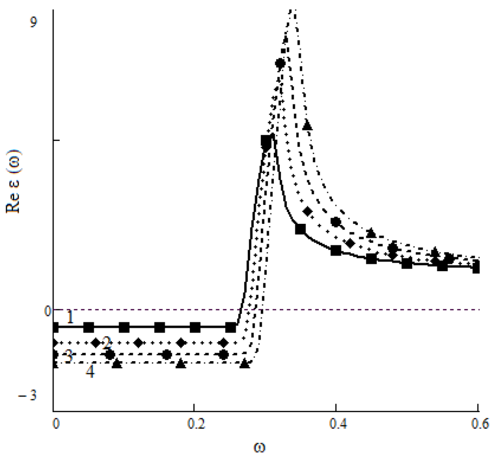

Fig. 3. The real part of the dielectric function of a two-dimensional electron gas in a medium with a quantum well for wave vectors $0.145 < q < 0.16$ 1 — $q = 0.145$, 2 — $q = 0.15$, 3 — $q = 0.155$, 4 — $q = 0.16$.

The behaviour of curves 1, 3, 4 actually reproduce the dependence for large wave vectors in Fig. 1. There are constant values of the dielectric function for a certain frequency range ($\omega \ll \omega_{kr}$), a sharp decline of the function to its smallest value, followed by its monotonic growth and following to its asymptote. However, in contrast to the previous case, there is a range of values for which the dielectric function is negative. Besides, curve 2 in Fig. 2 has an inverse tendency — the dielectric function is constant and negative for low frequencies with a sharp increase in the narrow area and a maximum at a certain point, and the monotonic decrease to the asymptotic value. As $\mathrm{Re}(\varepsilon)$ increases, we observe a change in its sign. For a narrow range of values of the wave vector (0.145; 0.15; 0.155; 0.16) we obtained the dependence presented in Fig. 3.

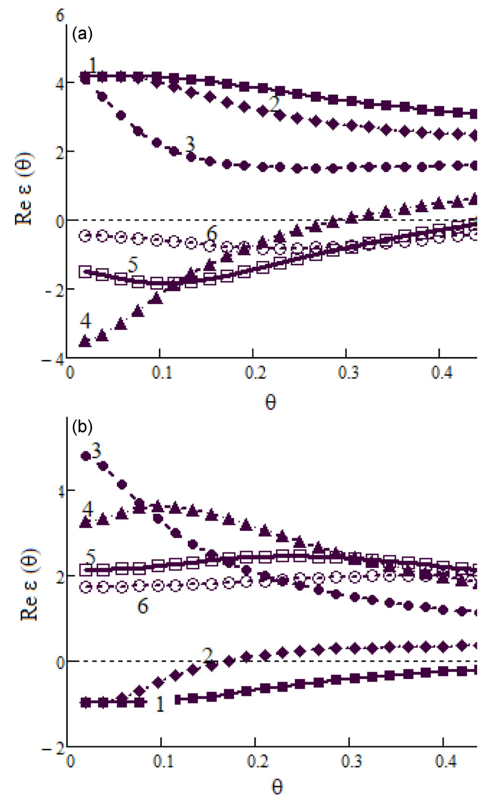

Fig. 4. $\mathrm{Re}(\varepsilon(t))$ for (a) $q = 0.15$ and (b) $q = 0.17$: 1 — $\omega = 0.2$, 2 — $\omega = 0.25$, 3 — $\omega = 0.3$, 4 — $\omega = 0.35$, 5 — $\omega = 0.4$, 6 — $\omega = 0.45$.

As one can see from curve 3 in Fig. 2, just after achieving the dimensionless pulse $q = 0.17$, we observe inversion dependence typical for the full range of wave vectors.

2.2. Temperature dependence

We also investigated the temperature dependence of the real part of the dielectric function for $q = 0.15$, which falls into a special region (Fig. 4a), and for $q = 0.17$ (Fig. 4b). We obtained the inverse trend of the temperature dependence for vibrations with the same frequencies but different wave vectors:

- curve 1 ($\omega = 0.2$) has negative values and increases monotonically for $q = 0.15$, and for $q = 0.17$ it has positive values and decreases monotonically;
- curve 2 ($\omega = 0.25$) increases monotonically and changes its sign for $q = 0.15$, and for $q = 0.17$ it decreases monotonically, always being positive;
- curve 3 ($\omega = 0.3$) is a positive and monotonically decreasing function for both cases;
- curves 5 ($\omega = 0.4$) and 6 ($\omega = 0.45$) are nonmonotonic, weakly dependent on temperature, positive for $q = 0.15$ and negative for $q = 0.17$;
- for some vibrations (curve 2 in Fig. 4a and curve 4 in Fig. 4b), increasing the temperature leads to the sign change in $\mathrm{Re}(\varepsilon)$.

The inverse tendencies that we observed in the dependence of the actual dielectric function on frequency also occur with an increase of the temperature (amplified by the temperature dependence). As our calculations show, for large wave vectors and high frequencies, the dielectric function is a constant asymptotic value independent of the parameters of the problem.

3. Conclusions

Investigations of the dielectric function of a two-dimensional electron structure with a quantum well, in which the exchange interaction between particles is taken into account, for room temperature showed that:

1. There is a large range of values of the wave vector ($0.17 < q < 1.5$) for which the dielectric function of the frequency is nonmonotonic in a minimum. It means that medium with a quantum well will attenuate electromagnetic oscillations for certain frequencies (decreasing part of the function) and reinforce for other ones (growing area). For high frequencies, in all cases the dielectric function goes to its asymptotic value and is independent of the wave vector, temperature and frequency.
2. For a small region of oscillations with the wave vector $0.145 < q < 0.16$, we get a region with a negative dielectric constant — such electromagnetic oscillations will not pass inside the structure, but will be reflected from the surface.
3. In both region cases, the many-body interaction of electrons leads to the fact that such a structure interacts with the electromagnetic field as an active material.
4. The temperature dependence of the dielectric function for the two analyzed regions reveals inverse dependence of the dielectric constant. Namely, $\mathrm{Re}(\varepsilon)$ is negative for: curve 1 ($\omega = 0.2$) at $q = 0.15$ (Fig. 4a) and curve 5 ($\omega = 0.5$) at $q = 0.17$ (Fig. 4b), or positive for: curve 1 ($\omega = 0.2$) at $q = 0.17$ (Fig. 4b) and curve 5 ($\omega = 0.5$) at $q = 0.15$ (Fig. 4a).
5. The temperature increase leads to the sign change in $\mathrm{Re}(\varepsilon)$ for some oscillations: curve 2 ($\omega = 0.25$) at $q = 0.15$ (Fig. 4a) and curve 4 ($\omega = 0.35$) at $q = 0.17$ (Fig. 4b).
6. Different temperature dependence of $\mathrm{Re}(\varepsilon)$ denotes that the frequency dependence is a strongly nonmonotonic function. We passed our calculations for room temperatures to follow the influences of electron quasi-momentum and frequencies. For small momentum, we obtained a family of nonmonotonic functions with singularity typical for

generalized functions. To the left of singularity (for small frequencies), we get the function almost independent on ω, with the values overcoming asymptotic, typical for the right side of singularity. After the singularity, our function increases rapidly and moves to the asymptotes (curve 1 for our dimensionless calculations). This actually means that we get higher values of $\mathrm{Re}(\varepsilon)$ for small ω. Such a conclusion is in good agreement with the fact that the layered systems are effective for low energies [7].

We see that the presence of a quantum well in a two-dimensional structure leads to an inhomogeneous and nonlinear response of the medium to the applied electromagnetic field. Some oscillations will not pass into such an environment, and some will be amplified or attenuated by the medium. However, the asymptotic values of the dielectric function are constant, independent of frequency, and change slightly with temperature. They are the same for $\mathrm{Re}(\varepsilon(\infty))$ and have different values for $\mathrm{Re}\varepsilon(0)$, depending on the wave vector of the particle.

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