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DIELECTRIC FUNCTION OF A QUANTUM-CONFINED THIN FILM WITH A MODIFIED PÖSCHEL–TELLER POTENTIAL

The spatial and time dispersions of the dielectric permittivity of an electron gas in quasi-two-dimensional quantum nanostructures are studied. The screening of the charge-carrier scattering potential in a quantum-confined film with a modified Pöschel–Teller potential is considered for the first time. Analytical expressions for the dielectric permittivity are obtained.

Keywords: quantum-confined thin film, quantum confinement effects, dielectric function, modified Pöschel–Teller potential, matrix element of the scattering potential, polarization operator.

1. Introduction

Large attention is currently paid to the creation and research of semiconductor nanostructures. In particular, these are quantum wells, quantum wires, and quantum dots. From the practical viewpoint, the electronic properties of nanostructures emerging due to quantum effects are of special interest. Quantum confinement effects begin to affect the electronic properties, when the size of the free charge carrier localization region becomes comparable with the de Broglie wavelength. These effects play a key role in the formation of optoelectronic properties of nanostructures [1]. Owing to the rapid development of nanoelectronics and the available technologies for the production of low-dimensional structures, a large number of theoretical and experimental works devoted to the physical properties of those structures have appeared in recent decades [2, 3].

The dielectric function is one of the most important characteristics that describe the electrical and optical properties of solids. The accurate modeling of the frequency-dependent dielectric function is of large importance, when studying the adsorption and long-range van der Waals interaction in solids [4]. In particular, the gain coefficient of semiconductor laser structures created on the basis of quantum wells directly depends on the dielectric permittivity [5]. Therefore, the knowledge of the corresponding spatial dispersion law is important for the calculation of the parameters of such structures to be correct. In work [6], an analytical model was proposed for the dielectric function of two-dimensional semiconductors, which can be used as a reliable tool for predicting the excitonic optical properties. Using the spectroscopic ellipsometry method, the dependence of the dielectric function of PbSe nanocrystals electrically deposited onto the Au substrate on the thickness of those crystals was studied in work [7], and the experimental results were compared with the results of electron structure calculations. The authors of work [8] combined the Maxwell–Garnett theory of effective medium with the Kramers–Krönig relations in order to obtain the complex dielectric function for PbS, PbSe, and PbTe quantum dots. The applied method allows the real and imaginary parts of the dielectric function to be determined from the experimental absorption spectrum. The spatial and time dispersions of the dielectric permittivity of an electron gas in quasi-two-dimensional quantum nanostructures was considered in work [9]. The cited authors analyzed expressions obtained for the dielectric permittivity of quasi-two-dimensional quantum structures, by using the finite-depth rectangular and δ-function models for the potential well.

When physical processes in semiconductor quantum nanostructures are described, it is very important to use a proper mathematic model for the confining potential. As the latter, potentials with rectangular or parabolic profiles are often used. An analysis of the results of long-term researches showed that the rectangular potential is more suitable for thin layers, whereas the parabolic potential produces better results in the case of thicker layers. In this work, we consider the screening of the scattering potential for charge carriers in a quantum-confined thin film with a modified Pöschel–Teller potential.

2. Theory

When many-body effects in solids are examined, it is basically important to elucidate the role of the screening of external perturbations that are imposed on the system. The relevant phenomena are explained by the redistribution of charge carriers under the action of an external perturbation field. It is known that, in the two-dimensional geometry, the screening results in an essentially different spatial dependence of the dielectric function, as compared with that obtained in the three-dimensional case. If the interaction between particles is considered, the screening of the electric field created by charges in those structures has to be taken into account correctly [10–12].

Nowadays, such effects as the impurity field screening, Kohn effect, appearance of a charge halo around the impurity, and others have been studied rather well. The solution of the corresponding self-consistent problem testifies that the potential that actually acts on an electron is equal to the applied potential divided by the dielectric permittivity function, with the latter depending of the wavelength and frequency of the applied perturbation.

The probability magnitudes for a quantum-mechanical system to transit from one state into another are mainly described by matrix elements. In terms of the dielectric function, the screening is determined as follows [13, 14]:

$$M_{\mathrm{scr}} = \frac{M}{\epsilon(q)}, \tag{1}$$

where M is the matrix element of the scattering potential,

$$\epsilon(q) = 1 + M_{\mathrm{ee}}\Pi(0,q) \tag{2}$$

is the dielectric function, M_{ee} is the matrix element of the electron-electron interaction potential,

$$\Pi(0,q) = \int g(\varepsilon)\left(-\frac{\partial f_0}{\partial \varepsilon}\right) d\varepsilon \tag{3}$$

is the polarization operator [15], g is the electron state density, and f_0 is the Fermi distribution function.

In quasi-two-dimensional quantum films, the electron Hamiltonian is known to have the following form:

$$H = \frac{1}{2m}p^2 + U(z), \tag{4}$$

where

$$U(z) = \frac{\hbar^2\alpha^2\lambda(\lambda+1)}{2m}\tanh \alpha z$$

is the modified Pöschel–Teller potential confining the electron motion. The energy spectrum and the one-electron normalized wave functions for the charge carriers were obtained in works [10–13]:

$$\varepsilon_{\nu,\lambda} = \frac{\hbar^2\alpha^2}{2m}\Big(\lambda(\lambda+1) - (\lambda-\nu)^2\Big), \tag{5}$$

$$\psi_{\nu,\lambda,k} = \frac{1}{\sqrt{L_y L_x}} e^{i(k_x x + k_y y)} \times$$
$$\times \left[\frac{\alpha(\lambda-\nu)\Gamma(2\lambda-\nu+1)}{\Gamma(\nu+1)}\right] P_\lambda(z), \tag{6}$$

where m is the effective mass of charge carriers, L_x and L_y are the film dimensions in the xy-plane, α and λ are the potential parameters ($\lambda > 1$), ν is the size quantum number ($\nu < \lambda$), $\Gamma(x)$ is the gamma function, and $P_\lambda(z)$ is the Legendre function.

In the case of Pöschel–Teller potential, the electron density of states looks like [13]

$$g(\varepsilon) = \sum_{\nu=0}^{[\lambda]} \frac{L_x L_y m}{\pi\hbar^2}\theta(\varepsilon - \varepsilon_{\nu,\lambda}), \tag{7}$$

where $\theta(x)$ is the Heaviside step function. The polarization operator equals

$$\Pi(0,q) = \sum_{\nu=0}^{[\lambda]} \frac{L_x L_y m}{\pi\hbar^2} \int\limits_{\varepsilon_{\nu,\lambda}}^{\infty} \left(-\frac{\partial f_0}{\partial\varepsilon}\right) d\varepsilon =$$
$$= \sum_{\nu=0}^{[\lambda]} \frac{L_x L_y m}{\pi\hbar^2} f_0(\varepsilon_{\nu,\lambda}). \tag{8}$$

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Taking formulas (5) and (6) into account, the matrix element of the electron-electron interaction operator can be calculated in the quantum limit $\nu = 0$ as follows:

$$M_{\rm ee} = \left(\frac{1}{L_x L_y}\right)^2 \left(\frac{\alpha(\lambda)\,\Gamma(2\lambda+1)}{\Gamma(1)}\right)^2 \times$$
$$\times \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} dx_1 dy_1 dz_1 dx_2 dy_2 dz_2 \times$$
$$\times e^{i\left[\left(k'_{y_1}-k_{y_1}\right)y_1+\left(k'_{x_1}-k_{x_1}\right)\right]x_1} \times$$
$$\times e^{i\left[\left(k'_{y}{}_2-k_{y_2}\right)y_2+\left(k'_{x_1}-k_{x_1}\right)\right]x_1} \times$$
$$\times \frac{e^2 P_\lambda^2(z_1)\,P_\lambda^2(z_2)}{\chi\left[(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2\right]^{1/2}}. \qquad (9)$$

Let us change the variables:

$x_1 - x_2 \to x, \quad x_1 + x_2 \to X,$

$y_1 - y_2 \to y, \quad y_1 + y_2 \to Y.$

The corresponding Jacobian equals $\frac{1}{4}$. Since

$$\int\limits_{-\infty}^{\infty} e^{i\left(k'_{x_1}-k_{x_1}+k'_{x_2}-k_{x_2}\right)\frac{1}{2}X} dX =$$
$$= 2L_x\delta(k'_{x_1}-k_{x_1}+k'_{x_2}-k_{x_2})$$

and

$$\int\limits_{-\infty}^{\infty} e^{i(k'_{y_1}-k_{y_1}+k'_{y_2}-k_{y_2})\frac{1}{2}Y} dY =$$
$$= 2L_y\delta(k'_{y_1}-k_{y_1}+k'_{y_2}-k_{y_2}),$$

we obtain

$$\left(k'_{y_1}-k_{y_1}+k'_{y_2}-k_{y_2}\right) = 0,$$
$$(k'_{y_1}-k_{y_1}-k'_{y_2}+k_{y_2}) = 2q_y,$$

so that

$$k'_{y_1}-k_{y_1} = q_y,$$
$$k_{y_2}-k'_{y_2} = q_y.$$

Substituting those expressions into Eq. (9) for the matrix element of the electron-electron interaction operator, we get

$$M_{\rm ee} = \left(\frac{1}{L_x L_y}\right)^2 \left(\frac{\alpha(\lambda)\,\Gamma(2\lambda+1)}{\Gamma(1)}\right)^2 \times$$
$$\times \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} dx dy dz_1 dz_2\, e^{iqr\cos\phi} \times$$
$$\times \frac{e^2 P_\lambda^2(z_1)\,P_\lambda^2(z_2)}{\chi\left[z^2+y^2+(z_1-z_2)^2\right]^{1/2}}. \qquad (10)$$

Now, using the realtions

$x = r\cos\phi, \quad y = r\sin\phi,$

let us change in Eq. (10) from the Cartesian coordinate frame to the polar one:

$$M_{\rm ee} = \left(\frac{1}{L_y L_x}\right)\left[\frac{\alpha(\lambda)\,\Gamma(2\lambda+1)}{\Gamma(1)}\right]^2 \times$$
$$\times \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{0}^{\infty}\int\limits_{0}^{2\pi} r dr d\phi dx_1 dx_2\, e^{iqr\cos\phi} \times$$
$$\times \frac{e^2 P_\lambda^2(z_1)\,P_\lambda^2(z_2)}{\chi\left[r^2+(z_1-z_2)^2\right]^{1/2}} =$$
$$= (2\pi)\left(\frac{1}{L_x L_y}\right)\left[\frac{\alpha(\lambda)\,\Gamma(2\lambda+1)}{\Gamma(1)}\right]^2 \times$$
$$\times \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{0}^{\infty} r dr dz_1 dz_2 J_0(qr) \frac{e^2 P_\lambda^2(z_1)\,P_\lambda^2(z_2)}{\chi\left[r^2+(z_1-z_2)^2\right]^{1/2}} =$$
$$= \frac{2\pi e^2}{\chi q}\left(\frac{1}{L_y L_x}\right)\left[\frac{\alpha(\lambda)\,\Gamma(2\lambda+1)}{\Gamma(1)}\right]^2 \times$$
$$\times \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} dz_1 dz_2\, e^{-q\sqrt{(z_1-z_2)^2}} P_\lambda^2(z_2),$$

where $J_0(x)$ is the Bessel function of the 0-th order [13]. At $\lambda = 1$, we have

$$P_\lambda^2(z) = \frac{1}{2}\,\mathrm{sech}\,\alpha z,$$

so that

$$M_{\rm ee} = \frac{2\pi e^2}{\chi q}\left(\frac{1}{L_y L_x}\right)(2\alpha)^2 \times$$
$$\times \int\limits_{-\infty}^{\infty} dz_1 dz_2 \left(\frac{1}{e^{\alpha z_2}+e^{-\alpha z_2}}\right)^2 e^{-q\sqrt{(z_1-z_2)^2}} \times$$
$$\times \left[e^{\alpha(z_1+z_2)} + e^{\alpha(z_1-z_2)} + \right.$$
$$\left. + e^{-\alpha(z_1+z_2)} + e^{-\alpha(z_1-z_2)}\right]^2. \qquad (11)$$

In formula (11), we change the variables:

$z = z_1 - z_2, \quad Z = z_1 + z_2.$

The corresponding Jacobian equals $\frac{1}{2}$. Then

$$M_{\rm ee} = \frac{2\pi e^2}{\chi q}\left(\frac{1}{L_y L_x}\right)\frac{1}{2}\times$$

$$\times\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} dz dZ \left(\frac{1}{\text{cosech } Z + \text{cosech } z}\right)^2 e^{-\frac{q}{\alpha}z} =$$

$$= \frac{\pi^3 e^2}{2\chi q}\left(\frac{1}{L_y L_x}\right)\left(\frac{q}{\alpha}\right)^2 \text{cosec}\left(\frac{\pi q}{2\alpha}\right)^2. \quad (12)$$

Substituting expressions (8) and (12) into Eq. (2), we obtain the following formula for the dielectric function:

$$\epsilon(q) = 1 + \frac{m\pi^2 e^2}{2\hbar^2 \chi q} f_0\left(\varepsilon_{0,1}\right)\left(\frac{q}{\alpha}\right)^2 \text{cosec}\left(\frac{\pi q}{2\alpha}\right)^2. \quad (13)$$

In the limiting case $q \ll \alpha$, the relation

$$\text{cosec}\left(\frac{\pi q}{2\alpha}\right)^2 \approx \left(\frac{2\alpha}{\pi q}\right)^2$$

is satisfied. Then formula (13) looks like

$$\epsilon(q \ll \alpha) = 1 + \frac{2me^2}{\hbar^2 \chi q} f_0\left(\varepsilon_{0,1}\right).$$

This expression describes the dependence of the dielectric constant on the wave vector q at $q \ll \alpha$ in the two-dimensional case.

3. Conclusion

In this work, an expression for the dielectric constant of a quantum-confined thin film with a modified Pöschel–Teller potential has been obtained. In the two-dimensional case, the screening leads to a substantially different spatial dependence of the dielectric function, as compared with the three-dimensional case. It is shown that, in the two-dimensional case, the dependence of the dielectric constant on the wave vector is determined by a characteristic potential size and has the form $\epsilon(q) \sim \text{const} \times q^{-1}$.

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ДІЕЛЕКТРИЧНА ФУНКЦІЯ
КВАНТОВО-РОЗМІРНОЇ ТОНКОЇ ПЛІВКИ
З МОДИФІКОВАНИМ ПОТЕНЦІАЛОМ
ПЕШЛЯ–ТЕЛЛЕРА

Р е з ю м е

Досліджено просторову та часову дисперсії діелектричної проникності електронного газу в квазідвовимірних квантових наноструктурах. Вперше розглядається задача про екранування потенціалу, що розсіює, носіїв заряду в квантово-розмірній плівці з модифікованим потенціалом Пешля–Теллера. Отримані аналітичні вирази для діелектричної проникності.