Statistical mechanics of screened spatially indirect excitons

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We study thermodynamic properties of spatially separated electron-hole plasma in double-layered systems using Green function formalism. The screening of the Coulomb interaction is considered in the framework of Thomas-Fermi approximation, and a qualitatively new mechanism of screening by indirect excitons is taken into account. The exciton density is shown to decrease sharply with increasing electron-hole separation up to one exciton Born radius. The strong mutual enhancement of screening and charge-separation effects is found.

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I. INTRODUCTION

Spatially separated quasi-two-dimensional (2D) electron-hole plasma can be found in different modern nano-heterostructure-based devices. There is a continuous attention to closely situated (so called double) quantum wells. This attention is mostly due to the possibility of the Bose-Einstein condensation of spatially indirect excitons in such a system [1]. Another physical object with spatially separated electron-hole plasma, which currently attracts increasing interest, is a GaN/AlGaN quantum well, grown on a sapphire substrate [2]. In the latter case electrons and holes are separated by huge (of the order of one MV/cm) internal electric field. Because of the enhanced binding energy in wide-gap semiconductors, excitons in nitride-based nanostructures are a subject of extensive experimental and theoretical research.

The aim of this work is to provide a consistent many-body theory, describing statistical mechanics of the quasi-2D exciton/free carrier plasma with spatial charge separation.

II. SCREENING IN THE SPATIALLY-SEPARATED ELECTRON-HOLE SYSTEM

First of all, the potentials of electron-electron and electron-hole interaction should be established. The Thomas-Fermi (or, as it is often called in the 2D case, Stern-Howard) approximation is one of the most frequently used methods for dealing with static screening of Coulomb interaction in semiconductor systems [3]. In the frame of this approximation the charge, induced by external perturbation, originates from a redistribution of free carriers and is proportional to a local electric field. The resulting electric field potential is given by the Poisson equation in the form:

$$\Delta \phi - 2q_a^s \bar{\phi}_e g_e(z) - 2q_h^s \bar{\phi}_h g_h(z) = -\frac{4\pi}{\kappa}Q_{ext},$$

(1)

where \(\bar{\phi}_a(\rho) = \int \phi(\rho, z) g_a(z) \, dz\), \(g_a(z)\) is a free-carrier-distribution function in the direction normal to the quantum well plane, \(\kappa\) is a background dielectric constant, \(Q_{ext}\) is an external charge density, and the screening parameter in the 2D case is

$$q_a^s = \frac{2\pi e^2}{\kappa} \frac{\partial n_a}{\partial \mu_a} = \frac{2}{a_B m_{eh}} m_a \left[1 - \exp \left(-\beta \pi \hbar^2 n_a / m_a \right)\right].$$

(2)

Here \(n_a\) is a free particle density, \(\mu_a\) is a quasi-Fermi level, \(m_a\) is an effective mass, \(\mu_{eh} = m_e m_h / (m_e + m_h)\) is the reduced effective mass, \(a_B = \hbar^2 / (\mu^* e^2)\) is the 3D exciton Bohr radius, and \(\beta = 1/(k_B T)\).

The contribution of excitons to screening in the conventional single quantum well can be treated within the Thomas-Fermi approximation as a reduction of free carrier densities entering Eq. (2). In the case of spatially separated plasma, screening by excitons can not be neglected even in the Thomas-Fermi approximation. The indirect exciton has the finite dipole moment, and the external electric field causes redistribution of excitons, which plays its own role in the

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resulting field reduction. Using the same approach as for a free-carrier plasma, the indirect-exciton part of the induced charge density can be written as

\[ Q_{\text{exc}}^{\text{ind}} = \frac{k}{2\pi} q_s^{\text{exc}} (g_h(z) - g_e(z)) \left[ e\phi_h(\rho) - e\phi_e(\rho) \right]. \]

Here we introduced the excitonic screening parameter

\[ q_s^{\text{exc}} = \frac{2\pi e^2}{k} \frac{\partial n_{\text{exc}}}{\partial \mu}, \]

where \( n_{\text{exc}} \) is the exciton density and \( \mu = \mu_e + \mu_h \).

In the present paper we consider a simple model of spatially separated electron-hole plasma, where electrons and holes are purely two-dimensional and reside in different planes with distance \( d \) between them. The generalization of this model to incorporate finite-width quantum wells will be presented somewhere else. The two-plane model is particularly valuable for studying the interplay between screening and spatial separation of different types of carriers.

The problem of finding electron-electron repulsion and electron-hole attraction potentials has cylindrical symmetry, so we use the following representation:

\[ \phi(\rho, z) = \frac{1}{2\pi} \int_0^\infty \phi_q(z) J_0(\rho q) q \, dq, \]

where \( J_0 \) is the Bessel function. Let us assume that the electronic charge resides in the plane with coordinate \( z = d \) and the holes are in the plane \( z = 0 \). In this model the distribution functions \( g_n(z) \) are given by delta-functions. The Poisson equation is reduced to a one-dimensional problem:

\[ \frac{d^2}{dz^2} \phi_q(z) - q^2 \phi_q(z) - 2q^2 \phi_q(0) \delta(z) - 2q^2 \phi_q(d) \delta(z - d) - 2q_s^{\text{exc}} \delta(z) - 2q_s^{\text{exc}} \delta(z - d) \]

\[ = -\frac{4\pi e}{k} \delta(z - d) \]

Solving Eq. (5), we obtain repulsion and attraction potentials in \( q \)-representation:

\[ V^{\text{eh}}_s(q) = e \phi_q(0) = -\frac{2\pi e^2}{k} q \exp(-q d) + q_s^{\text{exc}} \frac{1 - e^{-2qd}}{\Theta + q_s^{\text{exc}} \Xi}, \]

\[ V^{\text{ee}}_s(q) = -e \phi_q(d) = \frac{2\pi e^2}{k} q + (q_s^{(e)} + q_s^{\text{exc}}) (1 + e^{-2qd}) + q_s^{\text{exc}} \Xi, \]

where both terms \( \Xi = \left[ 1 - \exp(-qd) \right] \left[ 2k + (q_s^{(e)} + q_s^{(h)}) (1 + \exp(-qd)) \right] \), and \( \Theta = (q + q_s^{(e)}) (q + q_s^{(h)}) - q_s^{(e)} q_s^{(h)} \exp(-2qd) \) in denominators of Eqs. (6) do not depend on the excitonic screening parameter \( q_s^{\text{exc}} \).

### III. CORRELATED DENSITY

In order to provide a consistent treatment of many-body effects in a 2D electron-hole plasma, we base our theory on a quasi-particle picture and Green functions technique. Electrons and holes are redistributed among the quasi-particle states with a sharp spectral peak and dispersion \( \epsilon_a = \hbar^2 k^2 / 2m_a \) (where the energy is measured from the corresponding size-quantized level renormalised by the many-body shift) and some other "correlated" states originating from the interaction between quasi-particles.

The total density of electrons can be divided into two parts, the first part representing “free” particles with a quasi-Fermi level \( \mu_e \), and the second part incorporating interaction between quasiparticles. This second part, which is called the correlated density, is given by

\[ n_{\text{corr}}^{e} = 2 \sum_k \int \frac{d\hbar\omega}{\pi} \Gamma_{e}^{e}(k, \omega) \left[ f_{e}(\hbar\omega) - f_{e}(\epsilon_e(k)) \right] \frac{\partial}{\partial \hbar\omega} \frac{P}{\epsilon_e(k) - \hbar\omega}. \]
Here $\Gamma_\epsilon(k, \omega) = \text{Im} \Sigma_\epsilon(k, \omega)$ is an imaginary part of the single-particle self-energy, $f_\epsilon(\epsilon) = [\exp(\beta(\epsilon - \mu_\epsilon)) + 1]^{-1}$ is the Fermi distribution function, and the derivative of the principal value is given

$$\frac{\partial}{\partial h\omega} \frac{P}{e - h\omega} = \lim_{\nu \to 0} \frac{(\epsilon - h\omega)^2 - \nu^2}{((\epsilon - h\omega)^2 + \nu^2)^2}.$$ 

From the point of view of diagrammatic technique, exciton is a succession of electron-hole scatterings, which is represented by the series of diagrams serving as a basis for the ladder approximation. We use the ladder approximation to our many-body problem, keeping only ladder-type diagrams in the expression for the electron self energy:

$$\Sigma_\epsilon(\vec{k}, \beta_\epsilon) = -\frac{1}{\beta} \sum_{b, \vec{k}', \nu_b} \left[ 2\tilde{T}_{eb}(\vec{k}, \vec{k}' - \vec{k}, \beta_\epsilon, \beta_\epsilon + \nu_b) - \delta_{eb}\tilde{T}_{eb}(\vec{k}', \vec{k} - \vec{k}', \beta_\epsilon, \beta_\epsilon + \nu_b) \right] G_b(-\vec{k}, \Omega_b),$$

(10)

where the summation is taken over different types of particles, $b = e, h$, 2D wave-vector $\vec{k}'$ and Fermi-type Matsubara frequencies $\Omega_b$. The quantity $\tilde{T}$ represents a sum of ladder diagrams for electron-electron or electron-hole scattering and is given by the frequency-dependent T-matrix equation:

$$\tilde{T}_{ab}(\vec{k}, \vec{q}, \vec{k}', \Omega) = -V_{s}^{ab}(\vec{k} - \vec{k}') + \sum_{\vec{k}''} V_{s}^{ab}(\vec{k} - \vec{k}'') G_{ab}(\vec{k}'', \vec{q}, \vec{k}', \Omega) \tilde{T}_{ab}(\vec{k}'', \vec{q}, \vec{k}'', \Omega),$$

(11)

where the potentials $V_{s}^{ab}$ are given by Eqs. (8),

$$G_{ab}(\vec{k}, \vec{q}, \Omega) = \frac{N_{ab}(\vec{k}, \vec{q})}{\epsilon_a(\vec{k}) + \epsilon_b(\vec{q} - \vec{k}) - h\Omega},$$

and

$$N_{ab}(\vec{k}, \vec{q}) = 1 - f_a(\epsilon_a(\vec{k})) - f_b(\epsilon_b(\vec{q} - \vec{k})).$$

Following Zimmermann, who derived a similar formula for the 3D case, we obtain the expression for the correlated density in the 2D electron-hole system:

$$n_{\text{corr}}^a = \frac{2}{\pi \hbar^2} \sum_{m = -\infty}^{+\infty} \left[ \sum_n M_{ch} L_{ch}(\epsilon_{mn}) + \frac{1}{\beta} \sum_{\nu = e, h} M_{ab} \lambda_m \int_0^{\infty} dk L_{ab} \left( \frac{\hbar^2 k^2}{2m_{ab}} \right) 2\sin^2 \delta_{m}^{ab}(k) \frac{d\delta_{m}^{ab}}{dk} \right],$$

(12)

$$L_{ab}(\epsilon) = -\ln \left[ 1 - \exp \left( \beta(\mu_a + \mu_b - \epsilon) \right) \right],$$

$$M_{ab} = m_a + m_b, \quad m_{ab} = \frac{m_a m_b}{m_a + m_b}, \quad \lambda_m = 1 - \delta_{ab}(-1)^m/2.$$

Here $\epsilon_{mn}$ are the values of the exciton bound states energies, where the first index $m$ denotes the angular momentum and the second index $n$ enumerates different states for a given $m$. The bound state energies correspond to the poles of the T-matrix. The quantities $\delta_{m}^{ab}(k)$ give the phases of the coefficients in the Fourier series expansion of the T-matrix. The values of these quantities coincide with the scattering phase shifts when the k-space filling is neglected. Thus, the second part of Eq. (12) describes the scattering states contribution to the correlated density. In the low density/high temperature limit this expression differs from that of Portnoi and Galbright only by the factor $2\sin^2 \delta_{m}^{ab}$ in the integrand. The “e-e” part of the correlated density has a negative sign and is responsible for the reduction of the plasma density due to repulsion between the carriers of the same type. The electron-hole part of the density is positive and can be attributed to the presence of the excitons. As it was shown in Ref. [5] for dilute plasma, this part of the density does not change abruptly when one of the bound states disappears with increasing screening. We treat the electron-hole part of the correlated density as the density of excitons:

$$n_{\text{exc}} = \frac{2}{\beta \pi \hbar^2} \sum_{m = -\infty}^{+\infty} \left[ \sum_n L_{ch}(\epsilon_{mn}) + \frac{1}{\pi} \int_0^{\infty} dk L_{ch} \left( \frac{\hbar^2 k^2}{2m_{ch}} \right) 2\sin^2 \delta_{m}^{ch}(k) \frac{d\delta_{m}^{ch}}{dk} \right].$$

(13)
Substituting $n_{exc}$ from Eq.(13) into Eq.(4) we get the following expression for the excitonic screening parameter:

$$
q_{exc} = \frac{4M_{eh}e^2}{\kappa \hbar^2} \sum_{m=-\infty}^{+\infty} \left[ \sum_n f_B(\epsilon_{mn}) + \frac{1}{\pi} \int_{0}^{\infty} dk f_B\left( \frac{\hbar^2 k^2}{2m_{eh}} \right) 2 \sin^2 \delta_{eh}^m(\bar{\hbar}^2 k^2) \frac{d\delta_{eh}^m}{dk} \right],
$$

(14)

To calculate the exciton density we have to run the following self-consistent procedure. Firstly, for given electron-hole density we calculate the screening parameters from Eq.(2) and obtain corresponding bound state energies and phase shifts. Then, using these results we calculate the new values of excitonic screening parameter and free carrier density and recalculate bound state energies and phase shifts, repeating this procedure until the exciton density stops changing.

**IV. RESULTS AND DISCUSSION**

Throughout the calculations we neglect the phase shift dependence on the carrier density and obtain the values of $\delta_{ab}$ using the 2D modification of the variable phase approach. To find the bound state energies we use the method, proposed by Campi and co-workers, which is also based on the ladder approximation. We take into account only the ground exciton state. The material parameters are chosen to match these of the GaAs/AlGaAs quantum wells, and the difference between dielectric constants of the QW and the barrier is neglected.

In Figure 1 we present the dependence of the binding energy of the exciton ground state on the inter-plane distance. One can see (Fig. 1b) that the decrease of the exciton binding energy with increasing the distance is substantially enhanced by the presence of free carriers and indirect excitons, which screen the Coulomb attraction. Figure 2 shows the exciton density as a function of the total plasma density for different inter-plane distances. One can see that the exciton density has a maximum and then decreases sharply with increasing the total number of carriers, which reflects the action of both screening and k-space filing.

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FIG. 1. The ground state binding energy of the indirect exciton as a function of inter-plane separation for different free-carrier screening parameter: $q_e^* = 0$ (solid line), $q_e^* = 0.25 a_B^{-1}$ (long-dashed line), $q_e^* = 0.5 a_B^{-1}$ (dashed line), $q_e^* = a_B^{-1}$ (dotted line). (a) - measured in the 3D exciton Rydberg units, (b) - normalized by its maximum value.
FIG. 2. Exciton density as a function of plasma density for different inter-plane distances: $d = 0$ (solid line), $d = 0.25 \ a_B$ (long-dashed line), $d = 0.5 \ a_B$ (dashed line), $d = a_B$ (dotted line).