Exciton/free-carrier plasma in GaN-based quantum wells: Scattering and screening

M. E. Portnoi(a) and I. Galbraith(b)
(a) School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom
(b) Physics Department, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom

The degree of ionisation of a two-dimensional electron-hole plasma is calculated in the low-density (Boltzmann) limit. The electron-hole interaction is considered for all states: optically active and inactive, bound and unbound. The theory is applied to exciton/free-carrier plasma in GaN-based quantum wells at room temperature.

Room-temperature operation of blue quantum-well lasers, based on GaN [1] or ZnSe [2], is no longer a novelty. However, the nature of lasing in wide-gap semiconductors and quantum wells has not yet been completely understood. The large exciton binding energy in wide-gap semiconductors and quantum wells favours excitonic gain processes for which no satisfactory theoretical treatment exists [3]. A knowledge of the balance between excitons and free carriers is crucial in determining the dominant gain process. It is known that a naive application of the Mott criterion for the metal-insulator transition as well as the use of a single-bound-state law of mass action are insufficient, as screening of excitons by the electron-hole plasma and strong scattering of particles within the plasma both play a crucial role [4].

For a consistent description of the electron-hole plasma at a temperature which is higher then the exciton binding energy, bound states and unbound scattering states should be treated on the same footing. In what follows we present such a consistent treatment for the purely two-dimensional (2D) case in the low-density (Boltzmann) limit.

Following an approach applied in 3D to nuclear matter [5], an ionic plasma [6], and the electron-hole system in excited semiconductors [4], we divide the total electron (hole) density between two terms:

$$n_a \;=\; n_a^0 \;+\; n_a^{corr} \;. \tag{1}$$

The first term n_a^0 is the density of uncorrelated quasiparticles with renormalized energies. Only this term should be taken for the screening radius calculation [4]. All correlation effects both in the bound and continuum states are incorporated into the second term n_a^{corr} which is called the correlated density. The lower index in Eq. (1) is a species index, $a = e$ for electrons and $a = h$ for holes.

In the low-density limit there is no need to go beyond two-particle correlations. This allows us to separate clearly the role of the inter-particle Coulomb interaction from the phase-space filling effects. It is tempting to relate n_a^{corr} and n_a^0 by a simple law of mass action with the single exciton bound state energy reduced by screening [3,7]. The main shortcoming of this approach is a disregard of the strong scattering of unbound carriers. A complete account of scattering states as well as all (optically active and inactive) bound states requires the calculation of a two-body partition function which involves summation over all two-particle states. In the low-density (non-degenerate) limit, for which there is no Pauli blocking, a 2D analogue of the modified mass action law reads

$$n_a^{corr} \;=\; \sum_b n_a^0 n_b^0 \frac{2\pi\hbar^2}{\mu_{ab} k_B T} Z_{ab} \;, \tag{2}$$

where $\mu_{ab} = m_a m_b/(m_a + m_b)$ is the reduced effective mass, and Z_{ab} is the two-body interaction part of the partition function. Note that due to charge-neutrality the total electron-hole density $n_e = n_h = n$ is independent of species, whereas $n_e^0 \neq n_h^0$ and $n_e^{corr} \neq n_h^{corr}$ if the electron and hole have different masses.

The electron-hole part of the partition function which exhibits bound states (excitons) is given by

$$Z_{eh} = \sum_{m,\nu} \exp(-\beta E_{m,\nu}) \;+\; \frac{1}{\pi} \int_0^\infty \left(\sum_{m=-\infty}^{\infty} \frac{d\delta_m(k)}{dk} \right) \exp\left(-\beta \frac{\hbar^2 k^2}{2\mu_{eh}} \right) \; dk \;, \tag{3}$$

where $\beta = 1/(k_B T)$, $m\hbar$ is the projection of the angular momentum onto the axis normal to the plane of 2D motion ($m = 0, \pm 1, \pm 2, \;\ldots$), $\hbar^2 k^2/2\mu_{eh}$ is the energy of the relative motion of the unbound (scattered) electron and hole, k is the absolute value of the relative motion momentum, $\delta_m(k)$ are the 2D scattering phase shifts introduced in the standard way [8], $E_{m,\nu}$ are the bound-state energies (index ν enumerates bound states with given m), and the double sum in the first term ranges only over bound states. Equation (3) is the 2D analogue of the Beth-Uhlenbeck formula [9], and it is derived [10] in the same fashion as in the 3D case [11]. The scattering term in the right-hand side of Eq.(3) gives the contribution to Z_{eh} of the electron-hole attraction in the continuum part of the energy spectrum. The electron-electron and hole-hole parts of the partition function Z_{ee} and Z_{hh} contain the scattering term only.

Equations (1-3) provide a consistent description of the ionisation degree, defined as $\alpha = n_e^0/(n_e^0+n_e^{corr})$. Technically the most difficult problem is to calculate the binding energies and scattering phase shifts in a screened Coulomb potential. We use for this purpose the variable-phase method [12] known from scattering theory. In this method the scattering phase shift and the function defining bound-state energies can be obtained as a large distance limit of the phase function, which satisfies the first-order, nonlinear Riccati equation originating from the radial Schrödinger equation.

In this paper we model the screened Coulomb interaction in a 2D plasma by the well-known Thomas-Fermi expression for a statically screened Coulomb potential [8]:

$$V_s(\rho) = \mp\frac{e^2}{\epsilon}\int_0^\infty \frac{qJ_0(q\rho)}{q+q_s}dq = \mp\frac{e^2}{\epsilon}\left\{\frac{1}{\rho} - \frac{\pi}{2}q_s[\mathbf{H}_0(q_s\rho) - Y_0(q_s\rho)]\right\}\ , \tag{4}$$

where q_s is the 2D screening wavenumber (which depends on temperature and carrier density), ϵ is the static dielectric constant of the semiconductor, $J_0(x)$, $Y_0(x)$, and $\mathbf{H}_0(x)$ are the Bessel functions of the first and of the second kind and the Struve function. The upper sign in Eq. (4) is for electron-hole attraction, the lower sign is for electron-electron or hole-hole repulsion. Being the long-wavelength static limit of the random phase approximation for a purely 2D case, Eq. (4) is the simplest model for the screened Coulomb potential in 2D. Nevertheless, this expression reflects the fact that the statically screened potential in 2D decreases at large distances slower than in the 3D case. Despite numerous realistic corrections, Eq. (4) remains the most widely used approximation for the 2D screening, especially for the screened exciton problem. The variable-phase method application to scattering and bound states in the screened Coulomb potential (4) is described in detail in our recent paper [13]. The method is especially effective for calculation of shallow-state binding energies and low-energy scattering phase shifts. Applying the variable phase method together with a 2D analogue of the Levinson's theorem [14], we have found that with decreasing q_s several bound states with different angular momenta appear simultaneously at certain integer values of $1/(q_s a^*)$, where a^* is the effective (excitonic) Bohr radius. This degeneracy is different from the well-known degeneracy of the unscreened 2D exciton states. In the low-density limit ($q_s a^* \to 0$) the number of bound states oscillates around $1/(q_s a^*)$ with the period and amplitude of oscillations proportional to $1/\sqrt{q_s a^*}$. Then, using the expression for the Thomas-Fermi 2D screening wavenumber q_s for a two-component non-degenerate electron-hole plasma [15], $q_s a^* = 4\pi\ (\mathrm{Ry}^*/k_BT)\ (n_e^0 a^{*2} + n_h^0 a^{*2})$, Ry^* being the excitonic Rydberg, one can find the ratio of the free-carrier density to the total density. For a model semiconductor with $m_e = m_h$, this ratio is equal to 2/3 in the low-density limit. This result is different from the single-bound-state law of the mass action, which gives a complete ionisation of bound states ($\alpha \to 1$) in the same limit.

Figure 1 shows the results from the calculation of the electron-hole part of the partition function, Z_{eh}, which contains both the bound state sum and the scattering phase shift integral. In this figure Z_{eh} is plotted as a function of the inverse screening wave number $1/q_s$ measured in units of the effective Bohr radius a^*. The temperature is given in units of the bulk excitonic Rydberg Ry^*.

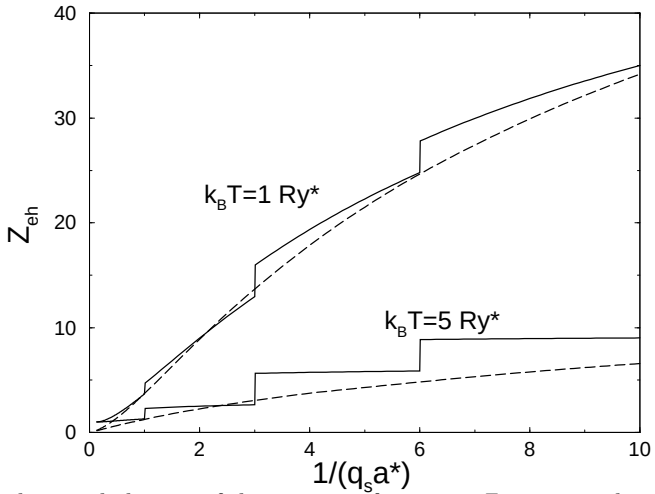

FIG. 1. The electron-hole part of the partition function, Z_{eh} versus the screening length $1/q_s$ for two values of k_BT/Ry^*. Solid lines show the bound state contributions Z_{bound} only. Dashed lines correspond to the total partition function with scattering states included.

To emphasize the role of scattering we show on the same plot the bound-state sum, $Z_{bound} = \sum_{m,\nu}\exp(-\beta E_{m,\nu})$,

which exhibits jumps whenever new bound states appear. These jumps become higher with increasing screening length $1/q_s$ since several bound states appear simultaneously [13]. A proper account of scattering eliminates these unphysical jumps.

We calculated the density dependence of the degree of ionisation α in the 2D low-density (Boltzmann) limit for $k_BT = 1$ Ry*, which roughly corresponds to GaN at room temperature. Over a wide range of pair densities, $0.01 < na^{*2} < 0.1$, α is almost independent of density, and it increases outside this range. The minimal value of the degree of ionisation, $\alpha_{min} \approx 0.34$, corresponds to $na^{*2} \approx 0.04$ ($n \approx 5 \times 10^{12}$cm^{-2} for GaN). Even at the relatively high densities of 10^{12} cm^{-2} we find that there is a single bound state having a binding energy of the order of k_BT which is available to participate in excitonic lasing.

We also calculated the second virial coefficient of the dilute 2D electron-hole plasma in GaAs and GaN-based quantum wells at room temperature. These calculations show a striking difference between a strongly correlated exciton/free-carrier plasma in GaN and a nearly ideal electron-hole gas in GaAs.

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