Vacancions in the two-dimensional Wigner crystal

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Abstract. From a new point of view, the recombination of two-dimensional electrons enclosed in a MgZnO/ZnO heterojunction with localized holes in the valence band is considered. It is suggested to consider quasi-holes in the two-dimensional electron system as quasiparticles in the Wigner crystal. The quasiparticles corresponding to electrons removed from the Wigner crystal are vacancions. Because of quantum tunneling effect, they are not localized. The vacancion energies $E(k)$ form a band of width $D$ which is proportional to the vacancy tunneling probability. The width $D$ corresponds to the photoluminescence band of the two-dimensional electron system. The shape of the photoluminescence band of the Wigner crystal is considered within the tight-binding approximation for dispersion $E(k)$ and compared with the experimental results.

1. Introduction
For many years there has been great interest in low-dimensional correlated quantum systems of many bodies. Most of theoretical methods work sufficiently well at high electron densities if the interaction energy is low compared to kinetic energy. Experimental research methods provide more and more information on the highly correlated the two-dimensional (2D) electron systems. To study the renormalization effects of the electron mass not only at the Fermi level, but within the entire energy range, the low-temperature photoluminescence spectra are analyzed. The recombination of 2D electrons with the valence-band holes created with the low-density optical excitation and localized at some distance from the two-dimensional electron system (2DES) is considered in [1–3]. It has been demonstrated [1] that in GaAs/AlGaAs quantum wells a rather strong renormalization of the electron mass (up to 35%) was detected for values of $r_s \sim 4.5$ ($r_s = (\pi n_s)^{-1/2}/a_B$, $n_s$ is the density of 2D electrons, $a_B = \varepsilon \hbar^2/(me^2)$ is Bohr radius for ZnO).

In recent works [2, 3] the low-temperature photoluminescence spectra from two-dimensional electron system (2DES) confined at MgZnO/ZnO heterojunctions are presented. The 2D electrons annihilate with the localized valence-band holes. The authors suppose that the width of the 2DES photoluminescence band gives the value of the quasiparticle optical density-of-states mass. The mass changes from 0.6 to 0.3 $m_0$ ($m = 0.3$ $m_0$ is the effective mass in bulk ZnO, $m_0$ is the electron mass) as the interaction parameter $r_s$ changes from 6.5 to 2.4. For experiments in high magnetic field the luminescence lines for all Landau levels are well defined, and the method demonstrates the existence of quasi-holes as quasiparticles not only near the Fermi energy. The many-body problem has no unified theoretical descriptions in this intermediate range of parameter $r_s$ neither for the ground state nor for its elementary excitations. The ground state of 2DES depends on $r_s$ and may be considered as the electron gas, electron Fermi or non-Fermi
liquid, Wigner crystal or Wigner glass (see, for example, [4,5]). It is shown that at low densities the potential energy dominates over the kinetic energy and the system forms a perfect triangular lattice, the Wigner crystal. Spin state may be ferromagnetic or spin glass. The crystallization at zero temperature occurs at $r_s = 37 \pm 5$ [5]. The liquid–solid transition calculations including the effect of impurities shift the transition density from $37 r_s$ to a milder value of about $7 r_s$ [6] thus providing a possibility to consider the quasi-holes occurring in the experiment of work [3] as quasiparticles in Wigner crystal. As shown in [7], at sufficiently low temperatures defects in crystals (vacancies or impurities) change into excitations that move practically free through a crystal. Because of the quantum-tunneling effect, a defect in a crystal is not localized. According to quantum mechanics, in such a case the possible defects are considered as quasiparticles and classified according to the values of quasimomentum $k$.

Associated with each type of defects is a branch of excitations. The electrons removed from the Wigner crystal are considered as vacancies. The vacancion energies $E(k)$ form a band of width $D$ which is proportional to the defect tunneling probability. The width $D$ should correspond to the 2DES photoluminescence band of [3].

2. The shape of the photoluminescence band for the Wigner crystal

The shape of the photoluminescence band for the Wigner crystal (WC) depends on the attenuation of vacancies $E(k)$. The one-particle excitation spectrum in the tight-binding approximation taking into account only the tunneling between nearest neighbors for a triangular lattice with interelectron spacing $a$ has the form [8]:

$$E(k) = 2t[\cos(k_x a) + 2 \cos(k_x a/2) \cos(\sqrt{3}k_y a/2)],$$  \hspace{1cm} (1)

where $t$ is the hopping integral (tunneling parameter). The sign of $t$ depends on the spin ordering.

At $t < 0$ (ferromagnetic case) $E(k)$ reached its minimum in the center of the Brillouin zone at point $\Gamma$ ($E(0) = 6t$) and its maximum at point $K$ ($E(K) = -3t$). The width of the allowed energy band is $D = 9|t|$.

The density of states is

$$N(E) = A(e)/[2\pi^2|t|(3 - 2e)^{1/4}],$$  \hspace{1cm} (2)

where $e = E/(2|t|)$, $A = K(k)$ at $k < 1$, $A = k^{-1}K(k^{-1})$ at $k > 1$; $K(k)$ is a complete elliptic integral of the first kind with its modulus $k = [2 + (3 - e^2)/\sqrt{(3 - 2e)}]^{1/2}/2$. The density of states tends to $\infty$ as $E \rightarrow -2t$ and has a singularity of the van Hove type:

$$N(E) \approx (3\nu/(4\pi^2|t|)) \ln(4/|1 - e|),$$  \hspace{1cm} (3)

where $\nu = 1$ for $e < 1$ and $\nu = 2$ for $e > 1$.

The shape of the photoluminescence band depends, although on the attenuation of vacancies (equivalent to the imaginary part of its energy). If the electron from the Wigner crystal annihilates with a localized hole, then a vacancion with the energy $\tilde{E}$ and damping $\delta(\tilde{E})$ is created. The luminescence line has the Lorenz form:

$$f(E, \tilde{E}) = \frac{\delta}{2\pi((E - \tilde{E})^2 + \delta(\tilde{E})^2/4)}. \hspace{1cm} (4)$$

The band shape $I(E)$ taking into account the damping has the next form:

$$I(E) = \int N(\tilde{E})f(E, \tilde{E})d\tilde{E}. \hspace{1cm} (5)$$

There is no singularity but a maximum in $I(E)$ is expected.

The damping $\delta(\tilde{E})$ is determined by relaxation mechanisms. In the experiment [3], the lower edge of the photoluminescence energy is more extended due to the reduced lifetime of quasiparticles (increased attenuation) with a higher excitation energy, but experiments in a
perpendicular magnetic field show that the lifetime does not change very significantly and all Landau levels are good resolved. Evaluation of the vacancion lifetime is a complicated problem. It should be affected by the interaction with impurities, with the phonon-type excitations at non-zero temperatures and by the vacancion-vacancion interaction. Due to the density of states singularity, most important is the damping around the singularity point, and therefore the simplest suggestions is to consider $\delta = \text{const.}$

The shapes of the photoluminescence bands for the recombination of a WC electron with a localized hole and the creation of a vacancy are shown in figure 1 for the different values of $\delta$. The band shapes in figure 1 and in the experiment [3] are similar. The next problem is to consider the band width $D$ for the Wigner crystal as a function of $r_s$. This dependence is determined by the ground state of 2DES. For the Wigner crystal in the tight-binding approximation $D = 9|t|$, and the dependence of tunneling parameter $t$ on $r_s$ is a subject of interest. The exchange energies calculated in the works [9–12] may be used to evaluate tunneling parameter. The expression for a $P$-particle exchange energy $J_P$ in the units of Ry is given as

$$J_P = A_P b_P^{1/2} r_s^{-5/4} e^{-b_P r_s^{1/2}}. \tag{6}$$

Assuming $b_P$ to be constant (see [10, 11]), the exchange energies vary exponentially with the density. The prefactors $A_P$ for the Wigner crystal are always of the order of unity. An effective pair electron exchange in the triangular lattice is introduced as $J_2^{\text{eff}} = J_2 - 2J_3$. If $J_2^{\text{eff}} < 0$, the Wigner crystal is ferromagnetic. If $J_2^{\text{eff}} > 0$, the ground state is antiferromagnetic, or Wigner glass. As follows from [10–12], the ground state for the systems with Coulomb interaction is ferromagnetic. However, for the electron crystal with impurities a transition to the Wigner glass

**Figure 1.** The photoluminescence intensity for the WC electrons and localized holes from the valence band with creation of vacancions: damping in units of $2|t|$ is 0.1 (solid line), 0.5 (dashed), 1.0 (dotted); $E = -3$ corresponds to the lower photoluminescence edge.
phase may occur [10]. The PL spectrum for this case must be reversed relative to the point $E = 0$ in figure 1. For the evaluation it is considered $t \approx J_2$.

The bandwidth $D$ can only be compared by the maximum experimental value $r_s = 6.4$. The evaluation for the Wigner crystal is $D_{WC} \approx 1$ meV. For the noninteracting electron gas it is $D_0 = E_F = 2.9$ meV. In the experiment [3] for the correlated electron gas it is $D_{exp} = 1.4$ meV. ZnO parameters are used. In figure 4 in [3], the dependence $m_{qh}(r_s)$ is presented, where the quasihole mass $m_{qh}$ is introduced by the following relation: $D_{exp} = \hbar^2 K_F^2/(2m_{qh})$, $K_F$ is Fermi momentum. For the Wigner crystal the parameter $m_{qh} \propto 1/(D_{WC}r_s^2)$ can be although used. The differential characteristic

$$\frac{1}{m_{qh}(r_s)} \frac{dm_{qh}(r_s)}{dr_s}$$

is more convenient to compare the theory and the experiment. In the experiment this value is $0.1–0.2$ ($\approx 0.13$ at $r_s = 6.4$), for the Wigner crystal it is $\approx 0.2$.

3. Conclusion
The analysis of the photoluminescence line shape and dependence of the band width on $r_s$ for the MgZnO/ZnO heterojunction at low densities of 2D electrons provides a possibility to consider the electron system as WC. The photoluminescence process may be interpreted as annihilation of a WC electron with a localized valence-band hole and creation of an elementary excitation in WC, a vacancion.

Acknowledgments
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